Three material decomposition in dual energy CT for brachytherapy using the iterative image reconstruction algorithm DIRA

Performance of the method for an anthropomorphic phantom

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A method for determining tissue composition via three material decomposition (3MD) from dual energy CT scans was developed at Linköping university. The method (named DIRA) is a model based iterative reconstruction algorithm that utilizes two photon energies for image reconstruction and 3MD for quantitative tissue classification of the reconstructed volumetric dataset.

This thesis has investigated the accuracy of the 3MD method applied on prostate tissue in an anthropomorphic phantom when using two different approximations of soft tissues in DIRA. Also the distributions of CT-numbers for soft tissues in a contemporary dual energy CT scanner have been determined. An investigation whether these distributions can be used for tissue classification of soft tissues via thresholding has been conducted.

It was found that the relative errors of mass energy absorption coefficient (MEAC) and linear attenuation coefficient (LAC) of the approximated mixture as functions of photon energy were less than 6% in the energy region from 1 keV to 1 MeV. This showed that DIRA performed well for the selected anthropomorphic phantom and that it was relatively insensitive to choice of base materials for the approximation of soft tissues.

The distributions of CT-numbers of liver, muscle and kidney tissues overlapped. For example a voxel containing muscle could be misclassified as liver in 42 cases of 100. This suggests that pure thresholding is insufficient as a method for tissue classification of soft tissues and that more advanced methods should be used.
Abstract

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Bror Robin Westin
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# Abbreviations

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<thead>
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<th>Abbreviation</th>
<th>Meaning</th>
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<tr>
<td>2MD/3MD</td>
<td>Two/three material decomposition</td>
</tr>
<tr>
<td>AMW</td>
<td>Adipose tissue, muscle tissue and water</td>
</tr>
<tr>
<td>CT</td>
<td>Computed tomography</td>
</tr>
<tr>
<td>DECT</td>
<td>Dual energy computed tomography</td>
</tr>
<tr>
<td>DIRA</td>
<td>Dual energy iterative reconstruction algorithm</td>
</tr>
<tr>
<td>FBP</td>
<td>Filtered back projection</td>
</tr>
<tr>
<td>HU</td>
<td>Hounsfield unit</td>
</tr>
<tr>
<td>HN</td>
<td>Hounsfield number</td>
</tr>
<tr>
<td>MAC</td>
<td>Mass attenuation coefficient</td>
</tr>
<tr>
<td>MBSCA</td>
<td>Model based dose calculation algorithms</td>
</tr>
<tr>
<td>MEAC</td>
<td>Mass energy absorption coefficient</td>
</tr>
<tr>
<td>LAC</td>
<td>Linear attenuation coefficient</td>
</tr>
<tr>
<td>LPW</td>
<td>Lipid, protein and water</td>
</tr>
<tr>
<td>UAF</td>
<td>Uncertainty amplification factor</td>
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</table>
Brachytherapy is radiation therapy performed by placing a radiation source near or inside a tumor. It can be used as a complement to external beam radiotherapy or as primary treatment. The radiation source can be placed at a tumor site either by placing it in a body cavity or by placing it using a needle or catheter (Hoskin and Coyle, 2011).

The need for improved dose calculation in brachytherapy is motivated in (Beaulieu et al., 2012). The authors stated that, in specific situations, difference between the current water-based brachytherapy dose formalism (TG-43) and new model-based dose calculation algorithms (MBSCAs) can differ by more than a factor of 10 in the calculated doses. The authors also stated that one of three major issues with MBSCAs is that there is a need for voxel-by-voxel cross-section assignment, ideally, both the tissue composition and mass density of every voxel should be known for individual patients. Therefore they encouraged further research in this area.

All major vendors of CT scanners have their own iterative reconstruction algorithms (IRAs), which are summarized in Table 1.1 (Beister et al., 2012). They are either statistical or model-based methods. A Statistical method only uses statistical models while the model-base methods also include geometrical and physical models. They all have the same basic structure as the DIRA, described in Section 2.3, and can work with either projection data or reconstructed images. Their main purpose has so far been dose reduction while maintaining image quality. Thus their possible benefit for quantitative CT measurements is unknown. The algorithms are kept secret by the vendors and consequently are "black boxes" to researchers outside of the companies (Beister et al., 2012).
Table 1.1: List of reconstruction software for the major vendors of clinical CT systems and the year of introduction.

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Meaning</th>
<th>Vendor</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>ASIR</td>
<td>Adaptive statistical iterative reconstruction</td>
<td>GE</td>
<td>2008</td>
</tr>
<tr>
<td>VEO</td>
<td>&quot;Product name&quot;</td>
<td>GE</td>
<td>2009</td>
</tr>
<tr>
<td>IRIS</td>
<td>Image reconstruction in image space</td>
<td>Siemens</td>
<td>2009</td>
</tr>
<tr>
<td>SAFIRE</td>
<td>Sinogram affirmed iterative reconstruction</td>
<td>Siemens</td>
<td>2010</td>
</tr>
<tr>
<td>iDose</td>
<td>&quot;Product name&quot;</td>
<td>Philips</td>
<td>2009</td>
</tr>
<tr>
<td>ADIR</td>
<td>Adaptive iterative dose reduction</td>
<td>Toshiba</td>
<td>2010</td>
</tr>
</tbody>
</table>

As part of a collaborative research project among the Division of Computer Vision, Division of Radiological Sciences and CMIV, Linköping University an iterative reconstructions algorithm for dual energy quantitative tissue classification (DIRA) has been developed. The main propose of DIRA is to provide tissue composition, via two and three material decomposition (2MD/3MD), for improved radiation treatment planning and absorbed dose calculations in brachytherapy.

1.1 Earlier master thesis work and publications

In 2010 Arif Muhammad made a first implementation of the DIRA and used it for beam hardening correction and estimation of mass fractions. The results showed that beam hardening artifacts were effectively removed and that accurate estimations of mass fraction for water, protein and adipose tissue could be achieved (Muhammad, 2010). His work was followed by Mattias Karlsson’s one that used Monte Carlo simulations to investigate the importance of knowing the tissue composition in brachytherapy radiation treatment planning to calculate the spatial distribution of absorbed dose in a patient (Karlsson, 2010). In 2012 Oscar Grandell extended Arif Muhammad’s work to include cortical bone and bone marrow. The algorithm performed well in aspects of both beam hardening correction and estimation of mass fractions (Grandell, 2012). In 2012 Merve Gürlüler experimentally estimated the accuracy of CT-numbers and resulting mass fractions when using the Siemens SOMATOM Definition Flash DECT scanner. The results showed that contemporary DECT scanners produce image artifacts that strongly affect the accuracy of the 3MD method and that the Siemens image reconstruction algorithm is unsuitable for accurate quantitative CT measurements (Gürlüler, 2012). The following publications have also been made on the DIRA: (Magnusson et al., 2011b), (Magnusson et al., 2011a) and (Malusek et al., 2013),

1.2 Aim

The main aim of this master thesis is to extend Arif Muhammad’s and Oscar Grandell’s work further. This will be done by investigating the accuracy of the 3MD method applied on prostate tissue in an anthropomorphic phantom when
using two different soft tissue approximations in the DIRA.

The secondary aim is to determine the distributions of CT-numbers for soft tissues in a contemporary DECT scanner and investigate if these distributions can be used for tissue classification of soft tissues via thresholding.

### 1.3 Outline

The master thesis has been divided into two studies. The first study focuses on the secondary aim of determining the distributions of CT-numbers as this information is used in the second study. The second study focuses on the investigation of the accuracy of the 3MD method for prostate tissue in an anthropomorphic phantom. The second study required an investigation that characterized the stability of equations of the 3MD method.
2.1 Computed tomography

In 1917 J.H. Radon proved a theorem that allowed reconstruction of images from projections. First experiments on medical applications were carried out by A.M. Cormack between 1957 and 1963. The first commercially available CT scanner was developed and constructed by G.N. Hounsfield in 1972 (Kalender, 2011). A schematic diagram showing a fan-beam geometry with a circular arc detector array is shown in Figure 2.1. An X-ray source emits photons that impinge on an object. When some of the photons interact with the matter, the X-ray beam becomes attenuated. The attenuation of the X-ray beam depends on the type of matter the imaged object consists of and the distance the beam travels through the object. The detector consists of many small detector elements. These detector elements give an electrical signal proportional to the amount of photons that impinge on the element itself. Combining the information from the individual detector elements gives an attenuation profile for a slice of the imaged object at a certain angle. If attenuation profiles are obtained for all angles a two dimensional function of position for the linear attenuation coefficients (LAC) of the imaged object can be calculated (Gonzalez and Woods, 2010).
In medical CT scanners the linear attenuation coefficients are converted to the Hounsfeld scale where water is defined as zero hounsfeld units (HU). This is done by the linear transformation

\[ HN = 1000 \cdot \frac{\mu_X - \mu_{water}}{\mu_{water}} \]  \hspace{1cm} (2.1)

where \( \mu_X \) is the linear attenuation coefficient of the imaged material and \( \mu_{water} \) is the linear attenuation coefficient of water.

The attenuation profile can be described by the following mathematics. For simplicity, a setup with parallel X-ray beams will be described rather than the fan-beam geometry shown in Figure 2.1. A line in the x/y-plane can be defined as

\[ x \cos \theta + y \sin \theta = \rho \]  \hspace{1cm} (2.2)

where the angle \( \theta \) and the distance of the line to the origin \( \rho \) are found in Figure 2.2. Using the \( \delta(t) \) function defined as

\[ \int_{-\infty}^{\infty} x(t) \delta(t) \, dt = x(0), \]  \hspace{1cm} (2.3)
one can construct a line integral over a two dimensional function $\mu(x, y)$ for a certain angle $\theta$, as

$$P_{\theta}(\rho) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mu(x, y) \delta(x \cos \theta + y \sin \theta - \rho) \, dx \, dy. \quad (2.4)$$

This creates a projection $P_{\theta}(\rho)$. $P_{\theta}(\rho)$ is an idealized mathematical description of an attenuation profile taken at the angle $\theta$, see Figure 2.2. By letting $\theta$ also be a variable, $P_{\theta}(\rho)$ can be written as $g(\rho, \theta)$. By varying $\theta$ from 0 to $\pi$ the two-dimensional function $\mu(x, y)$ can be calculated from its projection, $g(\rho, \theta)$ (Gonzalez and Woods, 2010). There are several methods that can be used for this task. The method of interest for this master thesis is filtered backprojection (FBP).

![Figure 2.2: Schematic parallel beam projection at angle $\theta$.](image)

### 2.1.1 Filtered backprojection

The theory of FBP is based on the Fourier-slice theorem. It states that the Fourier transform of a projection with respect to the parameter $\rho$ is equal to a slice taken along a line with the same angle as the projection of the 2D Fourier transform of the projected object, see Figure 2.3.
The mathematical expression for the Fourier-slice theorem is

\[ G(\omega, \theta) = F(\omega \cos \theta, \omega \sin \theta), \quad (2.5) \]

where \( G(\omega, \theta) \) is the 1D Fourier transform of the projection \( g(\omega, \theta) \) with respect to \( \rho \) and \( F(u, v) \) is the 2D Fourier transform of the object described by \( \mu(x, y) \).

The object described by \( \mu(x, y) \) can be calculated using inverse Fourier transform as

\[ \mu(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(u, v) e^{j2\pi(ux + vy)} du \, dv. \quad (2.6) \]

Using the variable substitutions \( u = \omega \cos \theta \) and \( v = \omega \sin \theta \), which have the Jacobian determinant \( \left| \frac{d(u,v)}{d(x,y)} \right| = \omega \), the expression becomes

\[ \mu(x, y) = \int_{0}^{2\pi} \int_{0}^{\infty} F(\omega \cos \theta, \omega \sin \theta) e^{j2\pi\omega(x \cos \theta + y \sin \theta)} \omega \, d\omega \, d\theta. \quad (2.7) \]

Using the Fourier-slice theorem and the symmetric property that the projections at \( \theta \) and \( \theta + \pi \) radians provides the same information i.e. \( g(\rho, \theta) = g(-\rho, \theta + \pi) \) the expression becomes

\[ \mu(x, y) = \int_{0}^{\pi} \int_{-\infty}^{\infty} \omega |G(\omega, \theta)| e^{j2\pi\omega(x \cos \theta + y \sin \theta)} \omega \, d\omega \, d\theta. \quad (2.8) \]
As $x \cos \theta + y \sin \theta = \rho$ is independent of the integration over $\omega$, the equation can be expressed as

$$
\mu(x, y) = \int_{0}^{\pi} \int_{-\infty}^{\infty} |\omega|G(\omega, \theta) e^{i2\pi \alpha \rho} d\omega d\theta.
$$

Equation (2.9) can be divided into two parts. The inner expression is a filtration of the projections by a ramp filter and the outer expression is a backprojection. It can also be expressed via convolution as

$$
\mu(x, y) = \int_{0}^{\pi} (\mathcal{F}^{-1}||\omega|| \ast g(\rho, \theta)) d\theta.
$$

FBP can therefore be implemented by performing the calculations in the spatial or in the frequency domain (Gonzalez and Woods, 2010). This concludes the basic theory of FBP, however there is a lot more needed for a full implementation. Among those are: the calculations are made using discrete mathematics so sampling and sampling rates become important, the ramp filter has to be band-limited, the geometry has to be changed to a fan-beam model and so on.

### 2.1.2 Beam hardening

In FBP the attenuation profile is calculated from Equation (2.4), which works for monoenergetic photons. In medical CT scanners polychromatic X-ray sources are used. They generate photons with energies distributed according to an energy spectrum. As the linear attenuation coefficient is energy dependent, the spectra will be shifted with increasing depth in the imaged object. Photons of higher energy are less likely to be removed from the beam than photons of lower energy; this will lead to a shift of the mean photon energy of the spectra towards higher energies. The phenomenon is illustrated in Figure 2.4. The shift will be dependent on the distance traveled through the object and on the object’s material. The shift leads to cupping artifacts and streaks between dense objects.
2.1.3 Dual energy computed tomography

In dual energy computed tomography (DECT) two datasets of linear attenuation coefficients are acquired, one for each tube voltage. There are several methods for obtaining them. One of them is rapid kV switching where the tube voltage switches between two values, one value for every other projection acquisition. Another is dual-source CT where two different x-ray tubes are used at the same time. This has the advantage of simultaneous projection acquisitions but it is more expensive and more difficult to construct as two detector arrays have to be fitted into the same gantry (Heismann et al., 2012).

2.2 Three-material decomposition

The two datasets containing linear attenuation coefficients obtained with DECT can be utilized for three-material decomposition (3MD). The purpose of 3MD is to determine the amounts of the three components that make up the mixture. This can be done for both volume and mass fractions.

The mathematical description that follows is for \( n \) components. The mass attenuation coefficient (MAC) of a mixture can be calculated as a weighted summation of the MACs of its components

\[
\frac{\mu_{\text{mix}}}{\rho_{\text{mix}}} = \sum_{i=1}^{n} w_i \left( \frac{\mu_i}{\rho_i} \right)
\]

(2.11)
where \( \mu_{\text{mix}} \) is the LAC of the mixture, \( \rho_{\text{mix}} \) is the density of the mixture, \( \mu_i \) is the LAC, \( \rho_i \) is the density and \( w_i \) the mass fraction of the component \( i \). The same is valid for LACs

\[
\mu_{\text{mix}} = \sum_{i=1}^{n} v_i \mu_i, \quad (2.12)
\]

where \( v_i \) is the volume fraction of the component \( i \) and the other symbols are the same as in Equation (2.11).

Summation formulas (2.11) and (2.12) are valid for any photon energy. This combined with the assumption that the summation of all fractions gives the entire mixture

\[
1 = \sum_{i=1}^{n} w_i \quad (2.13)
\]

and

\[
1 = \sum_{i=1}^{n} v_i \quad (2.14)
\]

gives matrix equations

\[
\begin{pmatrix}
\mu_{\text{mix}}(E_1)/\rho \\
\vdots \\
\mu_{\text{mix}}(E_{n-1})/\rho
\end{pmatrix}
= \begin{pmatrix}
\mu_1^b(E_1)/\rho_1 & \cdots & \mu_n^b(E_1)/\rho_n \\
\vdots & \ddots & \vdots \\
\mu_1^b(E_{n-1})/\rho_1 & \cdots & \mu_n^b(E_{n-1})/\rho_n
\end{pmatrix}
\begin{pmatrix}
w_1^b \\
\vdots \\
w_n^b
\end{pmatrix} \quad (2.15)
\]

for the mass fractions and

\[
\begin{pmatrix}
\mu_{\text{mix}}(E_1) \\
\vdots \\
\mu_{\text{mix}}(E_{n-1})
\end{pmatrix}
= \begin{pmatrix}
\mu_1^b(E_1) & \cdots & \mu_n^b(E_1) \\
\vdots & \ddots & \vdots \\
\mu_1^b(E_{n-1}) & \cdots & \mu_n^b(E_{n-1})
\end{pmatrix}
\begin{pmatrix}
v_1^b \\
\vdots \\
v_n^b
\end{pmatrix} \quad (2.16)
\]

for volume fractions, where \( E \) is the photon energy and the superscript \( b \) means component of base material. The assumption in Equation (2.14) is not always fulfilled, see for instance (Malusek et al., 2013). Nevertheless the assumption is needed and it works relatively well for soft tissues.
Equations (2.15) and (2.16) show that to decompose a mixture to $n$ materials there is a need for attenuation coefficients at $n - 1$ energies. The calculation of $\rho$ can be done using the assumption that the partial molar volumes of the base materials are conserved when mixed, this approximation works relatively well for soft tissues. With this assumption the reciprocal of $\rho$ can be calculated as

$$\frac{1}{\rho} = \sum_{i=1}^{n} \frac{w_i}{\rho_i}. \quad (2.17)$$

For $n = 3$ the system for 3MD with mass fractions can be deduced from Equations (2.15) and (2.17) as

$$\begin{bmatrix}
\frac{\mu_{\text{mix}}(E_1) - \mu^b_1(E_1)}{\rho_1} & \frac{\mu_{\text{mix}}(E_1) - \mu^b_2(E_1)}{\rho_2} & \frac{\mu_{\text{mix}}(E_1) - \mu^b_3(E_1)}{\rho_3} \\
\frac{\mu_{\text{mix}}(E_2) - \mu^b_1(E_2)}{\rho_1} & \frac{\mu_{\text{mix}}(E_2) - \mu^b_2(E_2)}{\rho_2} & \frac{\mu_{\text{mix}}(E_2) - \mu^b_3(E_2)}{\rho_3} \\
\frac{1}{\rho_1} & \frac{1}{\rho_2} & \frac{1}{\rho_3}
\end{bmatrix}
\begin{bmatrix}
w_1 \\
w_2 \\
w_3
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
1
\end{bmatrix}.$$  

(2.18)

### 2.3 Model based iterative reconstruction algorithm

The purpose of the dual-energy iterative reconstruction algorithm (DIRA) is to obtain images corresponding to a pre-specified photon energy. This is done by using 3MD to estimate the correction needed to convert polyenergetic projections to monoenergetic ones. Figure 2.5 shows the data flow of DIRA. $P(E_1)$ and $P(E_2)$ are the original projections acquired with a dual energy CT scanner. From the projections, voxel arrays of the linear attenuation coefficient are calculated as $\mu(E_1)$ and $\mu(E_2)$ via FBP. The voxels are classified for example into bone and soft tissue, $\mu_s(E_1)$ and $\mu_s(E_2)$. The classification can be done in several different ways, the simplest method is thresholding. The materials are then decomposed by 2MD and 3MD into mass fractions of different base materials $w_m$. The linear attenuation coefficients of the base materials are known, so by using the fractional amounts of the base materials both monochromatic and polychromatic projections can be calculated for the energies $E_1$ and $E_2$. By subtracting the monochromatic projections from the polychromatic the estimated error is obtained and by subtracting the error estimate from the original projections the polyenergetic projections are converted to monoenergetic ones and thus the error caused by beam hardening is reduced. Then the process starts over again with the new projection data and is repeated until the beam hardening artifacts are reduced to a satisfying level. By reconstructing the first reconstructions $\mu(E_1)$ and $\mu(E_2)$ using projections that have
been corrected with the simple water beam hardening correction, as described in (Grandell, 2012), the total number of needed iterations is decreased.

**Figure 2.5:** Data-flowchart of the dual-energy iterative reconstruction algorithm (DIRA).
Study 1: Feasibility of tissue classification via DECT

3.1 Introduction

One option for tissue classification using DECT is to use scatter plots. A scatter plot is a diagram that uses Cartesian coordinates to display values for two or more variables for a set of data and is used to visualize relationships between the variables (Reynard et al., 1995). In the case of DECT every voxel can be represented by two HN, one for each energy. When plotting a graph with the HN from one energy level on each axis for a set of CT voxels a scatter plot is obtained. Points originating from the same tissue type should, if CT images were noise and artifact free, have the same CT-numbers and therefore be placed in the same location. However the noise and reconstruction artifacts introduce errors to the CT-numbers.

The aim of this study is to determine the distributions of CT-numbers for soft tissues: adipose tissue, muscle, liver and kidney and if these distributions can be used for tissue classification using thresholding.

By selecting all points inside an elliptical region that is surrounding the mean CT-numbers for adipose tissue, the points should, ideally, originate from voxels containing adipose tissue. An example of this is shown in Figure 3.1 where the scatter plot was generated from a transversal CT slice of the abdominal region, green-colored pixels in the image corresponds to the green elliptical region in the scatter plot.
Figure 3.1: (a) A transversal CT slice of the abdominal region. CT numbers of green-colored pixels correspond to the green elliptical region in the scatter plot. (b) Scatter plot of CT numbers taken at 100 kV and 140 kV for all voxels in the transversal slice.

3.2 Theory

3.2.1 Error ellipse

An error ellipse is an ellipse (around a point which is an estimated solution to a problem) that contains a specified percentage of randomly distributed points (ASCE, 1994), for example an error ellipse with an 80% confidence level encloses 80% of the scatter in a distribution. The center of the error ellipse is placed at the mean of the CT-numbers for the two energies,

\[ m_{ei} = E[H_{E_i}] \quad i = [1, 2], \]

where \( H_{E_i} \) is the hounsfield number of the voxels inside a selected region of the CT image for the acquisition energies \( E_1 \) and \( E_2 \). The length of the semi major and semi minor axes are calculated as

\[ m_i = c \cdot \sqrt{\lambda_i \sigma_{cov}} \quad i = [1, 2], \]

where \( c \) is a constant defining the confidence level, for a 95% confidence level \( c = 2.45 \), and \( \lambda_i \sigma_{cov} \quad i = [1, 2] \), are the two eigenvalues of the covariance matrix \( \sigma_{cov} \) for \( H_{E_i} \quad i = [1, 2] \). The angle of the major axis \( \theta \) can be calculated as
\[ \theta = \tan^{-1}\left( \frac{2\rho \sigma_{H_{e_1}} \sigma_{H_{e_2}}}{\sigma_{H_{e_1}}^2 - \sigma_{H_{e_2}}^2} \right)/2, \]  
\[ (3.3) \]

where \( \rho \) is the correlation coefficient for \( H_{e_i} \), \( i = [1, 2] \) and \( \sigma_{H_{e_i}} \), \( i = [1, 2] \) the standard deviation of \( H_{e_i} \), \( i = [1, 2] \) (Ghilani, 2010).

### 3.3 Method

CT images of a woman were acquired with the Siemens SOMATOM Definition Flash DECT scanner. The following acquisition parameters were used: slice thickness of 1 mm, pitch factor of 0.7, tube voltages of 100 kV and 140 kV, and the date of the acquisition was 12th December 2011.

Scatter plots were created by selecting a homogeneous region of tissue, see Figure 3.2. The selected tissue types were muscle, liver, adipose, and kidney tissues. The scatter plots for the voxels inside these regions are shown Figure 3.3 (a). The properties of the distributions were determined by enclosing them with an error ellipse at the 95% confidence level. This is an ellipse that encloses 95% of the points originating from one of the regions, see Figure 3.3 (b). The parameters of the distributions are found in Table 3.1.

To determine if it is possible to use the CT-number distributions for tissue classification the probabilities of misclassification, when using thresholding as a classification method were calculated, see Table 3.2. By assuming that the CT numbers had Gaussian distributions, thresholding limits were set as the intersections between the probability density function (PDF) for the distributions, i.e. an image voxel is classified to belong to the distribution that has the largest PDF for the CT-number combination of that voxel.

The probability of misclassification can be calculated by integrating over regions of the intersecting distributions, however this is time consuming. Therefore a simple Monte Carlo simulation was used. By using the parameters in Table 3.1 1 000 000 samples and corresponding PDF values for each sample position from one of the distribution were generated. For each generated sample the PDF value at that position was calculated for all other distributions. The sizes of these PDF values were then compared with the PDF value from which the sample originated. If the PDF value from which the sample originated was smaller than the PDF value of one of the distributions it was counted as a misclassification. This procedure was done for all 4 distributions.

### 3.4 Results and discussion

The four selected tissue regions are shown in Figure 3.3. The regions were selected to contain as homogeneous tissue samples as possible.
Figure 3.2: Regions containing (a) muscle, (b) liver, (c) adipose, and (d) kidney tissues. A scatter plot of CT numbers for pixels from these regions is in Figure 3.3.

The scatter plots in Figure 3.3 show a large overlap which indicated that it would be difficult to do a correct tissue classification with the exception of the adipose tissue that was clearly separated from the other tissues.
Figure 3.3: (a) Scatter plot of CT numbers for pixels from regions in Figure 3.2. (b) Error ellipses marking the 95% confidence level of the corresponding bivariate distributions of CT numbers.

The parameters of the bivariate distributions are in Table 3.1. The expectations $m_{100}$ and $m_{140}$, semi major $w_1$ and semi minor $w_2$ axes and angle $\theta$ of the error ellipse are defined in Figure 3.4.
Figure 3.4: Schematic view of the semi minor axis $w_1$, semi major axis $w_2$, position and angle $\theta$ of the major axis of an error ellipse.

Table 3.1: Parameters defining the bivariate distributions of CT numbers for 100 kV and 140 kV: the mean values $m_{100}$ and $m_{140}$, standard deviations $\sigma_{100}$ and $\sigma_{140}$ and the correlation coefficient $\rho_c$. Corresponding parameters of the error ellipse: the semi major axis $w_1$, the semi minor axis $w_2$, and the position angle of the major axis $\theta$.

<table>
<thead>
<tr>
<th></th>
<th>$m_{100}$</th>
<th>$m_{140}$</th>
<th>$\sigma_{100}$</th>
<th>$\sigma_{140}$</th>
<th>$\rho_c$</th>
<th>$w_1$</th>
<th>$w_2$</th>
<th>$\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liver</td>
<td>60.8</td>
<td>57.7</td>
<td>21.5</td>
<td>20.1</td>
<td>0.0376</td>
<td>48.9</td>
<td>52.8</td>
<td>0.2553</td>
</tr>
<tr>
<td>Muscle</td>
<td>54.7</td>
<td>52.4</td>
<td>21.1</td>
<td>19.8</td>
<td>0.0694</td>
<td>47.6</td>
<td>52.4</td>
<td>0.4017</td>
</tr>
<tr>
<td>Adipose</td>
<td>-104.6</td>
<td>-84.5</td>
<td>18.5</td>
<td>16.2</td>
<td>0.3439</td>
<td>33.9</td>
<td>49.8</td>
<td>0.5998</td>
</tr>
<tr>
<td>Kidney</td>
<td>30.5</td>
<td>28.3</td>
<td>29.4</td>
<td>27.7</td>
<td>0.3123</td>
<td>57.7</td>
<td>80.2</td>
<td>0.6906</td>
</tr>
</tbody>
</table>

In the Monte Carlo simulations probabilities for misclassification were large for liver, adipose and kidney tissue while the probability for misclassification for the adipose tissue was small, see Table 3.2.

Table 3.2: Fraction of misclassified samples in the Monte Carlo simulation. The left most column contains the distributions from which the samples originated and the top row contains to which distribution the samples were classified. Values lower than $\varepsilon = 0.5 \times 10^{-3}$ were not significant.

<table>
<thead>
<tr>
<th></th>
<th>Liver</th>
<th>Muscle</th>
<th>Adipose</th>
<th>Kidney</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liver</td>
<td>-</td>
<td>0.43</td>
<td>&lt; $\varepsilon$</td>
<td>0.14</td>
</tr>
<tr>
<td>Muscle</td>
<td>0.42</td>
<td>-</td>
<td>&lt; $\varepsilon$</td>
<td>0.16</td>
</tr>
<tr>
<td>Adipose</td>
<td>&lt; $\varepsilon$</td>
<td>&lt; $\varepsilon$</td>
<td>-</td>
<td>&lt; $\varepsilon$</td>
</tr>
<tr>
<td>Kidney</td>
<td>0.28</td>
<td>0.34</td>
<td>&lt; $\varepsilon$</td>
<td>-</td>
</tr>
</tbody>
</table>
3.5 Conclusions

The distributions of CT-numbers from liver, muscle and kidney tissues overlapped; the probability of misclassification ranged from approximately 14% to 43%. The probability of misclassification was insignificant for adipose tissue.

The large probability of misclassifications for liver, muscle and kidney tissue suggests that pure thresholding is insufficient as a method for tissue classification for soft tissues. For some other soft tissues, as in this case the adipose tissue, there is a possibility that thresholding is sufficient.
4

Study 2: Performance evaluation of 3MD and DIRA

4.1 Introduction

Previous studies investigating DIRA are described in Section 1.1. Over time the original DIRA code was modified. The modifications included: mathematical corrections, generalization so that any number of material doublets and triplets could be used, speed improvements by converting loops to matrix operations and reorganization of code to improve its structure and remove repeating parts, see Appendix A.2. To ensure that the modifications did not affect the results, a comparison with two cases evaluated previously was done. It was of interest how this new code would perform in more realistic situations.

This study has two aims. The main aim is to extend earlier evaluations of the 3MD and DIRA to more realistic configurations. This was done by evaluating the accuracy of the 3MD method applied on a predefined prostate tissue when using the DIRA, an anthropomorphic phantom and two different soft tissue approximations. The second aim is to characterize the stability of the equations of the 3MD method.

4.2 Theory

4.2.1 Condition number

In Section 2.2 a system of linear equations of the form $Ax = b$ was deduced for calculation of the mass and volume fractions. In the ideal case this system always gives the exact mass fraction, however in a more realistic case there are inaccuracies introduced in the $b$ matrix. If an error $\delta b$ is introduced, the equation
\[ A(x + \delta x) = b + \delta b \]  

(4.1)

is obtained. It can be shown that the relative error of the mass and volume fraction satisfies (Elde’n and Wittmeyer-Koch, 2001):

\[
\frac{\|\delta x\|}{\|x\|} \leq \kappa(A) \cdot \frac{\|\delta b\|}{\|b\|},
\]

(4.2)

where \(\|\cdot\|\) is the vector norm and \(\kappa(A)\) is the condition number of the matrix \(A\).

Equation (4.2) shows that \(\kappa(A)\) is a scaling factor of the maximum relative error of \(b\) and thus a suitable measure of the equation system numeric stability for the selected material triplet. The condition number \(\kappa(A)\) can be calculated as

\[
\kappa(A) = \|A\| \cdot \|A^{-1}\|.
\]

(4.3)

The matrix norm \(\|A\|\) can be calculated according to

\[
\|A\| = \sqrt{\max_{1 \leq i \leq n} \lambda_i(A^T A)},
\]

(4.4)

where \(\lambda_i\) is the \(i\)th eigenvalue of the \(A^T A\) matrix. A small value of \(\kappa(A)\) close to 1 indicates a well-conditioned system and a large value indicates an ill-conditioned system.

In the case of the 3MD an intuitive graphical representation of the problem is in Figure 4.1. The drawings show LAC diagrams for two triplets. The left drawing shows a material configuration with a low condition number and the right drawing shows a configuration with a high condition number. A mixture composed of equal fractions of the materials in the triplet is found in the center of the triangle. When introducing a small error \(\Delta\) in one of the LACs the resulting error in mass fractions will be larger for the right drawing. It is clear that the size of the resulting error depends on the shape of the triangle.
4.2 Theory

4.2.2 Propagation of uncertainty

The guide to the expression of uncertainty in measurement (GUM) describes how to calculate the uncertainty of an output quantity from the uncertainties of input quantities in a mathematical model (JCGM, 2008). It states that you seldom measure a quantity $Y$ directly, but determine it from $N$ other quantities $X_1, X_2, ..., X_N$ via a functional relationship $f$ as

$$Y = f(X_1, X_2, ..., X_N).$$  \hfill (4.5)

An estimate $y$ of the quantity $Y$ is then given by the estimates $x_1, x_2, ..., x_N$ of the input quantities $X_1, X_2, ..., X_N$ as

$$y = f(x_1, x_2, ..., x_N).$$  \hfill (4.6)

If the input quantities are correlated then the combined standard uncertainty can be calculated as (JCGM, 2008)

$$u_c^2(y) = \sum_{i=1}^{N} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j),$$  \hfill (4.7)
where \( u_c(y) \) is the combined standard uncertainty, \( u(x_i) \) is the uncertainty of the \( i \)th input quantity and \( u(x_i, x_j) \) is the estimated covariance of the input quantities \( i \) and \( j \).

In the case of the 3MD method the combined uncertainty can be calculated analytically, because the functional relationship \( f \) for the 3MD method is linear. The derivation follows.

By using two uncorrelated random variables with Gaussian distributions describing the measured linear attenuation coefficients of the mixture, distributions of the resulting volume fractions can be calculated. A linear transformation of two independent Gaussian distributed random variables has the Gaussian distribution (Bickel and Doksum, 1977):

\[
ax_1 + bx_2 + c \sim N(a\mu x_1 + b\mu x_2 + c, a^2\sigma^2 x_1 + b^2\sigma^2 x_2).
\]

(4.8)

For a vector of volume fractions \( v \) Equation (2.16) can be written as

\[
\mu_{mix} = A_{base}v.
\]

(4.9)

This matrix equation can be transformed to

\[
v = A_{base}^{-1}\mu_{mix}
\]

(4.10)

which can be written for individual matrix elements as

\[
\begin{pmatrix}
v_1 \\
v_2 \\
v_3
\end{pmatrix} =
\begin{pmatrix}
a_{1,1} & a_{1,2} & a_{1,3} \\
a_{2,1} & a_{2,2} & a_{2,3} \\
a_{3,1} & a_{3,2} & a_{3,3}
\end{pmatrix}
\begin{pmatrix}
\mu(E_1) \\
\mu(E_2) \\
1
\end{pmatrix}.
\]

(4.11)

The corresponding system of linear equation is

\[
\begin{align*}
v_1 &= a_{1,1}\mu(E_1) + a_{1,2}\mu(E_2) + a_{1,3} \\
v_2 &= a_{2,1}\mu(E_1) + a_{2,2}\mu(E_2) + a_{2,3} \\
v_3 &= a_{3,1}\mu(E_1) + a_{3,2}\mu(E_2) + a_{3,3}
\end{align*}
\]

(4.12)

Statement (4.8) and formula (4.12) give the variance of the output quantity as a function of the variance of the input quantity.

### 4.2.3 Relative error of MEAC and LAC

The relative error of the approximated mass energy absorption coefficient (MEAC) can be defined as
\[ \delta_{MEAC}(E) = \left| \frac{\mu^{a}_{en}(E)/\rho - \mu_{en}(E)/\rho}{\mu_{en}(E)/\rho} \right|, \]  

(4.13)

where \( \mu^{a}_{en}(E)/\rho \) is the mass energy absorption coefficient of the approximated mixture and \( \mu_{en}(E)/\rho \) is the mass energy absorption coefficient of the original mixture. The mass energy absorption coefficient can be calculated as

\[ \mu_{en}(E)/\rho = \sum_{i=1}^{n} w_i \mu_{en,i}(E)/\rho_i, \]  

(4.14)

where \( n \) denotes the number of materials, in this case three, and \( \mu_{en,i}(E)/\rho_i \) the mass energy absorption coefficient for the \( i \)th material.

Similarly the relative error of the approximated linear attenuation coefficient can be calculated as

\[ \delta_{LAC}(E) = \left| \frac{\mu^{a}(E) - \mu(E)}{\mu(E)} \right|, \]  

(4.15)

where \( \mu^{a}(E) \) is the linear attenuation coefficient of the approximated mixture and \( \mu(E) \) is the linear attenuation coefficient of the original mixture.

4.3 Methods

4.3.1 Mathematical phantom

To create an anthropomorphic phantom, one transverse slice of the ICRP 110 voxel phantom, ICRP (2009), was approximated by ellipses fitting the tissue structures, see Figure 4.2. The slice was selected so that it included the prostate, which is of high interest in brachytherapy, and the complex bone structure of the pelvis which is a strong contributor to beam hardening artifacts.

The resulting mathematical model based on the position, size, rotation and corresponding elemental composition of the elliptical regions were then used as input to the CT simulation program Drasim, see Appendix A.1. The process of generating the input file was automated via a Matlab® script.

4.3.2 Numerical stability of the solution

Eight different base material triplets representing a variety of triangle shapes, see Figures 4.4 and 4.5, were used to investigate how the shape of the triangle relates to the condition number of the corresponding system of linear Equations (2.16). The conditioning number was calculated from Equation (4.3). The mean energy of the polyenergetic spectra used in the CT simulation, see Section 4.3.3, were 50
keV and 88.5 keV, respectively, therefore this were used for creation of the eight base material triplets.

Uncertainty of the output quantity $v$ was calculated from Statement (4.8) using the assumption that input quantities had equal variances. The resulting formula was

$$u(v) = \alpha u(\mu),$$

where the coefficient $\alpha$ is called uncertainty amplification factor (UAF) in this work.

The effect of translation and rotation of a base material triangle on the condition number and UAF was investigated by calculating the corresponding quantities for a set of translated and rotated triangles, see Figures 4.10 and 4.8.

### 4.3.3 Evaluation of 3MD and DIRA

The performance of the 3MD method and DIRA was evaluated by comparing results of the 3MD of a predefined prostate tissue obtained for two different base material triplets. The phantom described in Section 4.3.1 was used to calculate projection data. Projections were generated with Drasim for tube voltages of 80 kV and 140 kV. The filter used for the 80 kV projection generation consisted of 3 mm Al, 0.6 mm Ti and 1 mm C. For the 140 kV the filter also contained 0.4 mm Sn.

The projection data was reconstructed for each soft tissue approximation with DIRA using 4 iterations. The base triplets were: (i) muscle tissue, adipose tissue and water (AMW) and (ii) lipid, protein and water (LPW). Elemental compositions and mass densities are in Tables 4.2 and 4.3, respectively.

The linear attenuation coefficients obtained by DIRA for the prostate tissue were decomposed to a base material triplet consisting of prostate tissue, water and calcium.

Relative errors of MEAC and LAC were calculated from Equations (4.13) and (4.15).

### 4.4 Results and discussion

#### 4.4.1 Mathematical phantom

The ellipse approximation (the mathematical phantom) is shown in Figure 4.2 as an overlay on the ICRP 110 phantom. Table 4.1 contains tissue numbers (see Table 4.2), positions, sizes and rotation angles of the ellipses. Parameters defining an ellipse are described in Figure 4.3.
Figure 4.2: A colormap of material indices in a transversal slice of the pelvic region of the ICRP 100 voxel phantom. Ellipses approximating tissue boundaries were used to construct a mathematical model of the slice.
Table 4.1: Parameters of ellipses used to approximate the slice in Figure 4.2: coordinates of the center $x$ and $y$, the semi major and semi minor axes $\delta x$ and $\delta y$, respectively, and the rotation angle $\theta$ of the major axis.

<table>
<thead>
<tr>
<th>Tissue nr</th>
<th>$x$</th>
<th>$y$</th>
<th>$\delta x$</th>
<th>$\delta y$</th>
<th>$\sin \theta$</th>
<th>$\cos \theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>117</td>
<td>-28.5</td>
<td>8.8</td>
<td>176.3</td>
<td>89.1</td>
<td>0.017</td>
<td>-1.000</td>
</tr>
<tr>
<td>107</td>
<td>-38.7</td>
<td>-84.3</td>
<td>60.0</td>
<td>48.9</td>
<td>0.025</td>
<td>-1.000</td>
</tr>
<tr>
<td>107</td>
<td>-38.2</td>
<td>102.3</td>
<td>58.9</td>
<td>45.9</td>
<td>0.009</td>
<td>-1.000</td>
</tr>
<tr>
<td>107</td>
<td>-75.8</td>
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<td>50.0</td>
<td>17.4</td>
<td>0.122</td>
<td>-0.993</td>
</tr>
<tr>
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<td>-72.3</td>
<td>75.4</td>
<td>41.5</td>
<td>18.2</td>
<td>-0.233</td>
<td>-0.972</td>
</tr>
<tr>
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<tr>
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</tr>
<tr>
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<tr>
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<td>-0.412</td>
<td>-0.911</td>
</tr>
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<td>107</td>
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<td>98.2</td>
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<td>-0.088</td>
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</tr>
<tr>
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<tr>
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<td>-0.501</td>
<td>-0.865</td>
</tr>
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<td>0.560</td>
<td>-0.828</td>
</tr>
<tr>
<td>41</td>
<td>-52.9</td>
<td>-46.0</td>
<td>20.4</td>
<td>11.5</td>
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<td>-0.000</td>
</tr>
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<td>42</td>
<td>-53.4</td>
<td>-46.0</td>
<td>17.3</td>
<td>8.4</td>
<td>1.000</td>
<td>-0.030</td>
</tr>
<tr>
<td>41</td>
<td>-49.9</td>
<td>65.6</td>
<td>19.3</td>
<td>12.9</td>
<td>-1.000</td>
<td>-0.000</td>
</tr>
<tr>
<td>42</td>
<td>-49.9</td>
<td>65.6</td>
<td>16.3</td>
<td>10.3</td>
<td>-0.999</td>
<td>-0.032</td>
</tr>
<tr>
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<td>13.6</td>
<td>9.1</td>
<td>-0.822</td>
<td>-0.569</td>
</tr>
<tr>
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<td>10.8</td>
<td>6.0</td>
<td>-0.850</td>
<td>-0.527</td>
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<tr>
<td>41</td>
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<td>18.1</td>
<td>13.8</td>
<td>7.6</td>
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</tr>
<tr>
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<td>5.1</td>
<td>0.677</td>
<td>-0.736</td>
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<tr>
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<td>17.8</td>
<td>5.1</td>
<td>11.4</td>
<td>5.6</td>
<td>0.000</td>
<td>-1.000</td>
</tr>
<tr>
<td>115</td>
<td>-19.8</td>
<td>8.8</td>
<td>11.2</td>
<td>9.3</td>
<td>-1.000</td>
<td>-0.000</td>
</tr>
</tbody>
</table>
### Table 4.2: Elemental compositions and mass densities of materials used in the mathematical phantom and 3MD.

<table>
<thead>
<tr>
<th>Tissue nr</th>
<th>Tissue</th>
<th>Atomic composition by atomic fraction [%]</th>
<th>Density [g/cm³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>117</td>
<td>Adipose tissue</td>
<td>H 62.60 C 27.09 N 00.31 O 9.92 Na 0.02 S 0.01 Cl 0.0156</td>
<td>0.950</td>
</tr>
<tr>
<td>115</td>
<td>85% Prostate, 10% Water, 5% Ca</td>
<td>H 62.87, C 10.39, N 1.08, O 24.71, Na 0.02, P 0.03, S 0.05, Cl 0.03, K 0.02, Ca 0.79</td>
<td>1.044</td>
</tr>
<tr>
<td>107</td>
<td>Muscle tissue</td>
<td>H 63.16, C 7.37, N 1.51, O 27.73, Na 0.02, P 0.04, S 0.05, Cl 0.01, K 0.06</td>
<td>1.050</td>
</tr>
<tr>
<td>29, 42</td>
<td>Bone marrow</td>
<td>H 62.09, C 25.06, N 0.83, O 11.91, Na 0.01, P 0.01, S 0.02, Cl 0.02, K 0.01, Fe 0.01</td>
<td>1.005</td>
</tr>
<tr>
<td>28, 41</td>
<td>Mineral bone</td>
<td>H 40.31, C 14.93, N 3.38, O 31.60, Na 0.14, Mg 0.09, P 3.42, S 0.10, Ca 5.99</td>
<td>1.920</td>
</tr>
</tbody>
</table>

---

**Figure 4.3:** An ellipse is defined by its center \((x, y)\), semi major axis \(dx\), semi minor axis \(dy\), and rotation angle \(\theta\) of the major axis.
Table 4.3: Elemental compositions and mass densities of materials used in the 3MD.

<table>
<thead>
<tr>
<th>Material</th>
<th>Atomic composition by atomic fraction [%]</th>
<th>Density [g/cm$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lipid</td>
<td>H 11.8, C 77.3, O 10.9</td>
<td>0.92</td>
</tr>
<tr>
<td>Protein</td>
<td>H 6.6, C 53.4, N 17.0, O 22.0, S 1.0</td>
<td>1.35</td>
</tr>
<tr>
<td>Water</td>
<td>H 11.2 O 88.8</td>
<td>1.00</td>
</tr>
</tbody>
</table>

4.4.2 Numerical stability of the solution

The base material triangles used for calculation of the UAFs and condition numbers are found in Figures 4.4 and 4.5.

**Figure 4.4:** Base material triangles 1 to 4 of different shapes. Condition numbers $\kappa(A)$ of the corresponding equation systems are also listed. Blue circle represents material 1, red circle material 2 and green circle material 3.
Graphs in Figure 4.6 show how standard uncertainty of the input quantity is amplified by the 3MD with the base material triplets described in Figures 4.4 and 4.5. X-axis displays the standard deviation of the mixture's LAC and the Y-axis the standard deviation of the resulting volume fractions. The slope of the curve is the largest for the small and flat triangles.
Figure 4.6: Standard uncertainty of the calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for the triangles 1 - 8 in Figures 4.4 and 4.5.

The graph in Figure 4.7 shows a subset of the curves in Figure 4.6; for a given triangle (base material triplet) only the curve with the largest slope (the maximum UAF for materials 1 to 3) is plotted.

For triangles 1 to 8 the order of UAFs sorted according to size was the same as the order of condition numbers (Table 4.4) also sorted according to size. It indicates that there is an association between those quantities.
4.4 Results and discussion

Figure 4.7: Standard uncertainty of calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for the triangles 1 - 8 in Figures 4.4 and 4.5. Only the function with the steepest slope from the functions for materials 1, 2 and 3 is plotted.

Table 4.4: Condition number for base material triplets and corresponding triangle index.

<table>
<thead>
<tr>
<th>Triangle nr</th>
<th>$\kappa(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.287 \times 10^3$</td>
</tr>
<tr>
<td>2</td>
<td>$2.931 \times 10^2$</td>
</tr>
<tr>
<td>3</td>
<td>$3.900 \times 10^2$</td>
</tr>
<tr>
<td>4</td>
<td>$1.319 \times 10^2$</td>
</tr>
<tr>
<td>5</td>
<td>$5.236 \times 10^2$</td>
</tr>
<tr>
<td>6</td>
<td>$3.803 \times 10^2$</td>
</tr>
<tr>
<td>7</td>
<td>$2.339 \times 10^4$</td>
</tr>
<tr>
<td>8</td>
<td>$1.943 \times 10^2$</td>
</tr>
</tbody>
</table>

Figure 4.8 shows triangles rotated by $0$, $\pi/16$, $\pi/8$, $\pi/4$ and $\pi/2$ radians. The triangles are marked with their condition numbers, which also are in Table 4.5. The condition number was the smallest when the long side of the triangle was diagonal to the x and y axis and the largest when the long side of the triangle was parallel to either the x or y axis. This suggests that the system of equations in the 3MD method is more stable for triangles whose sides are not parallel to the x or y axis. The changes in the condition number was however so small that the effect on the stability was negligible.
Figure 4.8: Base material triplet triangles rotated by $0\,\pi/16\,\pi/8\,\pi/4$ and $\pi/2$ radians and corresponding condition numbers.

Table 4.5: Condition numbers of rotated triangles and corresponding rotation angles.

<table>
<thead>
<tr>
<th>Rotation angle</th>
<th>$\kappa(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0$</td>
<td>$1.139 \times 10^2$</td>
</tr>
<tr>
<td>$\pi/16$</td>
<td>$1.128 \times 10^2$</td>
</tr>
<tr>
<td>$\pi/8$</td>
<td>$1.120 \times 10^2$</td>
</tr>
<tr>
<td>$\pi/4$</td>
<td>$1.116 \times 10^2$</td>
</tr>
<tr>
<td>$\pi/2$</td>
<td>$1.149 \times 10^2$</td>
</tr>
</tbody>
</table>

Standard uncertainty of calculated volume fraction as a function of standard uncertainty of the linear attenuation coefficient for the triangles in Figure 4.8 is in Figure 4.9. The figure only shows two lines because: (i) the rotation does not change the curves slope (this follows the graphical solution of the system of equations) and (ii) the curve slopes are the same for two volume fractions of one triangle (the triangle is isosceles). The UAF is not affected by the rotation.
4.4 Results and discussion

**Figure 4.9:** Standard uncertainty of calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for the rotated triangles in Figure 4.8. Only two lines are visible because of the UAFs invariance to rotation and due to the isosceles triangle shape. The green line represent UAF for one of the base materials in the rotated base material triplet, the purple (red and blue mixture) line represent the UAF for the two other base materials.

Figure 4.10 shows a triangle positioned at five different locations. The triangles are marked with their condition numbers, which also are in Table 4.6. The condition number becomes larger the further away the triangle is placed from the origin. It follows from the fact that the relative error $\|\delta b\|/\|b\|$ of the input quantity in Equation (4.2) decreases with increasing distance from the origin while the relative error $\|\delta x\|/\|x\|$ of the output quantity should remain approximately the same; the condition number must compensate for this change by increasing its size.

**Table 4.6:** Condition numbers for base material triplets and corresponding triangle locations.

<table>
<thead>
<tr>
<th>Triangle position</th>
<th>$\kappa(A)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Center</td>
<td>$1.139 \times 10^2$</td>
</tr>
<tr>
<td>Bottom left</td>
<td>$1.063 \times 10^2$</td>
</tr>
<tr>
<td>Top left</td>
<td>$1.229 \times 10^2$</td>
</tr>
<tr>
<td>Top right</td>
<td>$1.327 \times 10^2$</td>
</tr>
<tr>
<td>Bottom right</td>
<td>$1.159 \times 10^2$</td>
</tr>
</tbody>
</table>
Figure 4.10: A triangle positioned at five different locations and corresponding condition numbers.

Standard uncertainty of calculated volume fraction as a function of standard uncertainty of the linear attenuation coefficient for the triangles in Figure 4.10 is in Figure 4.11. The figure only shows two lines because of similar reasons as in the case of rotated triangles (cf. Figure 4.9).
4.4 Results and discussion

Figure 4.11: Standard uncertainty of calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for the translated triangles in Figure 4.10. Only two lines are visible owing to similar reasons as in the case of rotated triangles, see Figure 4.9. The green line represent UAF for one of the base materials in the translated base material triplet, the purple (red and blue mixture) line represent the UAF for the two other base materials.

4.4.3 Evaluation of 3MD and DIRA

Figure 4.12 shows the triangle representation of the two base material triplets that were used in this study. The adipose tissue, muscle and water base material triplet (AMW) had $\kappa(A) = 1.413 \times 10^3$. The lipids, protein and water base material triplet (LPW) had $\kappa(A) = 2.911 \times 10^2$. The lower value for the LPW triplet indicated that the system of equations for the this triplet was more numerically stable and should therefore give better results for the 3MD. Also the lower UAF in Figure 4.13 suggests that the LPW triplet should perform better.
Study 2: Performance evaluation of 3MD and DIRA

Figure 4.12: Triangle representation of base material triplet adipose, muscle and water (AMW) in (a) and base material triplet lipid, protein and water (LPW) in (b).

Figure 4.13: Standard uncertainty of calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for base material triplet AMW in (a) and LPW in (b), see Figure 4.12. Each base material is represented by one line describing its UAF.

The triangle representation and standard uncertainty of calculated volume fraction as a function of standard uncertainty of the linear attenuation coefficient for the tabulated prostate tissue, water and calcium triplet used for material decomposition of the prostate are shown in Figure 4.14. The triplet had \( \kappa(A) = 1.158 \times 10^3 \). This large value indicated that the system of equation was numerically unstable. On the other hand the small UAF value for calcium shows that the resulting mass fraction was accurate. The accuracy of the calcium mass fraction
is important as it has a large impact on the mass energy absorption coefficient of the prostate tissue.

![Graph](image)

**Figure 4.14:** The base material triangle and the standard uncertainty of calculated volume fraction (the output quantity) as a function of standard uncertainty of the linear attenuation coefficient (the input quantity) for the lipid, prostate and water base material triplet.

Figures 4.15 and 4.16 show images reconstructed with DIRA using the AMW and LPW triplets, respectively, for the soft tissue approximation. The beam hardening artifacts are clearly visible, especially for the simulation with the tube voltage of 80 kV. Figures 4.17 and 4.19 show mass fractions calculated from the reconstructed images in Figures 4.15 and 4.16, respectively; here the beam hardening artifacts are even more expressed and corrupt the results to a large extent. In Figures 4.15 and 4.16 the beam hardening artifacts result in streaks and a shift of the LAC values. The shift affects the whole image but is most visible in the bone marrow.
Figure 4.15: Reconstructed images of the mathematical phantom for 0th (a, c) and 4th (b, d) iterations of the DIRA algorithm using the AMW base material triplet. Top row: 80 kV, bottom row: 140 kV. [cm$^{-1}$]
4.4 Results and discussion

Resulting mass fractions for the AMW and LPW base material triplets are in Figures 4.17 and 4.19, respectively. Larger inaccuracies in mass fractions of the 0th
iteration for the AMW triplet were caused by beam hardening artifacts that were amplified owing to the larger condition number for this triplet. These inaccuracies were mostly diminished in the 4th iteration.

Figure 4.17: Mass fractions in % of adipose tissue, muscle tissue and water for 0th (top row) and 4th (bottom row) iteration of the DIRA algorithm using the AMW base material triplet. Values below 0% and above 100% are represented by blue and red colors, respectively.
Figure 4.18: Mass fractions in % of mineral bone and bone marrow, and density of the bone in g/cm³ for 0th (a) and 4th (b) iteration of the DIRA algorithm using the AMW base material triplet. Values below 0% and above 100% are represented by blue and red colors, respectively.
Figure 4.19: Mass fractions in % of lipid, protein and water for 0th (top row) and 4th (bottom row) iteration of the DIRA algorithm using the LPW base material triplet. Values below 0% and above 100% are represented by blue and red colors, respectively.
Figure 4.20: Mass fractions in % of mineral bone and bone marrow, and density of the bone in g/cm$^3$ for 0th (a) and 4th (b) iteration of the DIRA algorithm using the LPW base material triplet. Values below 0% and above 100% are represented by blue and red colors, respectively.

Figure 4.21 shows mass fractions of the prostate after 4th iteration of DIRA using the AMW or LPW triplets. There was no major difference between the results. Both slightly deviated from the true values, especially the more unstable ones for prostate tissue and water. As these mass fractions were so sensitive they were highly effected by the remaining beam hardening artifacts, and the streaking is clearly visible for both cases. The average mass fractions for the three materials are shown in Table 4.7.
Study 2: Performance evaluation of 3MD and DIRA

Figure 4.21: Mass fractions in % of prostate tissue, water and calcium for the prostate region after 4th iteration of DIRA for the AMW (top) and LPW (bottom) triplets. Values below 0% and above 100% are represented by blue and red colors, respectively.

Table 4.7: Average mass fractions for the prostate.

<table>
<thead>
<tr>
<th>Base material triplet</th>
<th>Mass fraction of prostate tissue</th>
<th>Mass fraction of water</th>
<th>Mass fraction of calcium</th>
</tr>
</thead>
<tbody>
<tr>
<td>True values</td>
<td>0.85</td>
<td>0.10</td>
<td>0.05</td>
</tr>
<tr>
<td>Muscle t., adipose t. and water</td>
<td>0.995356</td>
<td>-0.041136</td>
<td>0.045780</td>
</tr>
<tr>
<td>Lipid, protein and water</td>
<td>0.973131</td>
<td>-0.018541</td>
<td>0.045410</td>
</tr>
</tbody>
</table>

Figure 4.22 shows relative errors in MEAC and LAC for the cases using AMW and LPW triplets. The values were less then 6% in the photon energy range considered in brachytherapy and they were approximately the same for both cases (the difference was less then 0.5%).
Figure 4.22: Relative error in mass energy absorption coefficients (top) and linear attenuation coefficient (bottom), for the two prostate approximation. Red = Tabulated data for lipid, protein and water were used for soft tissue approximation in the DIRA. Blue = Tabulated data for adipose tissue, muscle tissue and water were used for soft tissue approximation in the DIRA.
4.5 Conclusions

The 3MD method is based on a solution of a linear system of equations. The stability of this system can be determined via a so-called condition number. It was shown that the condition number strongly depended on the shape of the base material triangle, which was used in the 3MD method. Flat triangles resulted in numerically unstable systems of equations, the highest stability was achieved for equilateral triangles. It was shown that the condition number depended on the position and rotation of the base material triangle in the LAC diagram. This dependence was, however, quite small. Another parameter that reflected the stability of the system of equations was the uncertainty amplification factor that described how uncertainty of the resulting volume fraction (the output quantity) depended on the uncertainty of the linear attenuation coefficient of the mixture (the input quantity). Though this factor did not depend on rotations or translations of the base material triangle, it still well reflected the values of the condition number.

Performance of DIRA for 3MD in brachytherapy of prostate was tested for two approximations of soft tissues: the adipose tissue, muscle and water (AMW) and lipid, protein and water (LPW) triplets and for a realistic anthropomorphic phantom. It was shown that relative errors in LACs and MEACs of the approximated tissues were less than 6% for photon energies used in brachytherapy; the largest discrepancies were at 12 keV and 30 keV for the LACs and MEACs, respectively. These two energies were from the energy region where the photoelectric effect dominated. The results for the two cases did not differ much from each other. It indicated that DIRA was relatively insensitive to the choice of base material triplets for soft tissue approximations.
Improvements can be made in these areas: classification methods, realistic simulations and evaluation of measured CT data and estimation of the organ dose.

There is a possibility that more advanced methods than thresholding, which for example could include topological information, can improve the results for soft tissue classification. This would give a larger freedom in the selection of base materials to use in the DIRA, which in turn can lead to improved image reconstruction.

The simulation can be extended further by including statistical noise, variability in tissue composition and phantoms of different sizes. Noise from the projection acquisition can be added to the simulated projection data. The variability among patients can also be simulated by adding variability in the tissue composition and by using phantoms of different sizes and shapes.

So far the DIRA has not been tested with measured CT data. The ability to process measured data is a basic requirement for clinical usage of DIRA.

Precision of DIRA increases with decreasing statistical noise in the reconstructed images. The suppression of statistical noise is related to the increase in organ dose to the patient. It would be of interest to investigate the relation between DIRA’s precision and the organ dose.
A.1 Drasim

The following command were used to run Drasim:

```
drasim projection\_generationLow.txt \ 
  -P vpp -DNPROJ=560 -DNPHI=512 -run 0
drasim projection\_generationHigh.txt \ 
  -P vpp -DNPROJ=560 -DNPHI=512 -run 1
```

A.1.1 Drasim input files

A.1.1.1 projection\_generationLow.txt

```
#ifndef NPROJ
#define NPROJ 280 // default projection number
#define NPHI 256
#endif
#define RFOC 1000mm // radius of focus circle
#define RDET 1000mm // radius of detector circle
#define FAN 2*11.525 // fan beam angle
#define DZ 0.7884mm // detector element width
#include <materials>
```

Text "Calculation of projections for a sinogram."

Commands

```
{   no\_control\_print
    plot\_spectrum
    no\_noise
}
```
// 3 mm Al filter
Filter { ALUMINIUM d=0.3 }{TITANIUM d=0.06 }{GRAPHITE d=0.1} // Include phantom.
#include "pha113.txt"

$for i 1 NPROJ
Beam
{
    start(RFOC*cos((i-1)*228/NPROJ),
    RFOC*sin((i-1)*228/NPROJ),0)
    anode=W
    kV = 80 //polychromatic
    mAs = 1.7314
}

Detector
{
    [ Cylindrical_z: center(-RDET*cos((i-1)*228/NPROJ),
    -RDET*sin((i-1)*228/NPROJ),0) ]
    cx=RFOC*cos((i-1)*228/NPROJ) cy=RFOC *sin((i-1)*228/NPROJ)
    phi1=-FAN/2 phi2=FAN/2 nphi=NPHI // NPHI channels
    z1=-DZ/2 z2=DZ/2 nz=1 n_z_sub=10 // subdivision by 10 in
    s_phi(-0.1,0,0.1) s_z(-100,100)
    p_phi_z(0,0.9,0, 0,0.9,0) // phi collimator, no dependency on s_z
    ideal //ideal detector
    beam = i-1 // receives rays from beam i-1
}$forend

A.1.1.2  projection_generationHigh.txt

ifndef NPROJ
#define NPROJ 280 // default projection number
#define NPHI 256
#endif
#define RFOC 1000mm // radius of focus circle
#define RDET 1000mm // radius of detector circle
#define FAN 2*11.525 // fan beam angle
#define DZ 0.7884mm // detector element width
#include <materials>

Text "Test Tube Phantom: Calculation of projections for a sinogram."

Commands
{
    no_control_print
    plot_spectrum
    no_noise
}

// 3 mm Al + 0.4 Sn filter
Filter { ALUMINIUM d=0.3 }{TITANIUM d=0.06 }{GRAPHITE d=0.1}{ TIN ...
    d=0.04 }
// Include phantom.
#include "phantom.txt"

$for i 1 NPROJ
Beam
{
    start(RFOC*cos((i-1)*228/NPROJ),
          RFOC*sin((i-1)*228/NPROJ),0)
    anode=W
    kV = 140 // polychromatic
    mAs = 1.7314
}

Detector
{
    Cylindrical_z: center(-RDET*cos((i-1)*228/NPROJ),
                            -RDET*sin((i-1)*228/NPROJ),0)
    cx=RFOC*cos((i-1)*228/NPROJ) cy=RFOC*sin((i-1)*228/NPROJ)
    phi1=-FAN/2 phi2=FAN/2 nphi=NPHI // NPHI channels
    z1=-DZ/2 z2=DZ/2 nz=1 n_z_sub=10 // subdivision by 10 in z direction
    s_phi(-0.1,0,0.1) s_z(-10,100)
    p_phi_z(0,0.9,0, 0,0.9,0) // phi collimator, no dependency on s_z
    ideal // ideal detector
    beam = i-1 // receives rays from beam i-1
}
$forend
A.2 DIRA improvements

To exemplify the changes made to the DIRA two modifications, of representative types, are summarized in this section.

A.2.1 Extracting function and removing loops

By identifying similar code sections used several times and extracting them to functions readability of the code were increased. In Matlab® matrix operations are preferred to loop therefore some functionality were converted to reduce calculation time.

In the following example the same or very similar code were used to calculate polyenergetic projections at 4 different locations so it were extracted to a function. The code were revised to decrease the number of loops witch reduced the computational time substantially.

A.2.1.1 Old code

```matlab
%% Compute polychromatic 80kV projections No.1
% -------------------------------------
up = zeros(255,360);
sl = zeros(1,78);
for b = 1:1:360;
    for a = 1:1:255;
        for k = 2:79;
            sl(k) = (E(k)*N(E(k))) * ... 
                (exp((-mu1(E(k))*100*p1(a,b))+ ... 
                    (-mu2(E(k))*100*p2(a,b))+ ... 
                    (-mu3(E(k))*100*p3(a,b))+ ... 
                    (-mu4(E(k))*100*p4(a,b))+ ... 
                    (-mu5(E(k))*100*p5(a,b))))* ... 
                    (E(k+1)-E(k-1));
        end
        up(a,b) = sum(sl)/2;
    end
end
Ap80 = -log(up/u80);

% Compute polychromatic 140kV+Sn projections No.1
%------------------------------------------------
up = zeros(255,360);
sl = zeros(1,138);
for b=1:1:360;
    for a=1:1:255;
        for k=2:139;
            sl(k) = (E140(k)*N140(E140(k))) * ... 
                (exp((-mu1140(E140(k))*100*p1(a,b))+ ... 
                    (-mu2140(E140(k))*100*p2(a,b))+ ... 
                    (-mu3140(E140(k))*100*p3(a,b))+ ... 
                    (-mu4140(E140(k))*100*p4(a,b))+ ... 
                    (-mu5140(E140(k))*100*p5(a,b))))* ... 
                    (E140(k+1)-E140(k-1));
        end
end
Ap140 = -log(up/u80);
```
up(a,b) = sum(sl)/2;
end
end
Ap140 = -log(up/u140);

% Compute polychromatic 80kV projections No.2-6
% -------------------------------------------
up = zeros(255,360);
sl = zeros(1,78);
for b = 1:1:360;
    for a = 1:1:255;
        for k = 2:79;
            sl(k) = (E(k)*N(E(k))) * ...
                (exp((-mu1(E(k))*100*p1(a,b))+ ...
                    (-mu2(E(k))*100*p2(a,b))+ ...
                    (-mu3(E(k))*100*p3(a,b))+ ...
                    (-mu4(E(k))*100*p4(a,b))+ ...
                    (-mu5(E(k))*100*p5(a,b))))* ...
                (E(k+1)-E(k-1));
        end
        up(a,b) = sum(sl)/2;
    end
end

% Compute polychromatic 140kV+Sn projections No.2-6
%------------------------------------------------
up = zeros(255,360);
sl = zeros(1,138);
for b=1:1:360;
    for a=1:1:255;
        for k=2:139;
            sl(k) = (E140(k)*N140(E140(k))) * ...
                (exp((-mu1140(E140(k))*100*p1(a,b))+ ...
                    (-mu2140(E140(k))*100*p2(a,b))+ ...
                    (-mu3140(E140(k))*100*p3(a,b))+ ...
                    (-mu4140(E140(k))*100*p4(a,b))+ ...
                    (-mu5140(E140(k))*100*p5(a,b)))) * ...
                (E140(k+1)-E140(k-1));
        end
        up(a,b) = sum(sl)/2;
    end
end
Ap140 = -log(up/u140);

A.2.1.2 New code

function [Ap] = computePolyProj(E, uE, N, p, mu)
    sizeE = size(E);
    sizeP = size(p);
    sl = zeros(sizeP(1), sizeP(2), sizeE(1)-1);
    for k = 2:sizeE-1;
        tmpSum = zeros(size(p(:, :, 1)));
        for a = 1:1:255;
            for b = 1:1:360;
                sl(k) = (E140(k)*N140(E140(k))) * ...
                    (exp((-mu1140(E140(k))*100*p1(a,b))+ ...
                        (-mu2140(E140(k))*100*p2(a,b))+ ...
                        (-mu3140(E140(k))*100*p3(a,b))+ ...
                        (-mu4140(E140(k))*100*p4(a,b))+ ...
                        (-mu5140(E140(k))*100*p5(a,b)))) * ...
                    (E140(k+1)-E140(k-1));
            end
        end
    end
    Ap140 = -log(up/u140);

% Compute polychromatic 80kV projections No.2-6
for i = 1:sizeP(3)
    tmpSum = tmpSum+(-mu(E(k), i)*100.*p(:, :, i));
end
sl(:, :, k) = (E(k)*N(k))*(E(k+1)-E(k-1)).*exp(tmpSum);
end
up = sum(sl, 3)/2;
Ap = -log(up/uE);
end

A.2.2 Generalization of code

By introducing cell-structures the code both became shorter and more general. This makes it easier to adapt the DIRA for a specific situation, this can now be done in a single configuration file, rather than to have to make changes throughout the complete algorithm.

A.2.2.1 Old code

% Projection generation with Joseph No.2-6
%---------------------------------------
porig1 = sinogramJ(Wei1.*dens, degVec, r2Vec/pixsiz, interpolation)';
[~,X] = size(porig1);
p1 = porig1(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
p1 = pixsiz * p1;
p180 = p1 * Cross1(1) * 100;
p1140 = p1 * Cross1(2) * 100;

porig2 = sinogramJ(Wei2.*dens, degVec, r2Vec/pixsiz, interpolation)';
[~,X] = size(porig2);
p2 = porig2(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
p2 = pixsiz * p2;
p280 = p2 * Cross2(1) * 100;
p2140 = p2 * Cross2(2) * 100;

porig3 = sinogramJ(Wei3, degVec, r2Vec/pixsiz, interpolation)';
[~,X] = size(porig3);
p3 = porig3(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
p3 = pixsiz * p3;
p380 = p3 * Att3(1) * 100;
p3140 = p3 * Att3(2) * 100;

porig4 = sinogramJ(Wei4, degVec, r2Vec/pixsiz, interpolation)';
[~,X] = size(porig4);
p4 = porig4(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
p4 = pixsiz * p4;
p480 = p4 * Att4(1) * 100;
p4140 = p4 * Att4(2) * 100;

porig5 = sinogramJ(Wei5, degVec, r2Vec/pixsiz, interpolation)';
[Y,X] = size(porig5);
p5 = porig5(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
p5 = pixsiz * p5;
p580 = p5 * Att5(1) * 100;
p5140 = p5 * Att5(2) * 100;
A.2.2.2 New code

```matlab
if p2MD
    p2 = cell(length(Wei2), 1);
    for j = 1:length(Wei2)
        for i = 1:2
            porig2 = sinogramJ(Wei2{j}(:, :, i).*dens{tissueOrder2(j)}, degVec, r2Vec, ...
                                interpolation)';
            X = size(porig2, 2);
            p2{j}(:, :, i) = porig2(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
            p2{j}(:, :, i) = pixsiz * p2{j}(:, :, i);
        end
    end
    end
end

if p3MD
    p3 = cell(length(Wei3), 1);
    for j = 1:length(Wei3)
        for i = 1:3
            porig3 = sinogramJ(Wei3{j}(:, :, i), degVec, r2Vec, ...
                                interpolation)';
            X = size(porig3, 2);
            p3{j}(:, :, i) = porig3(:,1+(X-Nr2)/2:X-(X-Nr2)/2)';
            p3{j}(:, :, i) = pixsiz * p3{j}(:, :, i);
        end
    end
end
```


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