Material Identification using Multiple X-Ray Absorptiometry

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Abstract

Dual Energy X-ray Absorptiometry is a proven technique used to identify unknown materials, by measuring the transmission of two X-ray energies. This technique is limited to measuring a single chemical quantity and is not able to handle more chemical variation. To overcome this, one approach is to use multiple-energies to resolve more information. The differences in the processes controlling the X-ray transmission limits the theoretical resolution capability to three characteristics. Of these three, one is dependent on the sample geometry and density. The remaining two are purely chemical characteristics and are investigated in this thesis. It is found that using X-ray photon energies in the range 20-90 keV, it is possible to measure one chemical characteristic to a high precision. Two chemical characteristics can be measured in limited circumstances and even though the precision is good, the measurement is prone to inaccuracies in machine modeling and stability. A two step method is defined, first finding an approximation of the X-ray spectra and then reconstructing the attenuation coefficient of the sample to a high precision (< 0.2%) using a robust low-rank basis for the characteristics.
Referat

Kemisk identifiering med MXA

DXA (Dual Energy X-ray Absorptiometry) är en teknik för att identifiera okända material genom att mäta transmissonen för två olika röntgenenergier. Den här metoden är begränsad till att mäta en kemiskt variation. Vid mer än en varierande komponent, kan MXA (Multiple Energy X-ray Absorptiometry) användas för att utröna mer information. MXA är dock begränsat av de små skillnaderna i de fysikaliska processerna som styr röntgenfotonernas interaktion med materialet. Teoretiskt är det bara möjligt att mäta tre egenskaper med MXA, varav en är beroende på provets geometri och densitet. De kvarvarande kemiska egenskaper är utforskade i den här rapporten. Det är möjligt att mäta en kemisk material egenskap med hög precision med röntgenenergier mellan 20 - 90 keV. Två kemiska egenskaper går att mäta i vissa fall, dock är precisionen sämre och mätningen är känslig för fel i modelleringen av maskinen och mätningens stabilitet. I den tvästegs metod som används uppskattas först de använda röntgenspectra och sedan återskappas proovets attenueringskoefficient med en hög precision (< 0.2 %) med en lågranks bas av attenueringsegenskaperna.
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Chapter 1

Introduction

1.1 Background

High energy photons, often called X-rays are used to investigate material properties in many fields and applications. The high energy of the photons give them the ability to penetrate materials. Unlike other penetrating particles such as neutrinos and neutrons, the X-ray photons have a small probability to interact with atoms they pass through. An atom absorbs or scatters X-rays with a probability depending on the photon energy and the element. The simplest method is to measure the shadow of an object, i.e., how the photons are absorbed. It can visualize internal structures and composition of complex objects by projecting the combined mass as a shadow.

A single illumination can only hint at the relative density of materials. To obtain quantitative material properties more measurements are needed, either by measuring a object from many directions and performing a tomographic reconstruction [7]. Another approach is to measure how photons of different energy interact with material. This can be done by having an energy discriminative detector or changing the settings between two measurements of the same sample. Comparing the attenuation at two energy levels is known as dual X-ray absorptiometry. Dual-energy X-ray techniques are used in different fields, to measure bone density in medicine [4] and find foreign objects in food and other product flow [6]. It can also be used to measure moisture in wood and other organic matter [3]. The drawback of dual methods is that they can’t discriminate between more than 2 different materials. This limits the usefulness in applications where there are many different possible materials. This requires more information and more illuminations. Multi-energy X-ray techniques enable more information to be obtained from the sample.

1.2 Purpose

Multi Energy techniques rely on small differences in the way atoms interact with photons to separate materials. Each additional energy measurement adds information...
CHAPTER 1. INTRODUCTION

Estimation but makes the problem of separating materials more numerically unstable. In this thesis, my approach to this problem is separated into several parts.

1. Estimate the chemical information available using Multi-Energy X-ray techniques.
2. Create a simulation model for *in silico* measurements.
3. Develop a method to extract the chemical information *in silico*.
4. Estimate the uncertainty of the found chemical information *in silico*.
5. Test the method *in situ*.

1.3 Scope

The scope of this project is limited by working with simulated measurements *in silico*. This allows for total control of the measurement noise variance and keeps the variations machine state stable, as real X-ray measurement systems require control and calibrations for accurate measurements. The measurement variance is limited to the photonic Poisson noise for simpler analysis of the uncertainty quantification. Measurements *in silico* are assumed to be composed of homogenous samples and results should only be indicative of real world performance.

1.4 Comparisons to earlier works

In this thesis the two step method described in [1],[2] to estimate attenuation coefficient is improved by combining all available information from a measurement. The proposed method retains the non-linear problem formulation in [1],[2] but uses a non-linear solver to estimate the machine state and material composition. Both machine state and material composition have properties that are local for each image pixel and global, for each measurement. The samples in the considered applications are simpler as the elemental composition of the sample is homogenous. By requiring that some of the sought parameters are global for the entire sample, it is possible to regularize the problem and to reduce the impact of noise.
Chapter 2

Theory

2.1 The Mantex Desktop scanner

The machine modeled in this thesis is a Mantex Desktop scanner. It is a transmission based X-ray instrument, equipped with a X-ray tube capable to generate X-ray spectra with a peak energy between 35 and 95 keV. The X-ray radiation is collimated two times before and after it passes trough the sample in order to produce a narrow fan beam illuminating the sample. The intensity of the transmitted X-rays is measured by a scintillator coated linear array of ccd-pixels. The X-ray tube illuminates the sample, which is transported on a sled through the fan beam. The beam intensity is integrated by the ccd for many short times while the sample moves, to produce a 2D X-ray picture of the sample. This setup makes it possible to use multiple settings for peak X-ray energy and filters for illuminating the sample, using only one X-ray source and detector. Combining the absorption images from the different illuminations a multiple photon analysis is performed.

2.2 X-ray physics

The physical properties of X-rays and their interactions with matters form the basis of the possibility to characterize different materials. X-rays are composed of photons with a shorter wavelength and higher energy than visible light. Photons with energy to interact with the inner shell electrons was the classical definition of X-rays. Shorter wavelength photons with higher energy are classified as gamma photons and interact with the nucleus of the atoms. Longer wavelength photons such as microwaves interact with the bonds between atoms.

The photon is described either with its kinetic energy, frequency or wavelength. X-rays which are linked to the kinetic energy the electron they interact with is usually described using the photons kinetic energy $E$ in electron volts eV. Transmission based commercial systems use X-rays from a few keV up to several MeV depending on the application. A X-ray photon is uncharged and thus has excellent penetration properties compared to charged particles. A photon interacts with electrons
CHAPTER 2. THEORY

by a large number of mechanisms, but some have larger significance than others. The primary mechanisms for photon-atom interactions in the X-ray energy range are photoelectric absorption, Compton scattering, pair production and Rayleigh scattering.

2.3 X-ray generation

In the Mantex Desktop scanner, a tungsten X-ray tube is used to generate the X-ray photons. Tungsten is a common material in X-ray tubes, as its high density and heat resistance makes it an excellent electron target. The main components of the X-ray tube is a target of tungsten as the anode and small filament as the cathode, both placed inside a vacuum. A large electric potential is placed between them and when a current is passed through the filament, it heats up and electrons are freed and accelerated by the electric potential towards the tungsten target. As the high energy electrons hit the tungsten target they are slowed down, converting the kinetic energy to photons and heat.[14] The electrons and the created photon of sufficient energy can remove inner shell electrons of the target creating an exited ion. An outer shell electron then transition down to the inner shell filling the void. This transition produces a X-ray photon. The photons produced have distinct energies equal to the energy difference between the states characteristic for the atom.

The incident electrons produce X-rays by two different processes. The electrons interact with the electrical field created by the nucleus of the target atoms, which diverts the electrons, causing them to lose energy. This loss of energy and momentum is converted to X-ray photons, with energy varying from zero to the total kinetic energy of the electron. This broad spectrum of photons is called Bremsstrahlung.

![Figure 2.1. Schematic of the operating principle of a X-ray tube](image)

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2.3. X-RAY GENERATION

A classic model of the Bremsstrahlung spectra is Kramers Law[11]. This model (eq. 2.1) provides the intensity $S(E)$ of photons with energy $E$ emitted by a X-ray source with a source potential setting kVp and anode material with atomic number $Z$. The potential placed over the anode and cathode kVp controls the kinetic energy of the incident electrons, which limits the peak energy of the emitted photons $E_{\text{max}}$ to the source potential multiplied with the elementary charge $e$. The proportional constant $C$ is dependent on the current of electrons hitting the anode.

$$S(E) = CZ \left(1 - \frac{E}{E_{\text{max}}} \right) , \quad E < E_{\text{max}} \quad (2.1)$$

The intensity of the low energy photons are limited by the inherent filtration of the X-ray source. Lower energy photons are absorbed by the source enclosure materials. To optimize shape of the spectrum for specific applications additional filters are placed in the beam path to remove unwanted lower energy photons in the emitted spectrum. Changing the source potential and filtration produce different spectra (fig. 2.2), increasing the source potential increases the number of photons and the maximum energy, filtration reduces the number of photons and increasing the minimum energy.
2.4 X-ray interactions

The potential for material identification is highly dependent on the different interaction mechanisms and their relation with photon energy and element. In a transmission based setting such as the Mantex Desktop scanner the goal is to measure the ratio of transmitted photons i.e. photons that do not interact with the sample under investigation. When a x-ray photon passes through matter it can either be absorbed or scattered in a significant angle or proceed unchanged depending on which way the photon interacts with the atom. The combined probabilities of absorbance and scattering is known as attenuation. The attenuation $\mu$ of a material is combination of the effects of the different interaction mechanisms. Each mechanism has different dependence on photon energy $E$ and the atomic number $Z$ of the element it interacts with (fig. 2.3). This permits element identification.

2.4.1 Photoelectric Effect

In the photoelectric effect a photon interacts with the bound electrons in a atom by transferring sufficient energy from the photon to eject a electron from its original shell in the atom. This required energy is dependent on the element and the binding energy of the shell. This produces one free electron and leaves a ionized electron free to absorb a electron, a process which produces a characteristic x-ray photon of the element with known energy levels. These characteristic x-ray photons have a lower energy than the initial x-ray photon and are often absorbed close to the initial interaction position but some may escape and is detected.

The photoelectric effect is the predominant interaction mechanism for low energy x-ray photons. A approximate expression of the possibility for interaction [14] is

$$\mu_{\text{Photo}} \propto \frac{Z^n}{E^{3.5}}$$

The exponent $n$ for the atomic number $Z$ vary between 4 and 5 depending on the photon energy $E$. The high photoelectric absorbance for materials with high $Z$ elements makes them useful for X-ray shielding and good candidates for X-ray detectors.

2.4.2 Compton Scattering

Compton scattering is a process in which a photon interacts with a electron in a similar fashion as a inelastic collision. A part of the photon energy is lost and the photon direction is changed to preserve the total momentum of the photon-electron system. This scattering has the same effect as absorption in when measuring absorption in a good geometry setup. There is a possibility that a scattered photon is rescattered back into the detector and be counted as a unabsorbed electron from another part of the sample.

The probability of a Compton scattering to occur is dependent on the number of electrons available as target and the energy of the photon. Generally the energy
dependent probability of scattering \( \text{Compton}(E) \) decreases slowly with increasing energy and it is the dominant interaction mechanism for high energy X-ray photons \([14]\).

\[
\mu_{\text{Compton}} \propto \frac{Z}{A_m} \text{Compton}(E)
\]  

### 2.4.3 Rayleigh Scattering

If the energy transferred to the electron in a collision is not enough energy to change its quantum state, the photon reacts as if it collide with the whole atom. The larger mass of the atom compared to a electron makes the energy transfer necessary to preserve total momentum negligible and the photon is elastically scattered but retains its original energy. In the same way as Compton scattering this changes the photon direction and the amount of photons that reach the detector. The energy dependent probability \( \text{Rayleigh}(E) \), of elastic Rayleigh scattering decreases slower than photoelectric absorption, but only account of at most \( \approx 10\% \) of the total attenuation \([14]\).

\[
\mu_{\text{Rayleigh}} \propto \frac{Z^2}{A_m} \text{Rayleigh}(E)
\]

### 2.4.4 Attenuation coefficient

When an X-ray with photon energy \( E \) travels through a material, the beam intensity changes as photons are absorbed or scattered by atoms in the material though the different mechanisms.

The combined probability of absorption and scattering is the sum of the individual mechanisms as they are independent an the number of present atoms is much higher than the number interactions.

\[
\mu(E, Z) = \mu_{\text{Photo}}(E, Z) + \mu_{\text{Compton}}(E, Z) + \mu_{\text{Rayleigh}}(E, Z)
\]

It is practical to describe the attenuation by the mass attenuation coefficient \( \frac{\mu}{\rho} \), the attenuation divided by the density \( \rho \). The attenuation of a compound material \( c \) can be written as

\[
W \left( \frac{\mu(E)}{\rho} \right)_c = \sum_m w_m \left( \frac{\mu(E)}{\rho} \right)_m
\]

Where \( W \) is the mass thickness (density \( \times \) thickness) and \( w_m \) the partial mass of element \( m \).

Using the attenuation coefficient, photon transport through an object with a thickness \( t \) is modeled by the differential equation for the intensity \( I \) (eq. 2.7).
CHAPTER 2. THEORY

Photon energy

\[ 10 \ 20 \ 30 \ 40 \ 50 \ 60 \ 70 \ 80 \ 90 \ 100 \]

\[ \text{Attenuation (} \mu / \rho \text{)} \]

\[ 10^{-2} \]
\[ 10^{-1} \]
\[ 10^{0} \]
\[ 10^{1} \]
\[ 10^{2} \]

Components of attenuation coefficient

- Total Carbon
- Photoelectric Carbon
- Compton Carbon
- Rayleigh Carbon
- Total Aluminium
- Photoelectric Aluminium
- Compton Aluminium
- Rayleigh Aluminium

**Figure 2.3.** The components of the attenuation coefficient for carbon and aluminum

\[
\frac{dI}{dt} = -\mu(E, Z)
\]

(2.7)

Solving eq. 2.7 for a constant \( \mu \), the Beer-Lambert law is obtained (eq. 2.8).

\[
I = I_0e^{-\mu(E,Z)t} = I_0e^{-(\mu(E)/\rho)cW}
\]

(2.8)

By measuring the intensity \( I \) transmitted through an object and the intensity \( I_0 \) for the same setup without sample, the sample attenuation \( (\mu(E)/\rho)c \) can be computed from the radiographic reflex \( R \) computed using eq. 2.9 if the density and thickness is known.

\[
R = -\log \left( \frac{I}{I_0} \right) = \left( \frac{\mu(E)}{\rho} \right)_c W
\]

(2.9)

2.5 X-ray detection

To measure the X-ray photons, they have to interact with a photon capture device. To capture X-ray photons requires materials with high Z atoms for high probability of capture. This was done and is still done with photographic film containing for example silver atoms but this have disadvantages of requiring developing to produce a visible image. To speed up the acquisition digital CCD-chips are used to detect
2.5. X-RAY DETECTION

The photons. These chips are sensitive to visible light and the high energy X-rays have low probability of being detected. To improve the ability to detect X-ray photons, the CCD-chips are covered by a scintillating material. Common scintillator materials are CsI, Gd$_2$O$_2$S, CdWO and NaI. These materials contain high $Z$ atoms which absorb the X-ray photon and through interactions with the other elements, the energy is dissipated by a number of low energy optical photons proportional to the energy of incident photon. The Mantex Desktop scanner is equipped with a linear array of CCD elements coated with a 300$\mu$m film of Gd$_2$O$_2$S often known as Gadox.

![Figure 2.4. Operation principle for a scintillator coated CCD-detector.](image)

Photons that interact with the scintillator produce a flash of visible light detected by the CCD. The detected intensity is proportional to the original X-ray photon intensity and the total induced voltage is converted to a digital signal.

The CCD-detector integrates the deposited charge from the optical photons and the potential is measured and converted to a digital signal by an A/D converter (fig. 2.4). The resulting signal $N$ can be regarded as the total intensity of incident photons multiplied with the detector response $D(E)$ during the integration time $T$ (eq. 2.10).

$$N = \sum_n I_n D(E_n)T$$  \hspace{1cm} (2.10)

In an ideal model of a scintillator, the detector signal is proportional to the intensity of incident photons $I$, the photon energy $E$, and the absorption probability $(1 - e^{-\mu(E)abs})$. The detector gain $G$, converting absorbed energy to detector signal $N$ (fig. 2.4) is dependent on the light yield of the scintillator material, detector geometry and the CCD sensitivity [14]. The ideal detector model used for the detector response $D(E)$ is:

$$D(E) = GE \left(1 - e^{-\mu(E)abs} \right)$$  \hspace{1cm} (2.11)
Using different scintillators and thickness makes it possible to get different spectral response, as thicker scintillators have higher probability to detect high energy photons. It is also possible to stack detectors with different scintillators to obtain many energy responses using a single X-ray source[1].

### 2.6 Modeling X-ray transport

To create a model of X-ray transmission the characteristics of the material in the sample, emission of the source and the efficiency of the detector needs to be accounted for [1].

There exist complex models of X-ray transport that simulate photon showers and their interactions by tracking individual photons until the photon is fully absorbed. A common code for this is PENELOPE [16] which uses Monte-Carlo methods to model X-ray measurements. These Monte-Carlo methods can account for secondary photons created by fluorescence and the scattering of photons but have a large computational cost.

The secondary photons have a small impact for a 1D detector array as it is constructed with a internal lead shielding, designed to only allow photons originating from the X-ray source to be detected. If we assume the secondary photons have negligible contribution, the photon transport model becomes linear. In the linear model, the numbers of photons to reach the detector is given by Beer-Lambert’s law (eq. 2.8).
### 2.7 X-RAY NOISE

Applying Beer-Lamberts law for all photon energies in the polychromatic spectrum, the signal from the detector $N$ can then be approximated using the superposition principle:

$$N = \int_0^\infty D(E)S(E)e^{-\frac{\mu(E)W}{\rho}}dE$$  \hfill (2.12)

Where $S(E)$ is the spectrum of photons generated by the X-ray source and $D(E)$ is the spectral sensitivity of the detector.

Combining the source and detector term into a combined into a effective spectrum term $I(E)$

$$N = \int_0^\infty I(E)e^{-\frac{\mu(E)W}{\rho}}dE$$  \hfill (2.13)

and

$$N_0 = \int_0^\infty I(E)dE.$$  \hfill (2.14)

And the expression for the reflex of a polychromatic spectrum is:

$$R = -\log \left( \frac{\bar{N}}{N_0} \right) = -\log \left( \frac{\int_0^\infty I(E)e^{-\frac{\mu(E)W}{\rho}}dE}{\int_0^\infty I(E)dE} \right)$$  \hfill (2.15)

### 2.7 X-ray noise

X-ray production, attenuation and detection are random independent processes, thus all measurements using X-Rays are inherently noisy. For monochromatic photons, the number of detected photons $X$ are usually modeled [14] by a Poisson distribution (eq. 2.16). For Poisson distributed data the variance $\sigma^2$, is equal to its expected value $\bar{X}$.

$$\text{Pr}(X=k) = \frac{\lambda^k e^{-\lambda}}{k!}$$  \hfill (2.16)

$$E[X] = \lambda = \bar{X}$$  \hfill (2.17)

$$\sigma_X^2 = \bar{X}$$  \hfill (2.18)

As the scintillator equipped detector converts the absorbed energy of the photons to a digital signal, the expected value is scaled with the detector gain $G$ and the photon energy $E$, using the simplified model (eq. 2.11). The mean and variance measured signal $N$ are:

$$E[N] = (GE)\bar{X} = \bar{N}$$  \hfill (2.19)

$$\sigma_N^2 = (GE)^2\bar{X} = (GE)\bar{N}$$  \hfill (2.20)
Expanding this to measurements using polychromatic spectra $I(E)$, the measured signal $N$

$$
\mathbb{E}[N] = \int_0^{\infty} I(E)dE = \bar{N}
$$

(2.21)

$$
\sigma_N^2 = \int_0^{\infty} (GE)I(E)dE
$$

(2.22)

By comparing the measured signal mean $\bar{N}$ and variance $\sigma_N^2$ it is possible to calculate the effective gain $G_e$ and the approximate number of incident photons $X_e$.

$$
G_e = \frac{\sigma_N^2}{\bar{N}} = \frac{G}{\bar{N}} \int_0^{\infty} EI(E)dE
$$

(2.23)

$$
X_e = \frac{\bar{N}^2}{\sigma_N^2} = \frac{\bar{N}}{G_e}
$$

(2.24)

2.8 Beam Hardening

The polychromatic spectra generated by X-ray tubes contain photons of different energies, compared to monochromatic sources of X-rays, such as isotopes, monochromators and X-ray lasers [14], which have much lower intensity. Sources with lower intensity requires longer measurement times to measure a sample with the same accuracy. High intensity monochromatic photons can be generated using synchrotron radiation [14], but this requires a large facility.

X-ray tubes produce X-ray photons with a broad spectrum of photon energies. This complicates the analysis because the reflex $R$ for polychromatic spectra (eq. 2.15) is not linear with respect to sample mass thickness, as predicted by Beer Lamberts law for monochromatic spectra (eq. 2.9). This is caused by the hardening of the spectra as it passes through material. The so called soft low energy photons have a higher probability to be attenuated, compared to hard high energy photons. When the low energy photons are absorbed, the effective attenuation coefficient for the remaining photons is lower, and the change in $R$ by subsequent material is smaller.

To reduce the beam hardening effects, the low energy photons can be removed with a metal filter placed in the beam, creating a harder spectrum, as the low energy photons are removed independent of the sample. This prefiltering reduces the width of the spectrum but also reduces the total intensity, which increases the relative noise. This can be seen in fig. 2.6 where the reflex of aluminum measured with the unfiltered and filtered spectra in from fig. 2.2 are simulated.

For dual and multi energy methods it is desirable to have as different spectra as possible, while retaining a good signal-to-noise ratio. Multiple source potential settings, together with appropriate filters is required to create optimal measurement conditions depending on the application.
2.9 Measuring chemical information by the coefficient of attenuation

The amount of chemical information and the ability to discriminate chemical elements using X-ray absorptiometry depends on the difference between the attenuation coefficients of the elements. For low Z elements (Z < 50), the energy dependent attenuation coefficient is smooth and decreasing in the observed region between 20-95 keV. The majority of the attenuation are caused by the photoelectric effect for low photon energies and the Compton scattering for the higher (with hydrogen as an exception as it has a negligible photoelectric effect). Inelastic Rayleigh scattering play a minor role as it only account for maximum ≈ 10% of the total attenuation. For higher photon energies than considered here, the pair production of electrons becomes predominant.

In figure 2.3, the components of the attenuation coefficient of elemental carbon and aluminum is shown. It is possible to observe the small difference in the Compton scattering at high energies and a large difference in the photoelectric effect.

2.9.1 Dual energy methods

Dual energy methods measures the attenuation of a object in a lower energy setting, where the Photoelectric effect is dominant and in a higher energy setting, where
the Compton-scattering is dominant. By comparing the observed attenuations \( R = \log(N/N_0) \), in the high energy setting to the low energy setting the weight fractions of the two materials in the object can estimated. It is possible to calibrate two weight fractions \( w_1/W \) and \( w_2/W \) with a linear model [3].

\[
\frac{w_1}{W} = A_1 + A_2 \frac{R_{LE}}{R_{HE}} \\
\frac{w_2}{W} = 1 - \frac{w_1}{W}
\]

or by solving the system

\[
R_{LE} = w_1 \left( \frac{\mu(E_{LE})}{\rho} \right)_1 + w_2 \left( \frac{\mu(E_{LE})}{\rho} \right)_2 \\
R_{HE} = w_1 \left( \frac{\mu(E_{HE})}{\rho} \right)_1 + w_2 \left( \frac{\mu(E_{HE})}{\rho} \right)_2
\]

(2.26)

when the mass attenuation coefficients of the two materials at \( E_{LE} \) and \( E_{HE} \) is known [8]. These linear models does not work for polychromatic spectra because beam hardening creates a non-linear relation between \( R \) and \( W \) as the effective \( \mu \) decreases with increasing mass thickness \( W \). To overcome these obstacles, more complex models needs to be formulated, for example: [15]

\[
w_1 = A_0 + A_1 R_{LE} + A_2 R_{HE} + A_3 R_{LE}^2 + A_4 R_{HE}^2 + A_5 R_{LE} R_{HE} \\
w_2 = B_0 + B_1 R_{LE} + B_2 R_{HE} + B_3 R_{LE}^2 + B_4 R_{HE}^2 + B_5 R_{LE} R_{HE}.
\]

(2.27)

This type of model requires a more complex calibration procedure and is hard to expand to measure multiple energies and more than two material fractions.

### 2.9.2 Multi energy methods

Expanding the linear dual energy model (eq. 2.26), to a multi-energy setting with \( M \) materials and \( K \) measurements, the system becomes [17],[4]

\[
R_k = \sum_{m=1}^{M} w_m \left( \frac{\mu(E_k)}{\rho} \right)_m = \sum_{m} A_{km} w_m
\]

(2.28)

can theoretically resolve \( M \) materials with measurements at \( K > M \) different energies. But in a realistic setting, it is limited by the physical effects, that together make up the attenuation coefficient, in addition to the non-linearity introduced by beam hardening. Solving the linear system (eq.2.28) by the metod of least squares, the system becomes:

\[
A^T R = A^T A w = M_G w.
\]

(2.29)
2.10. NON-LINEAR MODEL FITTING

The resulting system is ill-conditioned when trying to resolve multiple materials. As seen in the table 2.1, the condition number of the matrix \( M_G \) becomes large as more candidate elements are considered even when the number of energies are high.

<table>
<thead>
<tr>
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<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>cond((M_G))</td>
<td>(8.0859 \cdot 10^4)</td>
<td>(1.6478 \cdot 10^6)</td>
<td>(1.4844 \cdot 10^7)</td>
<td>(1.1569 \cdot 10^{11})</td>
</tr>
</tbody>
</table>

To overcome this, Maitjean et. al.[1],[2] creates a set of orthogonal eigeneffects \( u_p(E_k) \), by diagonalizing the matrix \( M_G \),

\[
M_G = V A V^T
\]

(2.30)

to compute the principal components \( u_p \) of \( A \)

\[
u_p(E_k) = \sum_m \left( \frac{\mu(E_k)}{\rho} \right)_m V_{pm}
\]

\[
U = AV
\]

(2.31)

and solves the system for the eigeneffect parameters \( \alpha_p \) instead of the partial weight of the materials \( w_m \):

\[
U^T R = U^T U \alpha
\]

(2.32)

which is simplified as the principal components are orthogonal \((U^T U = \Lambda)\). By only using the \( P \) strongest principal components \( u_p \), linked to the eigenvalues \( \lambda_p \), they compute the parameters \( \alpha_p \) by:

\[
\alpha = \Lambda^{-1} U^T R.
\]

(2.33)

The eigeneffects \( u_p(E) \) is an approximation of the physical interaction phenomena and the weight fractions of mixtures can be calibrated against the computed \( \alpha \). The authors claim to be able to measure three eigeneffects capable to separate three different mixtures of elements using ten different energy spectra.

2.10 Non-linear model fitting

The fitting off non-linear models to measured data is often performed by finding the parameters that minimizes the sum of squares of the residual, in the same way as linear models. Compared to linear models, non-linear models can only be solved directly in special cases. Instead models are fitted using iterative methods, unless a direct method is available. A common method to find the optimal model parameters
\( \theta \) by minimizing the sum of the squared residuals of the model \( f_i(\theta) \) and the data \( b_i \).

\[
S(\theta) = \left\| \phi_i(\theta) \right\|_2^2 = \sum_{i=1}^{N} \phi_i(\theta)^2 \\
\phi_i(\theta) = f_i(\theta) - b_i
\]

This non-linear optimization problem can be solved with the Gauss-Newton method, by linearizing the sum of squares \( S(\theta) \) around a starting guess \( \theta^* \) and finding the parameters \( \theta \) minimizing

\[
\min \left\| \phi_i(\theta^*) + \frac{\partial \phi_i(\theta^*)}{\partial \theta_j}(\theta_j - \theta_j^*) \right\|_2
\]

The derivatives \( \frac{\partial \phi_i}{\partial \theta_j} \) constitutes the elements \( J_{ij} \) in the Jacobian matrix \( J \) and the linear least squares solution for the parameters \( \theta - \theta^* \) is

\[
(\theta - \theta^*) = (J^T J)^{-1} J^T \phi(\theta^*)
\]

Which is repeated with for \( \theta^* = \theta \) until the difference between \( S(\theta) \) and \( S(\theta^*) \) or the norm of the change \( \|\theta - \theta^*\|_2 \), is smaller than termination value.

### 2.10.1 Ill conditioned problems & Regularization

Solving the linear sub problem (eq. 2.37) is highly dependent on the matrix \( J^T J \). If the determinant of \( J^T J \) is zero, the matrix is not invertible and the problem lack a unique solution and are ill-posed. When the determinant of \( J^T J \) is small, the problem is ill-conditioned. For an ill-conditioned problem a small perturbation in the data \( b_i \) will give rise to a large perturbation in the computed parameters \( \theta \).

This effect can be observed using the singular value decomposition (SVD) of \( J \).

\[
J = U \Sigma V^T
\]

The linear problem eq. 2.37 then becomes:

\[
(\theta - \theta^*) = V \Sigma^{-1} U^T \phi(\theta^*)
\]

Thus a small perturbation in \( b_i \) can be amplified by \( \sigma_p^{-1} \). To overcome ill-conditioning, regularization methods are applied. They are used to artificially limit the variation in the completed parameters while retaining the properties of the original problem. One way to regularize the least squares problem is the simplest form of Tikhonov regularization [9], by adding the regularization parameter \( \lambda \) to the diagonal of to the system matrix \( J^T J \).

\[
(\theta - \theta^*) = (J^T J + \lambda I)^{-1} J^T \phi(\theta^*)
\]

\[
(\theta - \theta^*) = V(\Sigma + \lambda I)^{-1} U^T \phi(\theta^*)
\]
2.10. NON-LINEAR MODEL FITTING

The smallest singular value is then at least \( \lambda \), which limits the amplification. The choice of regularization parameter \( \lambda \) is important, too large, the original problem is lost, and too small, the problem remains ill-conditioned. This method is used in the Levenberg-Marquardt method for solving non-linear least squares. The regularization parameter \( \lambda \) is the updated for each iteration, depending on how well the linear subproblem predicts the reduction of the residuals [9].

2.10.2 Principal Component Regression

Another regularization method is principal component regression[12]. Then the principal components of the matrix \( J \) are computed using SVD 2.38. The variation captured for each principal component \( p \) is proportional to the singular value \( \sigma_p \). By restricting the problem to the \( P \) strongest principal components, a lower rank approximation \( J_P \) of the matrix \( J \) can be formulated as:

\[
J_P = U_P \Sigma_P V_P^T
\]  

(2.42)

where \( U_P \) and \( V_P \) contains the first \( P \) columns of \( U \) and \( V \) respectively. \( \Sigma_P \) is the diagonal matrix with the largest \( P \) singular values \( \sigma_p \) on the diagonal. Computing the parameters is then:

\[
(\theta - \theta^*) = V_P \Sigma_P^{-1} U_P^T \phi(\theta^*)
\]

(2.43)

The maximum amplification is then restricted to the smallest singular value \( 1/\sigma_P \). The number of principal components to use in the regression is problem dependent.

2.10.3 Error in the computed parameters

Fitting a model against noisy data introduces variance in the computed parameters caused by variance in the data. For small perturbations in the data \( b \), the perturbation of the fitted parameters are

\[
\Delta \theta = (J^T J)^{-1} J^T \Delta b
\]

(2.44)

Assuming that the noise in the data is normally distributed and uncorrelated the covariance matrix \( C_b \) is then diagonal with the variance estimate \( \sigma_i^2 \) on the diagonals. The covariance matrix of the computed parameters is then related to the covariance in the data [18] by

\[
C_\theta = (J^T J)^{-1} J^T C_b J (J^T J)^{-T}
\]

(2.45)

which for independent identically distributed deviations i.e. \( C_b = \sigma^2 I \) the expression in eq 2.45 simplifies to:

\[
C_\theta = \sigma^2 (J^T J)^{-1}
\]

(2.46)
As the noise distribution varies for the different X-ray signal levels and using the SVD of $J$ (eq. 2.38, 2.39) to simplify eq. 2.45.

$$C_\theta = (V\Sigma^{-1}U^T)C_b(U\Sigma^{-1}V^T) = (J^T C_b^{-1} J)^{-1} \quad (2.47)$$
Chapter 3

Methods & Implementation

To measure the chemical content using only the transmission of X-ray photons, the linear coefficient of attenuation is the only information available. The properties of linear attenuation is well known and can be measured with a high precision in a laboratory setting[13]. In addition the properties of X-ray photon attenuation does not change with temperature, material state, chemical bonds or density. This makes transmission analysis a robust method to measure the chemical composition. The proposed method measures the chemical composition by fitting the linear X-ray model

$$N_{ijk} = \int_0^\infty I_{ijk}(E)e^{\sum w_{mij}(\mu(E)/\rho)m}dE$$

(3.1)

to the measured signal $N_{ijk}^{\text{obs}}$, using non-linear regression. The data is produced as a set of $K$ images, where each image measured using a selected spectral setting $k$. Each row $i$ of the image pixels is constructed by measuring one detector pixel several times while the sample is moved in front of it (fig. 3.1). It have been shown that it is impossible to resolve the weight fractions $w_{mij}$ explicitly and only variations between up to three different chemical compositions can be resolved. The method used to reconstruct a samples linear mass attenuation coefficient from a multiple energy measurement is separated in three parts:

1. A low rank basis for the attenuation $\sum w_m(\mu(E)/\rho)_m$ is constructed, as the attenuation of candidate elements are co-linear and the inverse problem is ill-conditioned.

2. The effective X-ray spectra $I_{ik}(E)$ for each pixel of the detector, is estimated using a reference object with known attenuation at different thicknesses and fitting a spectral ansatz $I_{k}(E, c_{ik})$ using least squares.

3. Using the effective spectra, the image of the sample is reconstructed, by fitting the low-rank basis to the measured signal.
In all steps the fitting is done by minimizing the squared error of the logarithm of the signal.

$$\min \left\| \log \left( N(c_{ik}, w_{ij}) \right) - \log \left( N_{ijk}^{obs} \right) \right\|_2$$  \hspace{1cm} (3.2)

The ability for this method to resolve the chemical composition of a sample is estimated, as the measurements are affected by noise.

![Image](image.png)

**Figure 3.1.** The multi-energy data $N_{ijk}$ from the Mantex Desktop scanner is organized in 8 images, one image for each energy setting ($k$). Each image is composed by combining 400 illuminations ($j$) of 128 detector pixels ($i$).

### 3.1 Simulation model

To simplify the analysis of the method a simulation model of the Mantex Desktop scanner is created. This makes it possible to create *in silico* measurements with similar properties as the real measurements. The *in silico* machine and samples are in total control, removing drifts and noise sources. In order to create realistic measurements artificial noise is added.

#### 3.1.1 In silico Samples

The simulated samples in table 3.1 were chosen to represent real world objects available for testing. The samples have varying thickness and each sample is simulated as a wedge, with the thickness $t_i$ increasing for each simulated illumination $i$. The attenuation coefficient of the sample $\mu_s(E)$ is constructed by combining the attenuation coefficients of the present elements $m$, by their weight fraction $w_m$ and scaled
3.1. SIMULATION MODEL

with the measured sample density as follows:

$$\mu_s(E) = \rho_s \frac{\sum_m \left( \frac{\mu(E)}{\rho} \right) w_m}{\sum_m w_m}$$  \hspace{1cm} (3.3)

<table>
<thead>
<tr>
<th>Common name</th>
<th>Chemical Formula</th>
<th>Density $\rho_s$</th>
<th>Thickness $t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>PE500</td>
<td>$(CH_2)_n$</td>
<td>0.954 g/cm$^3$</td>
<td>0-4 cm</td>
</tr>
<tr>
<td>PTFE</td>
<td>$(CF_2)_n$</td>
<td>2.174 g/cm$^3$</td>
<td>0-4 cm</td>
</tr>
<tr>
<td>PVC</td>
<td>$(C_2H_4Cl)_n$</td>
<td>1.363 g/cm$^3$</td>
<td>0-4 cm</td>
</tr>
<tr>
<td>Acrylic</td>
<td>$(C_5H_8O_2)_n$</td>
<td>1.188 g/cm$^3$</td>
<td>0-4 cm</td>
</tr>
<tr>
<td>Acetal</td>
<td>$(CH_2O)_n$</td>
<td>1.432 g/cm$^3$</td>
<td>0-4 cm</td>
</tr>
<tr>
<td>Aluminum stair</td>
<td>Al</td>
<td>2.699 g/cm$^3$</td>
<td>1, 2, ... 8 mm</td>
</tr>
<tr>
<td>Water</td>
<td>$H_2O$</td>
<td>1.000 g/cm$^3$</td>
<td>2-6 cm</td>
</tr>
<tr>
<td>Wood Pellets</td>
<td>$C_6H_{10}O_5$</td>
<td>0.56 g/cm$^3$</td>
<td>2-6 cm</td>
</tr>
<tr>
<td>Stone</td>
<td>$SiO_2$</td>
<td>2.650 g/cm$^3$</td>
<td>1-3 cm</td>
</tr>
</tbody>
</table>

3.1.2 Source spectrum

The source spectrum is simulated using the program SpekCalc [10]. It is capable to simulate X-ray spectra from tungsten tubes with a peak energy $E_k$ up to 300 keV. SpekCalc calculates the emitted number of photons $S_n$ between $E_n$ and $E_{n+1} = E_n + 0.5$ keV hitting a area of 1 cm$^2$ at a distance of 1 m per mAs for discrete energy levels from $E_n = E_k/10, \ldots, E_k$. The spectrum is then modified with the estimated inherent filtration of the source.

3.1.3 Detector Model

The detector is modeled as a perfect Gadox scintillator. The number of photons $X$ absorbed in the detector is a product of independent random emission and absorption processes. This is usually modeled as a poisson distributed variable $X_n$, with the mean $E(X_n) = \bar{X}_n$ and variance $Var(X_n) = \bar{X}_n$ [14]

$$\bar{X}_n = S_ne^{-\mu_s(E_n)t} \left( 1 - e^{-\mu_{Gadox}(E_n)Gadox} \right)$$  \hspace{1cm} (3.4)

The detector signal $N$ is the total photon counts modified by the energy dependent gain $E_nG$.

$$N_k = \sum_{n=1}^{E_n+1=E_k} E_nG\bar{X}_n\Delta E$$  \hspace{1cm} (3.5)
3.1.4 Image construction

To replicate the measurement system, the simulated image pixels $N_{ijk}$ is constructed by varying the sample thickness $t_{ij}$. The mean output of each detector pixel varies. To model this, a detector pixel specific constant $C_i$ is multiplied to the number of absorbed photons.

3.1.5 Simulation model

The simulated measurement images $N_{ijk}$ is then constructed by sampling a random distribution with the mean:

$$N_{ijk} = E(N_{ijk}) = \sum_{n=1}^{E_{n+1}=E_k} E_n G C_i T_n e^{-\mu_s(E_n)t_{ij}} \left(1 - e^{-\mu_{Gadox}(E_n)t_{Gadox}}\right)$$ (3.6)

and the variance, the combined variance of the bins:

$$\text{Var}(N_{ijk}) = \sum_{n=1}^{E_{n+1}=E_k} E_n^2 G^2 C_i T_n e^{-\mu_s(E_n)t_{ij}} \left(1 - e^{-\mu_{Gadox}(E_n)t_{Gadox}}\right)$$ (3.7)

To replicate this distribution, using the Poisson distribution, the effective gain $G_{ijk}$ is calculated for each pixel using eq. 3.6 and eq. 3.6

$$G_{ijk} = \frac{\text{Var}(N_{ijk})}{N_{ijk}}$$ (3.8)

each pixel is a outcome from a poisson distributed random variable with the mean $\lambda = \frac{N_{ijk}}{G_{ijk}}$ and scaled with the effective gain

$$N_{ijk} = G_{ijk}\text{Poisson}\left(\frac{N_{ijk}}{G_{ijk}}\right)$$ (3.9)

3.2 Linearization of the minimization problem

Analysis and minimization of the non-linear least squares problem (eq. 3.2) with the X-ray model (eq. 3.1) by standard methods assume that the problem surface can be approximated. A linear approximation near the minimum should represent the problem characteristics with respect to perturbations in the data and covariances in the variables.

3.2.1 Choice of norm

By comparing the non-linear problem with the special case of monochromatic spectra with distinct energies $E_k$, the choice of minimizing the norm of the error in the
3.2. LINEARIZATION OF THE MINIMIZATION PROBLEM

logarithm of the signal $N$ is motivated. Using monochromatic spectra defined with
the dirac delta function

$$ I_k(E) = C_k \delta(E - E_k). $$ (3.10)

in the X-ray model (eq. 3.1), creates the simplified X-ray model:

$$ N_{ijk} = C_k e^{-\sum w_{mij} (\mu(E_k)/\rho)_m} $$ (3.11)

hence the least squares minimization problem (eq. 3.2) reduces to

$$ \min \| \log(N_{ijk}^{obs}) - \log(C_k) - \sum_{m=0}^{M} w_{mij} \left( \frac{\mu(E_k)}{\rho} \right)_m \|_2 $$ (3.12)

which is linear with respect to $w_{mij}$ and can be solved directly by the linear least
squares solution of the problem (eq. 3.12). This monochromatic assumption does
not hold for real X-ray spectra since errors introduced by beam hardening are not
taken into account [15]. However, the relationship between the X-ray model and
the linear problem, shows that minimizing the error of the logarithm of the signal,
the X-ray model is approximately linear.

3.2.2 Deriving the Jacobian

Instead of making the monochromatic assumption for the spectra $I_k(E)$, the prop-
erties of the first order linear Taylor approximation of the problem is used. This
requires the calculation of the Jacobian with respect to the different set of param-
eters used in the separate parts of the multi energy method.

Using a generalized version of the X-ray model (eq. 3.1) with a set of param-
eters $\theta$, representing the spectral and material parameters, fitted in the spectral
reconstruction and material reconstruction part of the method.

$$ N_k(\theta) = \int_{0}^{\infty} g_k(E)e^{\sum_p f_p(E) \theta_p} dE $$ (3.13)

Linearizing the generalized X-ray model (eq. 3.13) and the corresponding least
square problem (eq. 3.14) around a point $\theta^*$

$$ \min S(\theta) = \min \| \phi_k(\theta) \|_2 $$ (3.14)

with the gradient:

$$ \phi_k(\theta) = \log(N_k(\theta)) - \log(N_k^{obs}) = \log \left( \int_{0}^{\infty} g_k(E)e^{\sum_p f_p(E) \theta_p} dE \right) - \log \left( N_k^{obs} \right) $$ (3.15)

yields the Jacobian:

$$ J_{kp} = \frac{\partial \phi_k(\theta^*)}{\partial \theta_p} = \frac{1}{N_k(\theta^*)} \int_{0}^{\infty} g_k(E) \frac{\partial}{\partial \theta_p} e^{\sum_p f_p(E) \theta_p} dE $$ (3.16)

$$ = \int_{0}^{\infty} \hat{g}_k(E, \theta^*) f_p(E) dE $$ (3.17)
where

\[ \hat{g}_k(E, \theta^*) = \frac{g_k(E)e^{\sum_p f_p(E)\theta^*_p}}{\int g_k(E)e^{\sum_p f_p(E)\theta^*_p} dE} \]  

(3.18)

The elements of the Jacobian is the weighted mean of the functions \( f_p(E) \), with the weighting \( \hat{g}_k(E, \theta^*) \), the effective spectrum at \( \theta^* \).

### 3.3 Low rank reconstruction of the attenuation coefficient

To overcome the multi co-linear nature of the attenuation coefficients caused by the limited number physical phenomena, a set of basis functions \( u_p(E) \) constructed as a linear combination of attenuation coefficients. By reconstructing the measured data with:

\[ N_k(\alpha) = \int I_k(E)e^{\sum_p \alpha_p u_p(E)} dE \]  

(3.19)

using only \( P \) parameters \( \alpha_p \). The basis function \( u_p(E) \) is defined as a linear combination of the attenuation coefficients.

\[ u_p(E) = \sum_m V_{mp} \left( \frac{\mu(E)}{\rho} \right)_m \]  

(3.20)

The basis is constructed with the objective

\[ \min_{\alpha} \left\| \log (N_k(w)) - \log (N_k(V\alpha)) \right\|_2 \]  

(3.21)

for each \( P < M \). Which for monochromatic spectra \( I_k(E) = \delta(E - E_k) \) becomes:

\[ \min_{\alpha} \left\| \sum_m w_m \left( \frac{\mu(E_k)}{\rho} \right)_m - \sum_p \alpha_p u_p(E_k) \right\|^2 \]  

(3.22)

Without the monochromatic assumption the problem in 3.21 can be linearized around a point \( w^* \).

\[ J_{km}(w^*) = \frac{\partial \log(N_k)}{\partial w_m}(w^*) = \frac{1}{N_k} \int_{E_{min}}^{E_{max}} I_k(E)e^{-\sum_m w_m^*(\mu(E)/\rho)_m} \left( \frac{\mu(E)}{\rho} \right)_m dE \]  

(3.23)

\[ \min \left\| \sum_m J_{km} w_m - \sum_p \sum_m J_{km} V_{mp} \alpha_p \right\|^2 \]  

(3.24)

Which is minimized when \( V \) is the right eigenvectors of \( J \), computed using the singular value decomposition.

\[ J = U\Sigma V^T \]  

(3.25)

Using the matrix \( V \), the right eigenvectors of \( J \) from the linearized problem (eq. 3.24), the basis functions \( u_p(E) \) for the non-linear problem (eq. 3.21) is constructed.
3.3. LOW RANK RECONSTRUCTION OF THE ATTENUATION COEFFICIENT

using eq. 3.20. The basis functions related to the three largest singular values shown in figure 3.2 can be compared to the three major physical effects. Using the same reasoning as Maitrejean et. al. [2], the basis $u_1(E)$ is observed to have the similar shape as the photoelectric effect, $u_2(E)$ the Compton scattering relative to the Photoelectric effect, $u_3(E)$ to the Rayleigh scattering relative to Compton scattering and the Photoelectric effect. Functions related to the smaller singular values have no apparent physical relationship and are very dependent on the basis elements used.

![Figure 3.2. Plot of the basis functions related to the 4 largest singular values.](image)

3.3.1 Scaling

To balance impact of the individual elements on the basis, the columns in the Jacobian are scaled. The scaled Jacobian $J^S$ is created by multiplying column $i$, with a factor $D^S_{ii}$, computed from the diagonal of the covariance matrix $(J^T J)$ (eq. 3.26).

$$D^S_{ii} = (J^T J)^{-\frac{1}{2}}_{ii}$$

(3.26)

The basis $u_p(E)$ is then computed using the eigenvectors $V^S$ of the scaled Jacobian $J^S$ and the column weights.

$$V = D^S V^S$$

(3.27)

A basis computed using the scaled Jacobian have less emphasis on modeling the high $Z$ elements, where the variation in the Photoelectric effect is larger. Thus the basis work for both high and low $Z$ elements. The scaling also improves the
conditioning of the low rank basis. As seen in figure 3.3 the scaled Jacobian have smaller difference between the largest and smallest singular value for the same number of basis functions.

### 3.3.2 Choosing the number of basis functions

The relative size of computed singular values $\sigma_p^2$ (eq. 3.25) indicate the relative variance of $J$ that each singular vector captures. Changing the spectra $I_k(E)$ and the material basis $\mu_m(E)$ can improve the relative significance of the computed bases. The behavior of the computed basis functions $u_p(E)$ and the relative size of the singular values indicates that only three basis functions are required to reconstruct the material basis accurately. In addition the third basis function have a very small contribution, making measurement of $\alpha_3$ very uncertain.

![Figure 3.3](image)

**Figure 3.3.** The singular values of $J$ and $J^S$ show no clear cutoff only the importance of the basis functions linked to the two largest singular values. The singular values in the plot have been normalized with the largest value.

### 3.3.3 The error of approximation

The error introduced by restricting the number of basis functions in the non-linear function can only be estimated form the linearized version. The error introduced
3.3. LOW RANK RECONSTRUCTION OF THE ATTENUATION COEFFICIENT

by only using $P$ parameters to reconstruct a $M$ material basis is:

$$\text{Err} = \left\| \sum_{m} J_{km} w_m - \sum_{p} P \sum_{m} J_{km} V_{mp} \alpha_p \right\|^2 = \left\| M \sum_{p=P+1} M \sum_{m} J_{km} V_{mp} \alpha_p \right\|^2 = \sum_{p=P+1} M \sigma_p^2 \| \alpha_p \|$$

(3.28)

assuming that the magnitude of the computed parameters are decreasing i.e. $\| \alpha_p \| > \| \alpha_{p+1} \|$ the approximation error magnitude is

$$\sum_{p=P+1} M \sigma_p^2 \| \alpha_p \| < \| \alpha_P \| \sum_{p=P+1} M \sigma_p^2$$

(3.29)

If the approximation error is much smaller than the measurement noise $\text{Var}(\log(N))$, an approximation using only $P$ parameters can be considered to be enough to reconstruct the measured signal $\log(N)$.

3.3.4 Chemical information in the low rank approximation

The multi-collinearity of the attenuation coefficients makes it impossible to uniquely determine the elemental composition of an unknown mixture of elements. This complicates the material classification. To classify an unknown material using the reduced basis $u_p$ with only three parameters, prior knowledge is required. For example, if the sample is composed of one of many known material, or if the sample is a unknown mixture of up three known materials. This requirement, makes the classification procedure dependent on the type of application the method used for.

Since prior knowledge is needed to compute the weight fraction parameters $w_m$ they are impractical to use in the analysis. Instead of using $w_m$, the computed parameters $\alpha_p$ can compared to the $\alpha_p$ of samples with known material composition. The parameters $\alpha_p$ are dependent on the samples mass thickness $w_s$, unless the samples density and thickness is known. Without knowing the mass thickness, elements cannot be discriminated by their relative atomic weights.

To make it possible to retrieve the chemical information, the relative sizes of the parameters can be used, as done by Maitrejean et al. [2].

$$w_s \left( \frac{\mu(E)}{\rho} \right)_s \approx M \sum_{m} w_m \left( \frac{\mu(E)}{\rho} \right)_m \approx P \sum_{p} \alpha_p u_p(E)$$

$$= \alpha_1 \left( u_1(E) + \sum_{p=2}^{P} \frac{\alpha_p}{\alpha_1} u_p(E) \right)$$

(3.30)

The fractions $\alpha_2/\alpha_1$ and $\alpha_3/\alpha_1$ should then contain information independent of the samples mass thickness and the atomic weight of the elements. Since the first basis $u_1(E)$ is close to the mean attenuation of the material basis, the first coefficient $\alpha_1$ is zero for measurements without a sample, reducing the risk of division by zero.
The values for $\alpha_2/\alpha_1$ and $\alpha_3/\alpha_1$ for the elements in the material basis is plotted in figure 3.4.

In figure 3.4 it is possible to observe that the relative difference between elements with $Z = 2 - 15$ is limited when using a unscaled Jacobian, as they are placed on a single line, implying that the ratio $\alpha_3/\alpha_1$ have no additional information from $\alpha_2/\alpha_1$. Therefore a mixture of for instance carbon and fluoride is hard to separate form a mixture of carbon and oxygen. This is caused by the relative small variation of the Rayleigh scattering from the Photoelectric effect and Compton scattering. Using a scaled Jacobian (fig. 3.5), the lighter elements are better separated.

### 3.4 Spectral Reconstruction

To fit the effective source-detector spectrum $I_k(E)$ a known material is measured at different thicknesses and a ansatz function is fitted. The ansatz is constructed by combining the approximative Kramer’s law with the known detector response function and a unknown inherent filtering. The characteristic photons in not modeled. To mitigate this and other inaccuracies in the approximation, each energy setting is fitted separately with a approximate photoelectric filtering $\mu_{Photo} \propto E^{-n}$, with $n \approx 3 \ldots 5$ and Compton filtering $\mu_{Compton} \propto E^{-1}$. 

28
3.4. SPECTRAL RECONSTRUCTION

The spectral ansatz is:

\[
I(E) = N_f G E \left( 1 - \frac{E}{E_{\text{max}}} \right) e^{-\mu(E)_{\text{Gadox}}} w_{\text{Gadox}} E^{-5} - w_{\text{Photo}} E^{-3} - w_{\text{Compton}} E^{-1} \\
= e^{c_1} I(E)_{\text{fixed}}e^{-c_2 E^{-5} - c_3 E^{-3} - c_4 E^{-1}}
\]

with the unknown parameters \(c_1 = \log(N_f G), \ c_2 = w_{\text{Photo}}, \ c_3 = w_{\text{Photo}'}, \ c_4 = w_{\text{Compton}}\) and are added to account for the variation of Photoelectric effect. The separate photoelectric and Compton filtering enables the model to approximate a filter with unknown thickness and atomic composition. The source potential \(E_{\text{max}}\) for each setting is assumed to be known.

The parameters are fitted to the measured signal of an aluminum stair with 8 steps of thickness \(d_j = 0, 1, 2 \ldots 8\) mm. By minimizing the error of the logarithm \(\phi_j\), it is possible to create an approximately linear problem. For each energy setting \(k\) the square error sum is minimized.

\[
\min_c S(c) = \min \sum_{j=0}^{9} (\phi_j(c))^2
\]

\[
\phi_j(c) = \log(N_j) - \log(N_j^{\text{obs}}) = \log \left( \int_{E_{\text{min}}}^{E_{\text{max}}} I(E, c)e^{-\mu(Al(E)d_j dE)} \right) - \log(N_j^{\text{obs}})
\]

Figure 3.5. Chemical identification of the elements in the scaled material basis
CHAPTER 3. METHODS & IMPLEMENTATION

The Jacobian of $S(c)$ is (eq 3.16):

$$J_{jp} = \frac{\partial \phi_j}{\partial c_p} = \frac{1}{N_j} \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{\partial I_j(E,c)}{\partial c_p} e^{-\mu_A(E)\alpha_j} dE$$

$$J_{j1} = \int_{E_{\text{min}}}^{E_{\text{max}}} \dot{I}_j(E,c) dE = 1$$

$$J_{j2} = -\int_{E_{\text{min}}}^{E_{\text{max}}} \dot{I}_j(E,c) E^{-5} dE$$

$$J_{j3} = -\int_{E_{\text{min}}}^{E_{\text{max}}} \dot{I}_j(E,c) E^{-3} dE$$

$$J_{j4} = -\int_{E_{\text{min}}}^{E_{\text{max}}} \dot{I}_j(E,c) E^{-1} dE$$

(3.34)

where

$$\dot{I}_j(E,c) = \frac{I_j(E,c) e^{-\mu_A(E)\alpha_j}}{\int_{E_{\text{min}}}^{E_{\text{max}}} I_j(E,c) e^{-\mu_A(E)\alpha_j} dE}$$

(3.35)

3.5 Material Reconstruction

When the source-detector spectra $I_k(E)$ is estimated, the attenuation function of the sample $\mu(E)$ can be estimated using the constructed attenuation basis functions (eq. 3.20), by fitting the model to the measured signal $N_{k \text{obs}}$ for each energy measurement $k$.

To reconstruct the sample attenuation, find $\alpha$ that minimize

$$\min_{\alpha} S(\alpha) = \min_k \sum_{k=1}^{K} (\phi_k(\alpha))^2$$

(3.36)

$$\phi_k(\alpha) = \log(N_k) - \log(N_{k \text{obs}}) = \log \left( \int_{E_{\text{min}}}^{E_{\text{max}}} I_k(E) e^{-\sum u_p(E)\alpha_p} dE \right) - \log(N_{k \text{obs}})$$

(3.37)

The Jacobian of $S(\alpha)$ is (eq 3.16):

$$J_{kp} = \frac{\partial \phi_j}{\partial c_p} = \frac{1}{N_k} \int_{E_{\text{min}}}^{E_{\text{max}}} \frac{\partial I_k(E)}{\partial \alpha_k} e^{-\sum u_p(E)\alpha_p} dE$$

$$= -\int_{E_{\text{min}}}^{E_{\text{max}}} \dot{I}_k(E,\alpha) u_p(E) dE$$

(3.38)

(3.39)

where

$$\dot{I}_k(E,\alpha) = \frac{I_k(E) e^{-\sum u_p(E)\alpha_p}}{\int_{E_{\text{min}}}^{E_{\text{max}}} I_k(E) e^{-\sum u_p(E)\alpha_p} dE}$$

(3.40)
3.5. MATERIAL RECONSTRUCTION

The sought after chemical information in the ratios $\alpha_2/\alpha_1$ and $\alpha_3/\alpha_1$ can be computed directly by introducing the parameters $\beta$, where $\beta_1 = \alpha_1$, $\beta_2 = \alpha_2/\alpha_1$ and $\beta_3 = \alpha_3/\alpha_1$ and minimizing

$$\min_{\beta} S(\beta) = \min \sum_{k=1}^{K} \phi_k (\alpha(\beta))^2$$

(3.41)

using the Jacobian

$$J_{k1} = -\int_{E_{min}}^{E_{max}} I_k (E, \alpha(\beta)) (u_1(E) + \beta_2 u_2(E) + \beta_3 u_3(E)) dE$$

(3.42)

$$J_{k2} = -\beta_1 \int_{E_{min}}^{E_{max}} I_k (E, \alpha(\beta)) u_2(E) dE$$

(3.43)

$$J_{k3} = -\beta_1 \int_{E_{min}}^{E_{max}} I_k (E, \alpha(\beta)) u_3(E) dE$$

(3.44)

(3.45)

3.5.1 Image reconstruction

Each measurement is performed by measuring the signal in the 128 detector CCD-pixels while the sample is moved through the X-ray beam. The measured X-ray intensity is integrated in the ccd over 32 ms and stored. Depending on the size of the sample and the speed, the number of image pixels differs. For the tests the sample 400 columns of the image are used. The resulting data is organized in 8 images for each setting with the size $128 \times 400$. Each sample can be assumed to measured with $128 \times 400$ statistically independent sub measurements assuming only photonic noise.

The material model can be used to reconstruct the images by minimizing (eq. 3.41) for all image pixels . The resulting problem is then:

$$\min_{\beta_{ij}} \sum_{i=1}^{128} \sum_{j=1}^{400} \sum_{k=1}^{8} \phi_{ijk} (\alpha(\beta_{ij}))^2$$

(3.46)

$$\phi_{ijk}(\alpha) = \log \left( \int_{E_{min}}^{E_{max}} I_{ik}(E)e^{-\sum_{p} u_p(E) \alpha_p dE} \right) - \log(N_{ijk}^{obs})$$

(3.47)

This can be minimized by minimizing each pixel $(i,j)$ separately, as done by Maitjjean et. al [2]. The chemical composition parameters of the whole sample $\bar{\beta}_2$ & $\bar{\beta}_3$ is then computed by the weighted mean of the individual $\beta_{ij2}$ & $\beta_{ij3}$, weighted by $\beta_{ij1}$ (eq. 3.48).

$$\beta_1 = \beta_{ij1}$$

$$\beta_2 = \frac{\beta_{ij1} \beta_{ij2}}{\beta_1}$$

$$\beta_3 = \frac{\beta_{ij1} \beta_{ij3}}{\beta_1}$$

(3.48)
CHAPTER 3. METHODS & IMPLEMENTATION

This problem has $128 \times 400 \times 8$ data points and $128 \times 400 \times 3$ unknown parameters which can be separated into $128 \times 400$ subproblems, each with three unknowns. Due to the noise in the data, the individual problems are prone to overfitting and require regularization to obtain a stable result.

3.6 Regularization strategies

As the full image reconstruction of individual pixels separately (eq. 3.46) is non-linear, a bound for the individual parameters $\beta_{ij}$ cannot be constructed. To limit the impact of noise, regularization of the problem is required to limit the variation in the computed parameters $\beta$. A good regularization strategy should not limit the modeling capability while reducing the degrees of freedom in the fitting. To regularize the problem and improve performance different strategies are combined.

3.6.1 Low rank reconstruction

The low rank approximation (eq. 3.19) used instead of the attenuation coefficients of the individual materials (eq. 3.1), have regularizing properties and improves the stability of the problem, as the fitted parameters are fewer, compared to the fitting the weight fractions of the materials directly. The reduction in modeling capability is not significant since the low rank approximation is capable to model almost all the variation in the attenuation coefficients.

3.6.2 Identifying global and local parameters

The large number of parameters in (eq. 3.46) are unnecessary since only the composition of the whole sample is interesting. By constraining the individual pixel parameters to be equal over the image, $\beta_{ij2} = \beta_2$ and $\beta_{ij3} = \beta_3$ and only allowing $\beta_{ij1}$ to vary over the image pixels. This is based on the assumption that $\beta_2$ and $\beta_3$ only contain chemical information, and varying $\beta_{ij1}$ can handle variations in sample thickness and density on the local pixel. This assumption connects all the individual data pixels and each pixel $\beta_{ij}$ can not be solved separately.

3.6.3 Image Reduction

To reduce noise in the individual data points, similar data points can be combined. In addition to reducing the noise, the size of the problem is reduced, improving the performance. Depending on the underlying problem, reduction can introduce biases, in the data and the computed parameters.

To take advantage of the fast performance of the reduced problem, the unknown parameters are first fitted to mean of the images. The resulting parameters are then used to create a initial guess for the full problem. The full problem is only reduced by combining 10 pixels measured in by the same detector pixel, to keep the
computational time reasonable. The full problem is reduced to find $128 \times 40 \times 1 + 2$ unknowns, which takes $\approx 1$ min to solve on a 2.26 GHz Intel Core 2 Duo processor.

### 3.7 Implementation details

#### 3.7.1 Integral approximation

The integral calculation (eq. 3.49) is approximated numerically using the trapezoidal method. The photon energy $E$ is discretized using 120 uniformly distributed grid points, the lowest energy $E_1 = 5$ keV and the maximum $E_{120} = E_{max}$ is different for each energy setting $k$.

$$N = \int_{E_{min}}^{E_{max}} I(E)e^{-\mu(E)}dE$$

$$N = \frac{1}{2} \sum_{n=1}^{120} \left( I(E_{n+1})e^{-\mu(E_{n+1})} + I(E_n)e^{-\mu(E_n)} \right) (E_{i+1} - E_i) \tag{3.50}$$

To reduce the interpolation error, extra grid points are added around the discontinuities in the $I(E)$, where the detector absorption increases (fig 2.5) at the Gadolinium K-edge energy level $E_K = 50.189$ keV. Thus the grid points $E_n = E_K - 10^{-3}$ $E_n + 1 = E_K + 10^{-3}$ are added to the uniform grid.

#### 3.7.2 Initial parameters

Solving non-linear problems requires a set of initial guesses for the parameters to be fitted. To improve the convergence properties, the initial parameters should be close to the optimal parameters. For the fitting of the spectral parameters, initial guesses are $c_k = 0$. After fitting parameters for the reduced problem, the pixel dependent first parameter $c_{1ik}$ is initialized using eq. 3.51.

$$c_{1ik} = c_{ik} - \frac{1}{9} \sum_{j=1}^{9} \left( \log \left( N_{ijk}^{obs} \right) - \log \left( N_{ijk}(c_k) \right) \right) \tag{3.51}$$

The initial parameters for the material model in the reduced problem (eq. 3.41): $\beta_1 = 1$, $\beta_2 = 0$ and $\beta_3 = 0$. After the minimizing the reduced problem, the solution $\beta$ is used to initialize the full problem. The pixel dependent parameter $\beta_{1ij}$ is initialized from $\beta_1$ with eq. 3.52.

$$\beta_{1ij} = \beta_1 \frac{1}{8} \sum_{k=1}^{8} \frac{\log \left( N_{ijk}^{obs} \right) - \log \left( N(0)_{ijk} \right)}{\log(N(\beta)_{ijk}) - \log(N(0)_{ijk})} \tag{3.52}$$
3.7.3 Non-linear least squares solver

The minimization problems to fit the parameters in the spectral and material reconstruction models are all solved using the non-linear least squares. To find the least squares solution, the MATLAB routine \texttt{lsqnonlin} implementation of the Levenberg-Marquardt algorithm is used. To limit the computational time used for hard problems, the numbers of allowed iterations is limited. The reduced problem is limited to 50 iterations and the full problem is limited to 5 iterations.

3.7.4 Order of operations

1. Measure the calibration stair with 8 energy settings and extract the aluminum stair steps $N_{ij}^{\text{obs}}$.
2. Find parameters $c_{ik}$ for each detector pixel $i$ and energy setting $k$.
   For each setting $k$ do:
   a) Reduce the problem to a single mean detector pixel. Solve eq. 3.32 for $c_k$.
   b) Using the found $c_k$ compute $c_{ik}$ using eq. 3.51
   c) Compute the discretized $I_{ik}(E_n)$ using $I(E, c_{ik})$
3. Construct the low rank basis $u_p(E_n)$ using SVD and $I_{ik}(E_n)$
4. Optional: Estimate the current machine state the by measuring the stair and redoing steps 1 – 2, to recompute $I_{ik}(E_n)$
5. Measure the sample and extract the images $N_{ij}^{\text{obs}}$
6. Find the parameters $\beta$:
   a) Reduce the image $N_{ij}^{\text{obs}}$ to $N_{i}^{\text{obs}}$, and find $\beta$ with eq. 3.41
   b) Using eq. 3.52, construct the initial guess for $\beta_{ij1}$.
   c) Reduce $N_{ij}^{\text{obs}}$ by combining 10 adjacent pixels
   d) Calculate $\beta_{ij}$, by solving the the full image problem (eq. 3.46) for $N_{ij}^{\text{obs}}$ with global $\beta_2$, $\beta_3$.
7. Use $\beta_2$ and $\beta_3$ to classify the sample.

3.7.5 Error estimates

To analyze the fitting of the parameters, the photonic noise in the measurement is estimated. With a estimated gain function $G(E) = GE$ and a estimate of the spectral composition $I_k(E)$ for each measured datapoint, the variance of the observed values, $\log(N_{ij}^{\text{obs}})$ can be estimated using:
3.7. IMPLEMENTATION DETAILS

\begin{equation}
\text{Var} \left( N_{ijk}^{\text{obs}} \right) = \sigma_{N_{ijk}}^2 = \int_0^\infty GEI_{ik}(E) e^{-\sum u_p(E) \alpha_p} dE \quad (3.53)
\end{equation}

\begin{equation}
\text{Var} \left( \log \left( N_{ijk}^{\text{obs}} \right) \right) = \frac{\sigma_{N_{ijk}}^2}{\left( N_{ijk}^{\text{obs}} \right)^2} \quad (3.54)
\end{equation}

With the data noise estimates on the diagonal of the covariance matrix $C_\phi$, an estimate (eq. 2.47) of the covariance in of the computed parameters $\beta$ can be constructed using the computed jacobian (eq. 3.44).

\begin{equation}
C_\beta = (J^T C_\phi^{-1} J)^{-1} \quad (3.55)
\end{equation}
Chapter 4

Results

4.1 Simulation Accuracy

The simulation model described in section 3.1 requires a calibration to replicate the Desktop Scanner system. In the model the effective inherent filtration in the source and the detector gain $G$ is unknown for the real system. Using measurements of an aluminum phantom from three spectral settings, the models capacity to replicate the spectral response $R$ and noise level is determined. The aluminum stair phantom have 10 steps of increasing thickness from 0.5 mm to 5 mm can be seen in figure 4.1.

![Figure 4.1](image)

**Figure 4.1.** Raw image of stair phantom measured in a Desktop scanner. Darker steps have higher attenuation.
CHAPTER 4. RESULTS

4.1.1 Spectral Accuracy

The spectral response is independent of detector gain and the number of emitted photons. The attenuation reflex $R$ of the simulated spectra is compared to the attenuation of the measured stair. In figure 4.2 the simulated signal $N$ in each aluminum step, is normalized with the unattenuated signal $N_0$ to compute the attenuation reflex $R$:

$$R = -\log \frac{N}{N_0}$$

(4.1)

![Figure 4.2. Comparison between simulated R values and measured for 3 spectral settings.](image)

4.1.2 Determining gain

The detector gain $G$ in the simulation model (eq. 2.11) is found, using the assumption of Poisson distributed photon counts, which links the mean and the variance by the effective gain $G_e$. Comparing the mean and variance of the measured signal in air $N_0$ for three different machine settings and comparing the effective gain (eq. 4.2) of the measured data to the effective gain of the simulation model using $G = 1$.

$$G_e = \frac{\text{Var}(N_0)}{N_0}$$

(4.2)

The detector response form a photon in (eq. 3.5) is approximated from the computed $G$ for the three settings in table 4.1.2.

$$G = \frac{G_{\text{sim}}}{G_{\text{meas}}} = 0.03\text{keV}^{-1}$$

(4.3)
4.1. SIMULATION ACCURACY

<table>
<thead>
<tr>
<th>Setting</th>
<th>Measured $G_e$</th>
<th>Simulated $G_e$</th>
<th>Estimated $G$</th>
</tr>
</thead>
<tbody>
<tr>
<td>40kV</td>
<td>0.9800</td>
<td>29.1652</td>
<td>0.0336</td>
</tr>
<tr>
<td>60kV</td>
<td>1.3160</td>
<td>37.1059</td>
<td>0.0355</td>
</tr>
<tr>
<td>90kV + 0.5Cu</td>
<td>1.7417</td>
<td>61.6849</td>
<td>0.0282</td>
</tr>
</tbody>
</table>

4.1.3 Signal and Noise

The simulation model estimates the variance of the simulated values, enabling the generation realistic data. The simulated effective gain (eq. 4.2) is compared to the measured effective gain for each stair step (fig. 4.3). In figure 4.3 it is possible to see good conformity between measured and simulated signal level $N$. The variance of higher voltage settings is overestimated in the simulation when comparing to measured data. This is probably an effect of the ideal detector model used (eq. 2.11).

![Figure 4.3.](image-url) Comparison between simulated R values and measured for 3 spectral settings.
CHAPTER 4. RESULTS

4.2 Spectral Reconstruction

The eight used spectra are reconstructed by fitting the spectral model (eq. 3.31). This is done for the synthetic spectra generated using the calibrated simulation model and measured data from the real machine.

![Graphs showing residual of fit to simulated data](image)

**Figure 4.4.** Measured residual of fit to simulated data, with artificial noise added to the simulated data and without. The residual is scaled to thickness error in cm. Dashed line is the estimated standard deviation of the noise.

4.2.1 Reconstructed synthetic spectra

Using simulated X-ray data replicating a real measurement of a real aluminum star phantom to fit the spectral model (eq. 3.31) a good fit is found. With a realistic noise level in the simulated measurement, the residuals of the fit (fig. 4.4) is in the same range as the standard deviation of the estimated noise and indicate a good fit. The reconstructed spectra shown in figure 4.5 displays a good fit to the used synthetic spectra for the low energy spectra. The reconstructed high energy spectra with added Cu filtration have a larger variation in the high photon energy ranges over 50 keV. This large uncertainty in the computed spectra is probably caused by...
the small difference in the attenuation coefficient for high energy interactions and exclusion of the characteristic X-ray photons in the spectral model.

4.2.2 Reconstructed X-ray spectra

Fitting the spectral model to a real measurement of an aluminum stair with step thicknesses 1, 2, … 8 mm and observing the residuals of the fitted data (fig. 4.6), it is evident that the assumed thickness $d_j$ of the aluminum stair steps in the spectral model (eq. 3.33) is incorrect, since the residuals are highly correlated. An estimate of an accurate step thicknesses $d_{j}^{*}$ is found by scaling each step thickness with the relative error for each different spectra $k$ (eq. 4.4).

$$
 d_{j}^{*} = d_j \frac{1}{8} \sum_{k=1}^{8} \frac{\log(N_{jk}) - \log(N_{0k})}{\log(N_{jk}^{obs}) - \log(N_{0k}^{obs})}
$$

Using the corrected step thicknesses, the residuals of the fitted spectra (fig. 4.7) for the eight machine settings still show structure larger than the estimated noise. The residual structure is different for the low energy spectra and the filtered high energy spectra indicating that even when the step thicknesses are corrected, the 8 different real spectra can’t be modeled accurately with the spectral model.

The reconstructed real X-ray spectra (fig. 4.8) display the same behavior as the reconstructed simulated spectra (fig. 4.5). The fitted intensity for high energy spectra have a larger estimated confidence band, indicating accurate reconstruction is harder. Comparing the fitted measured spectra with the fitted simulated spectra
Figure 4.6. Initial residuals of the measured real aluminum stair phantom, indicating that the assumed thicknesses are incorrect.

and the used synthetic spectra (fig. 4.9) for three of the spectral settings, the low energy spectra match however the high energy spectrum differs.
4.3. MATERIAL RECONSTRUCTION

Reconstruction the sample material using the low-rank approximation (eq.3.19) with 3 material basis functions, the material parameters $\beta$ are obtained with the multi-energy method (sect. 3.7.4). For both simulated in silico and real measurements in situ the spectra was first measured and reconstructed. Using the calculated spectrum, basis functions are calculated using the basis elements defined. For each measurement the mean of the $\beta_1$ for all image pixels is computed together with global parameters $\beta_2$ & $\beta_3$. The $\beta$-parameters can be used to reconstruct the mean attenuation coefficient of the sample and elemental analysis of the sample contents. For accurate identification the properties of the computed parameters are vital. The noise present in the measurement and biases introduced from other sources limits the possible applications.

Figure 4.7. Measured residual of fit to measured data. The residual is scaled to thickness error in cm, Dashed line is the estimated standard deviation of the noise. The spectral model ansatz is not able to model both high and low energy spectra to the accuracy allowed by the noise level.
Figure 4.8. Reconstructed spectra from measured data

Figure 4.9. Comparison between reconstructed spectra from simulated data, measured data and used simulation model
4.3. MATERIAL RECONSTRUCTION

4.3.1 Reconstructed attenuation coefficient

With the estimated spectra, the test samples attenuation coefficients are estimated. In figure 4.10, the estimated attenuation coefficient for the test materials for *in silico* measurements are shown. Computing the relative error of estimated attenuation, it can be observed (fig. 4.11) that the error is small, with a relative error < 1% for all the test samples considered.

![Figure 4.10. Reconstructed attenuation coefficients for the test materials *in silico*.](image)

The relative error for the low energy attenuation is larger because the low rank basis is incapable to model the large variation between the elements and the inherent filtration in the X-ray source absorbs most of the photons in this energy range. For the photon energies present in the estimated spectra (20-90 keV) the attenuation is measured with a high precision.

Reconstructed attenuation coefficients from real *in situ* measurements, are not measured to the same precision as the simulated measurements. The relative error (fig. 4.12) of samples composed of heavier elements have a large error for lower energies. The cause is probably low transmission for these photon energies. The reconstructed attenuation of the stone sample have a large error over the whole energy range indicating a bad reconstruction or an incorrect assumption of the samples real elemental composition.
Figure 4.11. Relative error in reconstructed attenuation coefficients for different materials in silico

Figure 4.12. Relative error in reconstructed attenuation coefficients for different materials in-silico
4.3. MATERIAL RECONSTRUCTION

4.3.2 Properties of computed parameters

Comparing the computed parameters $\beta$ using the estimated simulated spectra and the real measurements in the multi-energy method. Using the estimated variance in the parameters from photonic poisson noise, a 95% confidence region can be approximated for the simulated and measured parameters. The variance of the all samples (tab. A.1, tab. A.2) is averaged and compared to the to the inverse of the singular value $\sigma_p$ related to each basis function.

Estimating the reconstruction precision from the 95% confidence interval for error relative to the range ($\Delta\beta_p = \max(\beta_p) - \min(\beta_p)$) of the test samples, it is possible to see that even the smallest parameter $\beta_3$ is computed with a high precision compared to the range (tab. 4.2, tab. 4.3).

<table>
<thead>
<tr>
<th>Table 4.2. Properties of the computed parameters from the simulated in silico measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta\beta_p$</td>
</tr>
<tr>
<td>-----------------</td>
</tr>
<tr>
<td>2.61</td>
</tr>
<tr>
<td>$\text{Err}_{95%}$</td>
</tr>
<tr>
<td>$\text{Err}_{95%}/\Delta\beta_p$</td>
</tr>
<tr>
<td>$\sigma_p^{-1}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 4.3. Properties of the computed parameters from the in situ measurements of real samples</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta\beta_p$</td>
</tr>
<tr>
<td>-----------------</td>
</tr>
<tr>
<td>2.68</td>
</tr>
<tr>
<td>$\text{Err}_{95%}$</td>
</tr>
<tr>
<td>$\text{Err}_{95%}/\Delta\beta_p$</td>
</tr>
<tr>
<td>$\sigma_p^{-1}$</td>
</tr>
</tbody>
</table>

For the first parameter $\beta_1$ in figure 4.13, linked to the mean thickness and density of the sample, the difference between measured and simulation is caused by differences in geometry and assumed density in the simulated samples compared to the real samples used in the measurements.

The second parameter $\beta_2$ (fig. 4.14), linked to the large variations in elemental composition, the parameter is estimated with a high precision. The computed parameters for the simulated and real measurements are a good match to theoretical parameters computed when reconstructing the simulated measurements with the same spectrum as the simulation.

The third parameter $\beta_3$ (fig. 4.15), linked to the small differences in the attenuation for the elements is computed with a larger uncertainty. The estimated precision of the parameter is good when comparing to the range in the samples but the accuracy is worse, as seen by plotting the computed chemical identification parameters $\beta_2$ and $\beta_3$ for the test samples (fig. 4.16). The samples group near the
### CHAPTER 4. RESULTS

#### Figure 4.13. Computed parameters $\beta_1$ for the used test materials. Deviation in $\beta_1$ is mainly caused by uncertain thickness of the measured object.

<table>
<thead>
<tr>
<th>Material</th>
<th>PE</th>
<th>PMMA</th>
<th>Acetal</th>
<th>Wood</th>
<th>Water</th>
<th>PTFE</th>
<th>Stone</th>
<th>Al</th>
<th>PVC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_1$</td>
<td>-2</td>
<td>-1.5</td>
<td>0.25</td>
<td>0.75</td>
<td>1.25</td>
<td>1.75</td>
<td>2.25</td>
<td>2.75</td>
<td>3.25</td>
</tr>
</tbody>
</table>

### Figure 4.14. Computed parameters $\beta_2$ for the used test materials show a good agreement of the simulated and measured data to the theoretical values.

<table>
<thead>
<tr>
<th>Material</th>
<th>PE</th>
<th>PMMA</th>
<th>Acetal</th>
<th>Wood</th>
<th>Water</th>
<th>PTFE</th>
<th>Stone</th>
<th>Al</th>
<th>PVC</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_2$</td>
<td>-1</td>
<td>-0.5</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>1.5</td>
<td>2</td>
<td>2.5</td>
<td>3</td>
</tr>
</tbody>
</table>

[Diagram showing the comparison of $\beta_1$ and $\beta_2$ for different materials, with theoretical, simulated, and X-ray data.]
4.3. MATERIAL RECONSTRUCTION

Figure 4.15. Computed parameters $\beta_3$ for the used test material show a larger deviation from the theoretical values for simulated and measured data.

Figure 4.16. Chemical identification parameters $\beta_2, \beta_3$ for used test materials form simulated and real measurements.
theoretical basis as predicted by the simulations. The variation between individual measurement of the same real sample is large for $\beta_3$ when compared to $\beta_2$.

Plotting the error (fig. 4.17) in the estimated chemical parameters when compared to the theoretical values, systematic errors in $\beta_2$ and $\beta_3$ for both simulated and real measurements can be seen. The heavier PVC and stone samples show large errors and the errors in $\beta_2$ and $\beta_3$ are linked. The lighter samples show a systematic error larger than the estimated precision for both simulated and real measurements.

![Error plots](image)

Figure 4.17. Systematic errors in the computed parameters $\beta_2$ and $\beta_3$ when compared to the theoretical parameters. Heavier PVC and Stone samples have a large error compared to the other samples.

### 4.3.3 Mass dependence

To test the claim that the computed parameters $\beta_2$ and $\beta_3$ are independent of the mass thickness of the sample, synthetic samples with mass thicknesses $W = 0.5$, 1 and 1.5 g/cm$^2$ for the elemental basis are computed. In figure 4.18, it can be observed that the beam hardening caused by different mass thickness is handled by the model for low $Z$ elements. Heavier elements however, shows a bias when
4.3. MATERIAL RECONSTRUCTION

the mass thickness vary indicating that the low rank model is unable to accurately model thickness variation for the full range of elements in the basis.

![Diagram](image)

**Figure 4.18.** Chemical identification parameters $\beta_2, \beta_3$ for basic elements with mass thickness 0.5, 1, 1.5 g/cm$^2$. The parameters is estimated using both the reconstructed spectra and the theoretical without added noise. The model can handle beam hardening for light elements, but have problems to accurately model thicker samples of high Z elements.

In addition, the models ability to handle beam hardening in practice was measured with a single object. The images from three measurements of a PMMA wedge was split into the thin and thick part and each half is reconstructed separately. The chemical parameters $\beta_2$ and $\beta_3$ for the thin and thick part of the wedge and the entire measurement for simulated data (fig. 4.19) and measured data (fig. 4.20) show differences outside the estimated 95% confidence region but compared to the range the differences in $\beta_2$ are small.

For both the simulated (fig. 4.19) and measured test objects (fig. 4.20), the confidence region of the parameters shows that errors in the two chemical parameters are weakly correlated. This indicate that the two parameters $\beta_2$ and $\beta_3$ are not independent as predicted by Maitrejean. et al.
CHAPTER 4. RESULTS

Figure 4.19. Repeated in silico measurements of a single PMMA wedge. Chemical identification parameters $\beta_2, \beta_3$ for the 2 halves of the wedge and the full wedge and the 95% confidence interval of each computed point.

Figure 4.20. Repeated in situ measurement of a single PMMA object. Chemical identification parameters $\beta_2, \beta_3$ for the 2 halves of the wedge and the full wedge together with the 95% confidence band. Three measurements were performed.
Chapter 5

Discussion

5.1 Conclusions

In this thesis, the method proposed by Maitrejean et. al. [2] is improved and adapted for measurements of low Z elements using transmission X-ray measurements in the 20-90 keV range. This problem is ill-conditioned and improvements are needed to reduce the impact of noise. The improvements of the proposed method in this thesis are summarized as:

- The method has a flexible calibration procedure, reconstructing the effective X-ray spectra directly. The transmission of a known object is modeled with a high precision. These estimated spectra have other uses than the multi-energy method.

- A non-linear formulation of the X-ray transmission allows for direct reconstruction of the attenuation and the chemical characteristics of a whole sample.

- Using a scaled low rank basis of attenuation coefficients and regularization improves conditioning of the problem and reduces the impact of photonic noise.

- Separating the global and local characteristics of the sample, the impact noisy local measurements are reduced while retaining the modeling capabilities.

A simple simulation model of transmission of polychromatic X-ray spectra is created and used to evaluate the method in a ideal setting. The simulation model is shown to have an accurate spectral response and noise level compared to a real measurement setup.

This multi-energy method improves on dual energy methods already in use. The ability to measure more chemical information than the dual energy methods is limited to the specific application. The theoretical limits to measure variations of only
two chemical quantities presented in [2] remain. Results from in \textit{slic}o simulation and \textit{in situ} measurements is summarized as:

- The attenuation coefficient of unknown materials can theoretically be estimated with a high precision ($\approx 0.2\%$) for photon energy levels 20-90 keV. Actual results for real homogenous samples show that the precision is worse ($\approx 1\%$).

- Measurement of a single chemical variation is possible. This single quantity can be measured accurately ($\approx 0.01\%$) and with low sensitivity to thickness and density variations.

- Measuring the additional chemical variations is limited to the application. Simulations yield a precision $\approx 1\%$ for a second chemical information, but practical tests indicate a high sensitivity to measurement and modeling errors.

Real world applications of the multi-energy method are the limited to the machine stability, sample geometry and homogeneity. The ability to measure a second chemical information accurately is limited as is the ability to measure on thick samples composed of heavy elements.

5.2 Future work

In this thesis I have limited my work to simple models and a very basic regularization method, it is a proof of concept and not readily applied. The Mantex Desktop scanner has not been modified and hardware improvements can be made to better utilize the multi-energy method. There are numerous improvements outside the scope of this thesis.

- Investigate the performance of the multi energy method on real world applications.

- The spectral model ansatz could be improved to better model the characteristic photons and the relativistic effects important to model high energy bremsstrahlung. Evaluating the models presented in [11] and replacing the classical Kramers law with a better model.

- Improvement in the machine hardware with more filtering options, could allow better separated spectra. Adding a calibration sample to allow of spectral measurement in conjunction with the sample measurement will increase the robustness against machine drifts.

- Adapt the regularization of the image so inhomogeneous parts of the sample are segmented and reconstructed separately.
5.2. FUTURE WORK

- Improve the calculation speed using multi-grid methods. This is probably required if inhomogeneous sample segmentation should be attempted to maintain current performance.

- Improve the robustness against real world samples. Both dense and thin parts of the sample introduce errors in the measurement. Weighting individual data points to reduce the impact of these errors can improve the accuracy of the method.
Bibliography


Computed parameters for the test samples

**Table A.1.** Computed parameters and 95% confidence for simulated *in-silico* test objects

<table>
<thead>
<tr>
<th>Material</th>
<th>$\beta_1$</th>
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**Table A.2.** Computed parameters and 95% confidence for measured *in-situ* test objects

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