Development of energy selective techniques in X-ray computed tomography

Mahsa Paziresh

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Patents


Abstract

X-ray micro computed tomography (μCT) has emerged as a powerful tool in petroleum industry for non-destructive 3D imaging of rock samples that offers micron-scale resolution images of the distribution of the rock specimens. μCT enables the modelling of the geomechanical and transport properties [Golab et al., 2010] of rocks. μCT obtains the radiographic projections of a sample at different angles and uses a mathematical procedure to reconstruct a 3D tomogram of the sample’s X-ray attenuation coefficients. Attenuation coefficient is a quantity that describes to what extent the X-ray beam is reduced as it passes through a sample. Through my thesis, the aim was to investigate and improve the two main issue from which μCT suffers:

1) μCT X-ray sources typically emit polychromatic X-rays. When an X-ray beam passes through a sample, the low energy photons (or soft X-rays) are attenuated more readily, leaving a beam consisting of more high energy photons (or hard X-rays), i.e., “X-ray beam hardening” (BH). Therefore the recorded attenuation, given by the logarithm of the ratio of the attenuated and incoming X-ray beam, i.e., Beer-Lambert law, is no longer a linear function of material thickness. If this nonlinear effect is not compensated for, the tomograms will be corrupted by severe edge, “cupping artefact” and “streaks” between dense materials. Apart from these visual aspects, quantitative problems may arise, thus, these artefacts make subsequent tomogram segmentation and analysis difficult.

2) μCT produce micro resolution structural images of a sample but not the compositional information. Although μCT can discriminate sample materials with totally different attenuation coefficients, there are samples such as rocks that include materials with similar attenuation coefficients at one energy spectra. In that case, the attenuation coefficients of materials in an altered energy spectra may be different.

This thesis contributes in addressing the above mentioned fundamental issues in μCT by providing “energy selective techniques” in: 1) BH correction and 2) material characterisation. These methods consider the energy dependency of attenuation coefficients and polychromatic nature of X-rays. The structure of thesis is as follows:

Chapter [1] provides an overview of the basics of tomography with special emphasis on the physics and production process of X-ray, the interaction of X-rays with matter at different energies, and presenting the full energy dependent form of attenuation coefficients and image reconstruction in CT. These concepts form the basis for understanding BH artefacts and correction techniques. One can proceed a step
further and use the energy dependency of \( \mu\)CT as a benefit to characterise the sample materials.

Chapter 2 presents an overview of the physics of BH and the existing correction methods with their advantages and disadvantages, followed by a brief review of the material characterisation methods and the recent advances in this field.

Chapter 3 assess the accuracy of five different linearisation BH correction models including polynomial, bimodal, power law, cubic spline and linear spline using the samples that have been imaged at the ANU \( \mu\)CT facility by measuring the BH curves directly from the projection data in a manner similar to that obtained by imaging wedge phantoms, and remapping the inverse of the models to data. The cubic spline, power law, and polynomial models were found to have the lowest root mean square errors, which for all samples were on average \(6.36 \times 10^{-1}\%\), \(6.24 \times 10^{-1}\%\), and \(6.41 \times 10^{-1}\%\) respectively. The number of parameters to be estimated in power law is the lowest, therefore, considering the small differences in comparing the errors of power law, polynomial and cubic spline models, the power law is a good, simple model for the ANU \(\mu\)CT system.

Chapter 4 is based on a published conference proceeding paper in the “International Conference of Tomography of Materials and Structures (ICTMS2013)” [Paziresh et al., 2013] which applies the power law linearisation BH correction method of chapter 3 to correct the BH artefacts of specimens composed of nested-cylinders, e.g., a rock core within a container. The amount of BH varies depending on the material composition of the specimen and the incident X-ray spectrum. BH can be corrected for each material provided a BH curve is known. The BH curves were obtained by assuming a uniform material for each cylinder. This chapter describes how to determine the centre and radius of each cylinder, generate their BH curves and fit them with a power law model to linearise the total projection data. The BH artefacts are significantly reduced in the tomographic reconstructions resulting from these corrected projections.

Chapter 5 is based on a published paper in the “Journal of Applied Physics” [Paziresh et al., 2016]. In this chapter, dual-energy imaging and the Alvarez and Macovski [Alvarez and Macovski, 1976] transmitted intensity (AMTI) model are used to estimate the maps of density (\(\rho\)) and atomic number (\(Z\)) of mineralogical samples. In this method, the attenuation coefficients are represented in the form of the two most important interactions of X-rays with atoms that is, photoelectric absorption (PE) and Compton scattering (CS) [Alvarez and Macovski, 1976]. This enables material discrimination as PE and CS are respectively dependent on the \(Z\) and \(\rho\) of materials. Dual-energy imaging is able to identify sample materials even if the materials have similar attenuation coefficients at single-energy spectrum. The AMTI model were used variously in simplified forms [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2011].
The model requires calibration and has several limitations, i.e., the model doesn’t account for K-edges and there’s no agreed value upon some parameters of the model. I calibrated and used the full model to estimate the \( \rho \) and \( Z \) of sample materials. This chapter describes the tomographic reconstruction of \( \rho \) and \( Z \) maps of mineralogical samples using the AMTI model. The full model requires precise knowledge of the X-ray energy spectra and calibration of PE and CS constants and exponents of atomic number and energy that I estimated based on fits to simulations and calibration measurements. The estimated \( \rho \) and \( Z \) images of the samples used in this chapter yield average relative errors of 2.62% and 1.19% and maximum relative errors of 2.64% and 7.85%, respectively. Furthermore, I demonstrate that the method accounts for the BH effect in \( \rho \) and \( Z \) reconstructions to a significant extent.

Chapter 6 implements two simplified forms of the full model of chapter 5: 1) Alvarez and Macovski polynomial (AMP) model [Alvarez and Macovski, 1976], Alvarez and Macovski presented the full model but used a polynomial simplified form of it to estimate \( \rho \) and \( Z \) of materials; and 2) Siddiqui and Khamees (SK) model [Siddiqui et al., 2004] that simplified the attenuation model, by assuming two monochromatic radiation. The AMP model, similar to the AMTI model performs the analyses on the projections, but unlike the AMTI doesn’t account for the energy dependency of the attenuation coefficients and X-rays, thus, the image captured in the PE energy range and, so the resultant \( Z \) image, includes BH artefacts. The results from the SK method are more stable since analysis is performed directly on the tomogram. However, since BH correction must be performed on the low-energy reconstructions, this hinders any accurate estimation of \( \rho \) and \( Z \). The results for the AMTI model are, on average for the reference materials used, more accurate than both the AMP and SK models for both atomic number and density estimation. That is, more accurate for atomic number estimation by 7.81% and 15.9%, and more accurate for density estimation by 4.73% and 13.00%, than the AMP and SK models, respectively.

Chapter 7 presents a method to estimate the properties of sample materials from measurements of transmitted intensity and its statistical variance (TIV model). The method only requires single-energy imaging, i.e.; eliminates the requirement of dual-energy. The registered intensity on the detector is proportional to a form of “average” energy of detected quanta of X-ray spectra. The statistical variance of images is then modelled as a Poisson distribution. The variance images can serve the same purpose as the higher energy information required in dual-energy imaging. This chapter examines the effect of energy and spectra on \( Z \) and \( \rho \) calculations. More registered photons and a higher number of collected radiographs provide less relative error in \( Z \) and \( \rho \) estimations. The proposed model yields average estimated \( \rho \) and \( Z \) values 4.29% and 2.47% error. The model correct the BH artefacts reasonably well.

Chapter 8 modified the TIV model of chapter 7 to apply it directly for BH correction without the need to estimate the properties of sample materials. This chapter
also presents a simplified form of the TIV model (STIV) that normalises the average intensity image. These methods notably reduce BH artefacts in the resultant tomosgrams.
Contents

Acknowledgments vii
Publications ix
Patents xi
Abstract xiii

1 X-ray micro Computed-Tomography 1
  1.1 Introduction ......................................................... 1
  1.2 X-ray micro computed-tomography (µCT) 2
    1.2.1 Comparison of clinical CT and µCT 2
    1.2.2 X-rays ......................................................... 3
    1.2.3 X-ray source ................................................... 3
      1.2.3.1 X-ray micro-focus tube 6
    1.2.4 X-ray detector ................................................. 8
      1.2.4.1 Scintillator ................................................ 8
    1.2.5 Basic interaction of X-rays with matter 9
      1.2.5.1 Photoelectric absorption 9
      1.2.5.2 Compton scattering ..................................... 9
      1.2.5.3 Rayleigh scattering ................................... 10
    1.2.6 Attenuation of X-rays ....................................... 11
      1.2.6.1 Linearisation ............................................. 13
    1.2.7 Image reconstruction ....................................... 14
      1.2.7.1 Line integrals and projections 14
      1.2.7.2 The Fourier slice theorem 17
      1.2.7.3 The filtered back-projection (FBP) .................. 20
      1.2.7.4 Fan beam ................................................ 24
      1.2.7.5 Cone beam .............................................. 26
  1.3 Conclusion ....................................................... 26

2 Energy selective techniques 29
  2.1 Introduction ...................................................... 29
  2.2 Beam hardening (BH) artefacts and correction techniques in CT 30
    2.2.1 Hardware filtering ......................................... 34
    2.2.2 Linearisation BH software correction methods ............ 35
2.2.2.1 Linearisation BH correction by minimising re-projection distance ........................................ 36
2.2.2.2 Linearisation iterative expert-guided BH correction for heterogeneous specimens .................. 38
2.2.3 Post-reconstruction iterative BH software correction methods ............................................. 40
  2.2.3.1 Post-reconstruction iterative, reference-less BH correction method ................................... 40
  2.2.3.2 Post-reconstruction iterative BH correction based on a physical model ............................ 43
2.3 Material characterisation in CT ............................................................................................ 45
  2.3.1 Correction on Siddiqui and Khamees (SK) method ................................................................. 46
  2.3.2 Source-weighting method ................................................................................................. 49
2.4 Conclusion .......................................................................................................................... 51

3 Assessment of several linearisation X-ray beam hardening correction methods .......................... 53
  3.1 Introduction .......................................................................................................................... 53
  3.2 Measuring beam hardening curves ...................................................................................... 55
    3.2.1 Wedge and cylinder phantoms ...................................................................................... 55
    3.2.2 Beam hardening curves of common materials at the ANU µCT facility ......................... 56
  3.3 Fitting BH curve models and performing BH correction ....................................................... 61
    3.3.1 Polynomial model .......................................................................................................... 63
    3.3.2 Bimodal energy model .................................................................................................... 65
    3.3.3 Power law model ............................................................................................................ 67
    3.3.4 Cubic spline model ........................................................................................................ 69
    3.3.5 Linear spline model ....................................................................................................... 70
  3.4 Performance assessment of the applied linearisation BH correction models ......................... 72
  3.5 Conclusion .......................................................................................................................... 73

4 Beam hardening correction of concentric cylindrical specimens using power law model .......... 75
  4.1 Introduction .......................................................................................................................... 75
  4.2 Fitting the cylinder (or circles) ............................................................................................ 76
  4.3 Fitting material attenuation .................................................................................................. 77
  4.4 Fitting the beam hardening correction model ....................................................................... 77
  4.5 Applying the beam hardening correction .............................................................................. 78
    4.5.1 Single cylinder ................................................................................................................ 78
    4.5.2 Nested-cylinders .............................................................................................................. 78
  4.6 Conclusion .......................................................................................................................... 83
## 5 Material characterisation using dual-energy imaging and the AM attenuation model

### 5.1 Introduction

85

### 5.2 Alvarez and Macovski attenuation coefficient (AMAC) and transmitted intensity (AMTI) models

88

### 5.3 Modelling the physics of X-ray energy spectrum \( S(E) \)

90

#### 5.3.1 Measuring the X-ray energy spectrum

93

#### 5.3.1.1 Correction of the partial registry of the measured X-ray spectra on the detector

93

#### 5.3.2 Correction of the characteristic peaks of the simulated X-ray spectra

95

#### 5.3.3 X-ray dual-spectra

96

### 5.4 Simulation: Validating and calibrating the model

97

#### 5.4.1 AMAC model calibration using NIST data

98

#### 5.4.2 AMTI model calibration using simulated cylinder images

101

#### 5.4.3 Testing the AMTI model calibration using the real cylinder images

105

### 5.5 Experimental analysis

108

#### 5.5.1 Material discrimination of rock using AMTI model

110

#### 5.5.2 Beam hardening correction in AMTI model

113

### 5.6 Conclusion

115

## 6 Assessment of the full AM model in comparison with two simplified forms

117

### 6.1 Introduction

117

### 6.2 Alvarez and Macovski Polynomial (AMP) transmitted intensity model

118

#### 6.2.1 The AMP model calibration using the real cylinder images

118

#### 6.2.2 Material discrimination of rock using AMP model

122

### 6.3 Siddiqui and Khamees (SK) attenuation model

126

#### 6.3.1 The SK model calibration using the real cylinder images

128

#### 6.3.2 Material discrimination of rock using SK model

129

### 6.4 Assessing the atomic number and density estimations of AMP and SK models in comparison with the results of the full AMTI model (from chapter 5)

131

### 6.5 Conclusion

133

## 7 Material characterisation using single-energy imaging and statistical variance

135

### 7.1 Introduction

135

### 7.2 The correlation of Transmitted Intensity and Variance

137

### 7.3 Transmitted Intensity and Variance (TIV) model for material characterisation

138

### 7.4 Testing the TIV model using simulated intensity and variance images

141

### 7.5 Testing the TIV model using simulated images including noise

144
## 7.5.1 Accuracy assessment of TIV model for different X-ray energy spectra

147

## 7.5.2 Accuracy assessment of TIV model for detected X-ray photons

148

## 7.6 Conclusion

149

## 8 Beam hardening correction using single-energy imaging and statistical variance

151

### 8.1 Introduction

151

### 8.2 The performance of energy in beam hardening correction (BH) methods

153

### 8.3 Transmitted intensity and statistical variance (TIV) model for BH correction

154

### 8.4 Simplified Transmitted Intensity and Variance (STIV) model for BH correction

157

### 8.5 Conclusion

158

## 9 Conclusion and Future Work

159
List of Figures

1.1 Schematic overview of an X-ray source tube and its component (http://doctorspiller.com/Dental%20radiologyx-ray_characteristics.html). .................................................. 4
1.2 Schematic overview of: a) characteristic and b) Bremsstrahlung X-ray productions [Mohamed, 2013]. ................................................................. 5
1.3 X-ray spectrum of a tungsten source for a maximum tube voltage of 100 keV, filtered by 0.1mm Cu measured using Amptek CdTe spectrum analyser. ............................................................. 6
1.4 Schematic overview of an micro-focus X-ray source tube and its component (http://www.yxlon.com/Technology). ............................................................. 7
1.5 The fine focus imaging geometry. ................................................................ 7
1.6 Mass Attenuation Coefficient for a soft tissue [Ajaja, 2010]. ...................... 9
1.7 For X-ray imaging in the energy ranges used in medical CT and μCT two interactions are important: (a) the photoelectric absorption and (b) the Compton scattering (http://www.studyblue.com). ......................... 11
1.8 Coordinate transformation of sample μ(x, y) to the projection Pθ(t) [Kak and Slaney, 1988]. ................................................................. 15
1.9 A parallel projection is formed by measuring set of parallel rays of different angles [Kak and Slaney, 1988]. .................................................. 16
1.10 The Fourier slice theorem relates the Fourier transform of a projection to the Fourier transform of a sample along a radial line [Kak and Slaney, 1988]. ................................................................. 18
1.11 Collecting projections of the sample at a number of angles provides estimation of the Fourier transform of the sample along radial lines [Kak and Slaney, 1988]. ................................................................. 20
1.12 Schematic of 1D projection of a sample at three different angles and the corresponding reconstruction from the obtained projection data (http://bruker-microct.com/home.htm). ................................................. 21
1.13 The dependency of the quality of the reconstruction image of a point sample on the available projection data from different angles (http://bruker-microct.com/home.htm). .................................................. 21
1.14 The blur around the reconstructed image after back-projection reconstruc- construction and the correction of the blur using a filter (http://bruker-microct.com/home.htm). .......................................................... 22
1.15 Schematic view of the projection filter, h(t), in the spatial domain [Kak and Slaney, 1988]. ................................................................. 24
# LIST OF FIGURES

1.16 A fan beam projection is collected if all the rays meet in one location [Kak and Slaney, 1988]. .................................................. 25

2.1 Attenuation of a) Silicon and b) Platinum as a function of photon Energy (http://physics.nist.gov/PhysRefData/XrayMassCoef/tab4.html). These plots are presented to show that the nonlinear trend of the attenuation coefficients result in the nonlinearity of the beam hardening artefacts (see Eqn. 1.2). Plots of the attenuation for the energy range of imaging in this thesis, [1, 120] keV, are presented in figure 5.7 for several samples used in the experiments. ........................................ 31

2.2 Effect of beam hardening on reduction of spectra’s photon counts as the beam is passing through the aluminium filters with thickness of 0.25, 0.5, 1, 2, 4, 6 mm shown subsequently in green, blue, red, purple, yellow and black colours. The spectra is recorded using Amptek CdTe spectrum analyser. .......................................................... 32

2.3 Illustration of BH effect; (i) a sample made of PMMA and aluminium, (ii) reconstruction including BH artefacts, (iii) BH corrected reconstruction and (iv) a line through the reconstructions [Van Gompel et al., 2011]. 33

2.4 Hardware Filtering. The spectra imaged at 60 keV with 0.25 mm Al filter and 100 keV with 0.25 mm Cu filter, using Amptek CdTe spectrum analyser ................................................................. 34

2.5 Flowchart of the linearisation BH correction by minimising re-projection distance (Section 2.2.2.1) [Kingston et al., 2012]. .......................... 37

2.6 Flowchart of the iterative expert-guided BH correction method (Section 2.2.2.2) [Ketcham and Hanna, 2014]. .............................................. 39

2.7 Flowchart of the iterative reference-less BH correction (Section 2.2.3.1) [Krumm et al., 2008]. ................................................................. 41

2.8 (a) shows the polychromatic and (b) the monochromatic approximation of the point cloud propagation path length versus ray sum plot of a two-material specimen, by a two-dimensional plane and surface with 400 nodes. Black dots indicate computed attenuation values [Krumm et al., 2008]. ................................................................. 42

2.9 Flowchart of the iterative physical energy distribution BH correction (Section 2.2.3.2) [Van Gompel et al., 2011]. ........................................ 44

2.10 Flowchart of estimation of the corrections to be applied on the SK method; with \( \epsilon \) being the relative error and \( \delta \) being the absolute error (Section 2.3.1) [Derzhi, 2012]. ................................................................. 47

2.11 Flowchart of applying the corrections of Fig. 2.10 on the SK method (Section 2.3.1) [Derzhi, 2012]. ................................................................. 48

2.12 Plots of the numerical results of \( Z \) and \( \rho \) projections: a) shows a function, \( F(Z) = \frac{\mu_1}{\mu_2} \), and b) shows \( \rho(\mu_1, \mu_2) \) for recorded images at 80 and 140 keV (\( \mu_1 \) and \( \mu_2 \) are normalised to CT values \( C \); where \( C = 1000 \times \frac{\mu}{\mu_{\text{water}}} \)) [Heismann et al., 2003]. ................................................................. 50

Draft Copy – 21 November 2016
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1</td>
<td>Illustration of the BH (i) the quantitative measurement of source with different filters corresponding to the thickness of the shown sample ($S_1 = 0.5\text{mm}$ and $S_2 = 2\text{mm}$ Al filter), and (ii) schematics drawing of beam hardened and the ideal projection.</td>
</tr>
<tr>
<td>3.2</td>
<td>Schematic of plotting the BH curve, i.e., the intensity of the projection versus the path length of X-ray (s) for a cylindrical sample.</td>
</tr>
<tr>
<td>3.3</td>
<td>The attenuation of the X-ray spectra using different filters or container, as the beam is passing through the sample. This plots are quantitative measurement of source with different filters corresponding to the thickness of the shown sample: (i) $S_1 = 0.5\text{mm}$ and $S_2 = 0.5\text{mm}$ Al filter, (ii) $S_1 = 0.5\text{mm}$ Al and $S_2 = 1\text{mm}$ Al filter, (iii) $S_1 = 0.5\text{mm}$ Al and $S_2 = 2\text{mm}$ Al filter.</td>
</tr>
<tr>
<td>3.4</td>
<td>BH curve of (i) NaI, (ii) CsI, (iii) CsCl, (iv) 100 per BrC, (v) BrC$_8$ in oil, and (vi) IC$_x$ with different salinities.</td>
</tr>
<tr>
<td>3.5</td>
<td>A cross-sectional reconstructed uncorrected image of 2M CsI in cylindrical container.</td>
</tr>
<tr>
<td>3.6</td>
<td>Flowchart of linearisation BH correction. The BH curve of samples can be obtained having prior knowledge of sample shape, i.e., wedge or cylindrical specimens of uniform composition, i.e., homogeneous samples (see section 3.2.1 and Fig. 3.1 and 3.2).</td>
</tr>
<tr>
<td>3.7</td>
<td>Plot of the uncorrected (main) data, polynomial of order eight fit and the corrected (linearised) data.</td>
</tr>
<tr>
<td>3.8</td>
<td>(i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the polynomial model of order (a-four, b-six, c-eight), (ii) profile through the centre of the uncorrected (blue line) and corrected (red line) images.</td>
</tr>
<tr>
<td>3.9</td>
<td>Plot of the uncorrected (main) data, bimodal fit and the corrected (linearised) data.</td>
</tr>
<tr>
<td>3.10</td>
<td>(i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the bimodal model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.</td>
</tr>
<tr>
<td>3.11</td>
<td>Measured X-ray BH curves at our facility [Paziresh et al., 2013].</td>
</tr>
<tr>
<td>3.12</td>
<td>Plot of the uncorrected (main) data, power law fit and the corrected (linearised) data.</td>
</tr>
<tr>
<td>3.13</td>
<td>(i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the power law model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.</td>
</tr>
<tr>
<td>3.14</td>
<td>Plot of the uncorrected (main) data, spline fit and the corrected (linearised) data.</td>
</tr>
</tbody>
</table>
3.15 (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the spline model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image. ................................................. 70

3.16 (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the linear spline model with (a-2_lines, b-3_lines), and (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image. ......................... 71

3.17 The average RMS error of corrected images compared with uniform disc. 72

4.1 Horizontal slices through two single cylinder specimens (a). (i) reconstructions with beam-hardening artefacts, (ii) reconstructions after correction, and (iii) profile through the centre of images as indicated by dashed lines .................. 79

4.2 Horizontal slices through two single cylinder specimens (b). (i) reconstructions with beam-hardening artefacts, (ii) reconstructions after correction, and (iii) profile through the centre of images as indicated by dashed lines ...................... 80

4.3 Flowchart of the BH correction of nested-cylinders. ......................... 81

4.4 A horizontal slice through a three cylinder specimen including the rock, fluid and the holder. (i) reconstructed using measured attenuation, (ii) reconstructed using corrected attenuation, and (iii) profile through the centre of images as indicated by dashed lines .................. 82

5.1 Flowchart of the Modelling the physics of X-ray energy spectrum \( S_\epsilon(E) \), with \( \epsilon \) being the energy label. ............................... 91

5.2 Simulated spectrum at 100 maximum energy; modified to match that seen for our experimental protocol, meaning that the spectrum is modified to be as measured by the detector with CsI scintillator. The plot shows a jump at 33.169 keV that relates to the K-edge of Iodine. .... 92


5.4 Plot of partial register correction using the stripping algorithm for a) 80 (blue line [Redus et al. 2009]), b) 60, c) 100 and d) 120 keV spectrum measured using the Amptek spectrum analyser. The yellow line is the measured partial registry corresponding to the four terms \( f_j(E - E_j)N_d(E) \) in Eqn. 5.7 ......................... 95

5.5 Plot of the partial registry corrected measured spectrum fitted to simulated spectrum to match the XRFs amplitude for: a) 80 ([Redus et al. 2009]), b) 60, c) 100 and d) 120 keV ................. 96

5.6 Simulated dual-energy spectra at 60 (red line) and 120 keV (blue line) maximum energies; modified to match that seen for our experimental protocol (section 5.3), and the spectra weight (dashed cyan line) that is the absolute difference of the dual-energy spectra. This weight is added to the AMAC model in section 5.4.1 ......................... 97
5.7 Plot of $\ln(\mu)$ versus $(E = [1,120]keV)$ of NIST data (red line) and AMAC model (blue dashed line) fits applying the the estimated $K_1$, $K_2$, $m$ and $n$ constants in section 5.4.1 for a) glass, b) acrylic, c) titanium and d) marble. ........................................... 100

5.8 Flowchart of the AMAC model calibration (Section 5.4.1). .................. 101

5.9 A line through a simulated projection cylinder and the AMTI model fit: at 60 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a) glass and b) marble. .................. 102

5.10 Flowchart of the AMTI model calibration and $\rho$ and $Z$ estimation, using simulated projections of cylinders of 7 reference materials (Section 5.4.2), with $\epsilon$ being the energy label and pre-processing step explained in section 5.5 $P = \int L_p(s,E)$ and $C = \int L_c(s,E)$ from Eq. 5.3 .................................................. 104

5.11 A line through an imaged projection cylinder and the AMTI model fit: at 60 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a) glass and b) marble. .................. 106

5.12 Flowchart of the AMTI model calibration and $\rho$ and $Z$ estimation, using real intensity images of cylinders of 7 reference materials (Section 5.4.3), with $\epsilon$ being the energy label and pre-processing step explained in section 5.5 $P = \int L_p(s,E)$ and $C = \int L_c(s,E)$ from Eq. 5.3 .................................................. 107

5.13 Flowchart of $\rho$ and $Z$ estimation using real intensity images of cylinders of rocks and the calibrated AMTI model (Section 5.5), with $\epsilon$ being the energy label and pre-processing step explained in section 5.5 $P = \int L_p(s,E)$ and $C = \int L_c(s,E)$ from Eq. 5.3 .................................................. 109

5.14 a-i) reconstructed slice of Berea sandstone at $E_{max} = 60keV$, b-i) reconstructed slice of Berea sandstone at $E_{max} = 120keV$, a-ii) reconstructed slice of the estimated $Z$ using the AMTI model 5.5 and b-ii) reconstructed slice of the estimated $\rho$ using the AMTI model. The cupping artefacts are evident around the edges in a-i, while a-ii and b-ii don’t have the BH artefacts. The image contrast in enhanced to illustrate the existence of the cupping artefact in a-i and no visible BH in b-i, however the a-ii and b-ii images shows the original grey scales of the images. .................................................. 111

5.15 a-i) reconstructed slice of the carbonate masked $Z$, b-i) reconstructed slice of the carbonate masked $\rho$, a-ii) reconstructed slice of the estimated $Z$ using the AMTI model 5.5, b-ii) reconstructed slice of the estimated $\rho$ using the AMTI model, a-iii) the plot of fitted Gaussian to histogram of masked $Z$ and b-iii) the plot of fitted Gaussian to histogram of masked $\rho$. .................................................. 114
6.1 Flowchart of the AMP model calibration and $\rho$ and $Z$ estimation, using real intensity images of cylinders of 7 reference materials (Section 6.2), with $\varepsilon$ being the energy label and pre-processing step explained in section 5.5. $P = \int_L p(s, E) \, ds$ and $C = \int_L c(s, E) \, ds$ from Eq. 5.3.

6.2 a-i) reconstructed slice of the estimated $Z$ of Berea sandstone, using the AMP model (6.1), b-i) reconstructed slice of the estimated $\rho$ of Berea sandstone using the AMP model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$, and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.14a-ii and b-ii for reconstruction slice of Berea sandstone imaged at $E_{\text{max}} = 60$ and 120 keV).

6.3 a-i) reconstructed slice of the estimated $Z$ of the carbonate, using the AMP model 6.1, b-i) reconstructed slice of the estimated $\rho$ using the AMP model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$, and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.15a-i and b-i for more details about masked $Z$ and $\rho$).

6.4 Flowchart of the SK model calibration and $\rho$ and $Z$ estimation, using reconstructed images of cylinders of reference materials (Section 6.3). One can choose to have different number of reference materials, $\omega$. We have chosen 7 reference materials, commonly used at the Anu $\mu$CT facility, for the calibration of the models in chapter 5 to 8. This materials are over a range of atomic number and density.

6.5 a-i) reconstructed slice of the estimated $Z$ of the Berea sandstone, using the SK model 6.3, b-i) reconstructed slice of the estimated $\rho$ of the Berea sandstone using the SK model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$ and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.14a-ii and b-ii for reconstruction slice of Berea sandstone images at $E_{\text{max}} = 60$ and 120 keV).

6.6 a-i) reconstructed slice of the estimated $Z$ of the carbonate, using the SK model 6.3, b-i) reconstructed slice of the estimated $\rho$ of the carbonate using the SK model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$ and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.15a-i and b-i for more details about masked $Z$ and $\rho$).

7.1 Simulated energy spectra at 100 keV maximum energy with 0.5 mm aluminium filter (red line) and the spectrum including higher mean energy (blue line); modified to match that seen for our experimental protocol.

7.2 A line through a simulated projection cylinder and the TIV model fit: at 100 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a)glass and b) aluminium.
7.3 Flowchart of the TIV model calibration and \( \rho \) and \( Z \) estimation, using simulated projections of cylinders of 7 reference materials (Section 7.4), with \( \varepsilon \) being the energy label. \[ P = \int_L p(s, E) \] and \[ C = \int_L c(s, E) \] from Eq. 5.3. ................................................................. 143

7.4 A line through a simulated projection and the TIV model fit of the cylinders of a) glass and b) carbon imaged at 100 keV. ................. 145

7.5 Flowchart of the TIV model calibration and \( \rho \) and \( Z \) estimation, using simulated projections of cylinders of 7 reference materials (Section 7.5), with \( \varepsilon \) being the energy label. \[ P = \int_L p(s, E) \] and \[ C = \int_L c(s, E) \] from Eq. 5.3. ................................................................. 146

8.1 Simulated energy spectra at 40 keV maximum energy with no filter (red line) and the spectrum including higher mean energy (blue line); modified to match that seen for our experimental protocol. .......... 154

8.2 A line through reconstruction of glass, showing the average intensity captured at 40 keV (blue line), statistical variance (green line) and the applied TIV BH correction in section 8.3 (red line). The reconstruction of this study are from a single radiograph. Since the same noise copied to the all projection angles, the line profile of the reconstructed image also include ring artefacts. ......................................................... 155

8.3 Flowchart of the modified TIV model for beam hardening correction, using simulated projections of cylinders of 7 reference materials (Section 8.3), with \( \varepsilon \) being the energy label. \[ P = \int_L p(s, E) \] and \[ C = \int_L c(s, E) \] from Eq. 5.3. ................................................................. 156

8.4 A line through reconstruction of marble, showing the average intensity captured at 40 keV (blue line), statistical variance (green line) and the applied TIV BH correction in section 8.4 (red line). ...................... 158
List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>Relative error between NIST attenuation coefficient and AMAC model for reference materials using AMAC model (Section 5.4.1)</td>
<td>100</td>
</tr>
<tr>
<td>5.2</td>
<td>Estimated effective atomic number and bulk density of reference materials using AMTI model (Section 5.4.2 and 5.4.3)</td>
<td>106</td>
</tr>
<tr>
<td>5.3</td>
<td>Estimated effective atomic number and bulk density of rocks using AMTI model (Section 5.5.1)</td>
<td>110</td>
</tr>
<tr>
<td>6.1</td>
<td>Estimated calibration parameters for AMP model (Eqn. 6.1)</td>
<td>119</td>
</tr>
<tr>
<td>6.2</td>
<td>Estimated effective atomic number and bulk density of reference materials using AMP model (Eqn. 6.1)</td>
<td>120</td>
</tr>
<tr>
<td>6.3</td>
<td>Effective atomic number and bulk density of rocks using AMP model</td>
<td>123</td>
</tr>
<tr>
<td>6.4</td>
<td>Estimated calibration parameters for SK model (Eqn. 6.4)</td>
<td>128</td>
</tr>
<tr>
<td>6.5</td>
<td>Estimated effective atomic number and bulk density of reference materials using SK model (Eqn. 6.3)</td>
<td>129</td>
</tr>
<tr>
<td>6.6</td>
<td>Effective atomic number and bulk density of materials</td>
<td>130</td>
</tr>
<tr>
<td>7.1</td>
<td>Estimated effective atomic number and bulk density of reference materials using TIV model (Section 7.4)</td>
<td>144</td>
</tr>
<tr>
<td>7.2</td>
<td>Estimated relative error of effective atomic number of reference materials using TIV model for different X-ray spectra (Section 7.5.1)</td>
<td>147</td>
</tr>
<tr>
<td>7.3</td>
<td>Estimated relative error of the bulk density of reference materials using TIV model for several X-ray spectra (Section 7.5.1)</td>
<td>147</td>
</tr>
<tr>
<td>7.4</td>
<td>Average estimated relative error of the ρ and Z of the seven samples for a) detected photon with 1000 image acquisition, and b) acquisition number with 100,000 detected photon</td>
<td>148</td>
</tr>
<tr>
<td>7.5</td>
<td>Estimated effective atomic number and bulk density of reference materials using TIV model for chosen acquisition time and photon counts (Section 7.5.2)</td>
<td>149</td>
</tr>
</tbody>
</table>
1.1 Introduction

In 1895, Wilhelm Rontgen [Röntgen, 1896] discovered the X-ray beam while he was experimenting an electric discharge in a vacuum tube in his laboratory. He noticed a radiation on a phosphor screen in front of the tube. He positioned different materials in front of the screen to examine which one could block the beam. When he put his hands in front of the screen, he saw a shadowed image of his bones. As such, X-rays were discovered and at the same time radiography was born. Rontegen received the Nobel Prize in 1901 for his discovery [Röntgen, 1896].

A radiograph only provides a two dimensional (2D) projected image (projection) of a three dimensional (3D) sample; where projection is the line integral of X-ray beam attenuation along the direction of X-ray propagation. This 2D projection of 3D sample can help to diagnose a broken bone but, having the information about the depth (3rd dimension) could facilitate more precise examination. Tomography solved this limitation by capturing these projected radiographs of the sample at different angles, this way, depth could be taken into account in reconstruction. The word tomography is a combination of two Greek words: “tomos” and “graphos” which respectively mean “slice” and “to draw”.

The problem of how to mathematically reconstruct a function from its projections was first solved in 1917 by Johann Radon [Radon, 1917]. A set of projections of a function at different angles is called the Radon transform. Tomographic reconstruction performs the inverse Radon transform to reconstruct the function. The practical use of the computed-tomography happened in 1972 when Godfrey N. Hounsfield developed the first X-ray computerised tomographic scanner (the EMI head scanner) [Hounsfield, 1973]. His mathematical and experimental methods were based on the work presented a decade earlier by A. M. Cormack [Cormack, 1963, 1964]. Housfield and Cormack shared the Nobel prize in 1979.
Micrometer-scale computed-tomography (µCT), like medical computed-tomography, uses X-ray imaging combined with the inverse Radon transform to reconstruct the cross-sections, or the even full 3D view, of a sample without destroying the original specimen. µCT allows quantitative analysis of the thickness or composition of the sample material. The first X-ray µCT system was built by Jim Elliott in the early 1980s [Elliott and Dover, 1982].

X-ray µCT system have a micro-focus source that emits polychromatic X-ray beam. When the X-ray beam is passing through a sample, the X-rays interact with matter and are attenuated. Attenuation coefficient describe the extent to which the X-ray photons are attenuated and is dependent on the applied X-ray energy and the density and atomic number of the sample material.

In this chapter, section 1.2 is a survey of the X-ray µCT systems including X-ray source, detector, production of X-ray spectrum, interaction of X-ray with matter and the energy-dependent attenuation of X-rays. This chapter also includes a summary of a µCT image reconstruction method including measurements of projections, the filtered back-projection reconstruction algorithm and X-ray imaging geometries. This background study lays the foundation for understanding the challenges of energy related issues in µCT and possible solutions.

1.2 X-ray micro computed-tomography (µCT)

X-ray computed-tomography (CT) or computerised axial tomography (CAT) use a combinations of several X-ray images at different angles to produce cross-sectional images of a sample. These cross-sectional images provide information about the internal structure of the sample and allow investigation of the specific areas of the sample without cutting into it. Since the introduction of CT in 1970s, the most common applications are found in medicine.

X-ray micro computed-tomography (µCT), like CT, uses X-rays to create cross-sectional images of a sample that can be used to reconstruct a virtual (computerised) 3D model without destroying the original sample. The prefix µ indicates that the pixel sizes of the cross-sections are in the micro-metre range. µCT has found applications both in medical and industrial imaging.

1.2.1 Comparison of clinical CT and µCT

The most significant difference between clinical CT and µCT is the set-up and size of the scanner. A clinical CT set-up is a gantry based where the patient is stationary and the tube-detector unit is rotating around the patient. The tube-detector unit consists of an X-ray tube and a detector array covering the entire field of view. In µCT, the source and detector are stationary while the sample is rotating. This produces
a more stable set-up than clinical CT where the rotating source-detector unit causes vibrations during image acquisition. This supports the ability of a μCT system to produce an enhanced resolution, which is an advantage of this system over clinical CT. Also in μCT, while the sample is rotating, projections can be taken using fan beam (see section 1.2.7.4) or a cone beam geometry (see section 1.2.7.5) along the optical axis. These two imaging geometries cause a magnification of the sample image and therefore the pixel resolution can be optimal for small samples. Further information about the CT imaging in medical scanners are available in [Hsieh, 2009; Seeram, 2001; Mihailidis, 2009] and about μCT imaging and reconstruction algorithms are available in [Stock, 2008].

Another difference between the μCT and medical CT is the type of scanner. μCT uses a source-detector unit that consists of a micro-focus X-ray tube and an X-ray detector. The X-ray detectors is a matrix covering the field of view in two directions, and at this time, they can cover to 2048 × 2048 pixels, however 4096 pixel detectors are appearing [Konstantinidis et al., 2012]. Both source and detector play an important role in the resolution of the image of the X-ray μCT. An arbitrary position of the sample can also impact on the resolution of the projections. Generally, the resolution of projections can be determined by spread of the source, resolution of the detector system, and the geometric magnification. For further information regarding the resolution of image in μCT, please refer to [Stock, 2008].

1.2.2 X-rays

X-rays are part of the electromagnetic spectrum. They are photons, each with an energy, \(E\), which is inversely proportional to its wavelength [Soper, 2012]:

\[
E = \frac{hc}{\lambda} = hv, \tag{1.1}
\]

where \(h = 6.62 \times 10^{20}\) Js is Planck’s constant, \(c = 3 \times 10^8\) m/s is the speed of light and \(v\) is the frequency. X-rays have a wavelength in the range of 0.01 to 10 nanometers, corresponding to frequencies in the range 3 × 10^{16} Hz to 3 × 10^{19} Hz and energies in the range 100 eV to 140 keV. The energy of the X-ray radiation used in most commercial CT scanners ranges from 30 keV to 140 keV [Van de Casteele et al., 2002].

1.2.3 X-ray source

A typical X-ray source consists of an anode and a cathode inside a vacuum tube as shown in Fig. 1.1. Electrons are ejected from the cathode and the electrical field between cathode and anode divert them toward the anode. These electrons interact with the atoms of the target material and transfer their kinetic energy in the process [Behling, 2015].
X-rays are produced through two different interaction processes: characteristic X-rays and Bremsstrahlung. Characteristic X-rays are produced when an electron interacts with electrons in the target material. When the incoming electron has enough energy to remove a target material’s electron from its shell and so ionise the atom, the resulting hole is filled with an outer shell electron and an X-ray photon with the energy greater than or equal to the difference in the binding energies of the orbital electrons is emitted. The X-ray photon is called characteristic X-ray because it is material dependent [Van de Casteele, 2004]. This is shown in Fig. 1.2 (a). The second process for X-ray production occurs when the electron interacts with the nucleus of an atom in the target material (tungsten). The electron is slowed and continues in a different direction with reduced energy. The kinetic energy lost from the electron is converted into a photon and emits an X-ray. This type of X-ray production is called “Bremsstrahlung” which is originated from two German names of “Bremsen” which means “to brake” and “Strahlung” which means “radiation”, i.e. “braking radiation” or “deceleration radiation” [Röntgen, 1896]. This process is illustrated in Fig. 1.2 (b). Bremsstrahlung has a continuous spectrum, while characteristic radiation results in a discrete X-ray spectrum with characteristic peaks corresponding to the difference in the binding energy of the atom shells between which electron has been transmitted. Fig. 1.3 shows the measured spectrum of a tungsten source that is normalised over area. The spectrum is filtered with a 0.1mm Cu filter. The filtering effect is obtained by placing a plate of a certain material and thickness in front of the source, which causes the preferential attenuation of the lower X-ray energies out of the spectrum.
Figure 1.2: Schematic overview of: a) characteristic and b) Bremsstrahlung X-ray productions [Mohamed, 2013].
1.2.3.1 X-ray micro-focus tube

Fine and broad focal spot sizes are available on general X-ray tubes. Fine focus X-ray sources are used predominantly to enhance visualisation of fine detail in imaging. The main difference between micro-focus X-ray tubes and conventional X-ray tubes are the centring coils (or the alignment unit shown in Fig. 1.4) and the focusing coils (or the objective lens/aperture shown in Fig. 1.4). The centring coils centre the beam of electrons so that it hits the tungsten target in the centre and the focusing coils focus the electrons on the tungsten target. Consequently, the effective source of the X-ray beam is so small that it only measures a few micro-metres across. Placing the sample in a short distance to the source results in geometric magnification of the image on the detector. The fine focus imaging geometry is shown in Fig. 1.5.
§1.2 X-ray micro computed-tomography (μCT)

Figure 1.4: Schematic overview of an micro-focus X-ray source tube and its component (http://www.yxlon.com/Technology).

Figure 1.5: The fine focus imaging geometry.
1.2.4 X-ray detector

The imaging geometry in Fig. 1.5 shows a detector that detects the X-rays after they have been transmitted through the sample. This X-ray radiation is polychromatic as mentioned in section 1.2.3. A detector in its ideal form should be able to detect every incident photon of the complete spectrum of the X-ray energies and the detector response should be linear over a large range of intensities. When X-ray radiography was first introduced, photographic films were used as detectors. The main disadvantage of using photographic films is that they have to be erased and reloaded into a cassette, because of this, CT systems started using the detectors that use digital storage of information. Currently, flat-panel scintillator detectors are the most commonly used detectors in µCT systems. Flat-panel detectors are more sensitive than films because they require a lower dose of radiation for a given image quality. Flat-panels are more accurate, durable, lighter, smaller and record images in larger sizes with less distortion [Seibert 2006].

1.2.4.1 Scintillator

There are two types of flat-panel detectors: direct and indirect detectors. Indirect flat-panel detectors contain a layer of scintillator material, either caesium iodide or gadolinium oxysulphide, which converts X-rays into light. The scintillator materials are of type that produce flashes of light in response to the absorption of ionising radiation. The amount of light emitted is proportional to the amount of energy absorbed by the material. This luminescence in solids has an efficient process for the conversion of energetic radiation (electrons and X-rays) into photons. The scintillator detector converts photons to digital signals using light-sensitive sensors in the second layer exactly behind the scintillator. This layer is an amorphous silicon glass detector array. Millions of pixels containing a thin-film transistor, form a grid patterned in amorphous silicon on the glass substrate, similar to a thin-film-transistor liquid-crystal-display (TFT-LCD). Each pixel also contains a photodiode that converts the light produced by the portion of scintillator layer in front of the pixel to an electrical signal. Additional electronics at the edges or behind the photodiodes amplify and encode these signals and produce an accurate and sensitive digital representation of the X-ray image.

Direct flat-panel detectors convert the X-ray photons directly into electrical signals. The radiated X-ray photons on the detector material and produces electron-hole pairs. The outer layer of these flat-panel detectors are typically a high-voltage bias electrode. The transit of these electrons and holes depends on the potential of the bias voltage charge. The electrical signals are then read by TFT arrays as explained in indirect flat-panel detectors above. For further information, please see [Ballabriga et al. 2016].
1.2.5 Basic interaction of X-rays with matter

In the typical μCT X-ray radiation energy range, [10, 120] keV, the three most important interactions of X-ray photons with matter are the photoelectric effect, Compton scattering and Rayleigh scattering. Pair production is another X-ray interaction with matter that happens in energy ranges over one MeV which is outside the range of [10, 120] keV. Our X-ray source energy generally uses an accelerating voltage in the range of 50 to 120 keV. Figure 1.6 shows the relative contribution of these interactions of X-ray with soft tissue.

![Attenuation Coefficient](image)

Figure 1.6: Mass Attenuation Coefficient for a soft tissue [Ajaja, 2010].

1.2.5.1 Photoelectric absorption

Photoelectric absorption is predominant at low energies. This event occurs when an incident X-ray interacts with an electron of an atom within the material. The electron is ejected from that atom and the photon is totally absorbed. If the X-ray photon was carrying even more energy, the extra energy would be transferred to the ejected electron in the form of kinetic energy [Attix, 2008]. This process is shown in Fig. 1.7a.

1.2.5.2 Compton scattering

Compton or incoherent scattering is predominant at intermediate energies [Attix, 2008]. It occurs when the incident photon interacts with an electron and the X-ray is scattered through an angle and emerges at a different energy related to the angle
to conserve the mass-energy and momentum of the system. The amount the energy (wavelength) changes by is called the Compton shift. This process is shown in Fig. 1.7b.

1.2.5.3 Rayleigh scattering

Lord Rayleigh discovered Rayleigh or “coherent” scattering in 1871 [Attix, 2008]. This event is elastic because the photon energy is conserved and results in occasional redirection of the X-ray photon. Rayleigh scattering is more evident at lower energies because the scattering angle is larger at lower energies. For the energy range considered here, relative to photoelectric absorption and Compton scattering, Rayleigh scattering has negligible effect on the attenuation coefficient. For more details and the simulations, please refer to [Boone and Seibert, 1997].
§1.2 X-ray micro computed-tomography ($\mu$CT)

1.2.6 Attenuation of X-rays

The Beer-Lambert law describes attenuation of monochromatic radiation as the line integral of attenuation coefficient ($\mu$), as follows [Beer 1852]:

$$\int_{L} \mu(s) ds = - \ln \left( \frac{I}{I_0} \right),$$

where $I_0$ and $I$ are the intensity of the incident and the transmitted radiation respectively, along the X-ray propagation ($L$) as the beam travels through the thickness of sample materials ($s$).
However, the attenuation coefficient ($\mu$) is a function of energy ($E$), and X-ray radiation in a lab-based $\mu$CT system spans a range of wavelengths. Consequently, the Beer-Lambert law is adapted to account for the polychromatic nature of X-rays such that the transmitted intensity ($I$) is presented as follows:

$$I = -\int_0^{E_{\text{max}}} S_\epsilon(E) \exp\left[ -\int L \mu(s,E)ds \right] dE. \quad (1.3)$$

where energy label ($\epsilon$) is the peak voltage energy of the X-ray radiation and $S_\epsilon(E)$ of ($\epsilon$) with X-ray of maximum energy ($E_{\text{max}}$) is the respective incident X-ray intensity spectrum modulated by detector quantum efficiency and spectral transmission of non-sample attenuating materials between source and detector. For further information, i.e., modelling and measurement of $S_\epsilon(E)$, please refer to section 5.3.

As mentioned in section 1.2.5, the two important interaction of X-rays with matter in energy range [1, 120] keV are photoelectric absorption and Compton scattering. Thus, the linear attenuation coefficient of Eqn. 1.3 can be written as:

$$\mu(s,E) = \mu_p(s,E) + \mu_c(s,E) \quad (1.4)$$

with $\mu_p(E)$ and $\mu_c(E)$ being, subsequently, the contribution of the photoelectric absorption (PE) and Compton scattering (CS) in the attenuation coefficient. $E$ is the X-ray energy, $\rho$ and $Z$ are the density and atomic number of the sample material and $n$ is the exponent to $Z$. The PE effect is highly dependent on atomic number ($\mu_p \propto \rho Z^{n-1}$) and CS is proportional to the density of the sample material ($\mu_c \propto \rho$).
1.2.6.1 Linearisation

Generally, before placing a sample in its position in a µCT system, shown in Fig. 1.5, two sets of information are obtained. Firstly, an image is recorded without X-ray illumination that is called a “dark field” image ($I_{DF}$). This image represents background and environmental noise. The second set of images are recorded after turning on the X-ray source and are called “clear field” images ($I_{CF}$). They represent the incident X-ray radiation ($I_0$ in Eqn. 1.2) on the detector in absence of a sample.

After placing the sample and recording projections ($I$), $\frac{I - I_{DF}}{I_{CF} - I_{DF}}$ is used to linearise the projection data and Eqn. 1.5 estimates the attenuation when assuming the X-ray radiation is monochromatic.

$$\int_{L} \mu(s) ds = -\ln \left( \frac{I - I_{DF}}{I_{CF} - I_{DF}} \right).$$

Where a sheet of material is used before or after the sample to filter the low-energy X-rays (e.g., to reduce artefacts), it is called hardware filtering (see section 2.2.1). The direct effect of filtering on the intensity is removed by the above mentioned linearisation using the clear field image, since identical filtering is present for $I$ and $I_{CF}$.

Temporal imaging characteristic of flat panel X-ray detectors can be separated into two categories including Lag and ghosting. These inaccuracies may affect the accuracy of the linearisation. Lag is the carryover of image charge generated by previous X-ray exposures into the next image. Ghosting is the change in X-ray sensitivity as a result of detector’s exposure to radiation which can be seen by the next X-ray exposures. Both lag and ghosting can lead to image artefacts in projection and reconstructed images [Shaw, 2014].
1.2.7 Image reconstruction

Projections are a set of measurements of line integrals of transmitted X-rays at different angles. One can recover the image of the cross-section of a sample from the projection data. The simplest case for reconstructing this image from the projection data is for the parallel set of X-rays. In this case, each point on the projection contains the information of the attenuation of the 3D sample integrated along the direction of X-ray propagation. This section demonstrates the theory of line integrals and projections. It also discusses the filtered back-projection reconstruction algorithm that is based on the Fourier slice theorem [Kak and Slaney, 1988].

1.2.7.1 Line integrals and projections

A line integral represents the integral of some measurement of the sample along a line. In this sense, the sample is modelled as a 2D distribution of the X-ray attenuation constants and a line integral represents the total attenuation of a beam of X-rays as it travels in a straight line through the sample. The coordinate system presented in Fig. 1.8 can be used to describe line integrals and projections. Figure 1.8 represents the sample in form of a 2D function $\mu(x, y)$ and each line integral in form of the $(\theta, t)$ parameters. Then the equation of an X-ray with the incident angle of illumination, $\theta$, and a distance, $t$, with respect to the origin can be presented as:

$$x \cos \theta + y \sin \theta = t$$  \hspace{1cm} (1.6)

This relationship can define line integral, $P_\theta(t)$, as:

$$P_\theta(t) = \int_{-\infty}^{\infty} \mu(x, y) \, ds$$  \hspace{1cm} (1.7)

Using a delta function, this can be rewritten as:

$$P_\theta(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mu(x, y) \, \delta(x \cos \theta + y \sin \theta - t) \, dx \, dy$$  \hspace{1cm} (1.8)

The function $P_\theta(t)$ is the Radon transform [Radon, 1917] of the function $\mu(x, y)$ with a constant $\theta$ for a collection of parallel X-rays shown in Fig. 1.9.
Figure 1.8: Coordinate transformation of sample \( \mu(x, y) \) to the projection \( P_\theta(t) \) [Kak and Slaney 1988].
Figure 1.9: A parallel projection is formed by measuring set of parallel rays of different angles [Kak and Slaney, 1988].
1.2.7.2 The Fourier slice theorem

The Fourier slice theorem is a fundamental part of tomographic imaging that relates measured projections from Radon transform to a radial profile in Fourier space. To derive the Fourier slice theorem, a one-dimensional (1D) Fourier transform of a parallel projection is derived that is equal to a slice of the 2D Fourier transform of the sample. As such, to reconstruct the sample, a 2D inverse Fourier transform of the projection data should be estimated. The 2D Fourier transform of the attenuation coefficient of the sample is defined as:

\[ F(u, v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mu(x, y) e^{-i2\pi(ux + vy)} \, dx \, dy \]  (1.9)

Likewise, the Fourier transform of a projection \( P_{\theta}(t) \) at an angle \( \theta \) is defined as:

\[ S_{\theta} = \int_{-\infty}^{\infty} P_{\theta}(t) e^{-i2\pi wt} \, dt \]  (1.10)

The simplest form of the Fourier slice theorem is given for a projection at \( \theta = 0 \). First, the Fourier transform of the sample along the line in the frequency domain of Eqn. 1.9 when \( v = 0 \), simplifies into:

\[ F(u, 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mu(x, y) e^{-i2\pi ux} \, dx \, dy \]  (1.11)

In that case, the phase factor is not dependent on \( y \) anymore and the integral can be split into two parts as below:

\[ F(u, 0) = \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \mu(x, y) \, dy \right] e^{-i2\pi ux} \, dx \]  (1.12)

As shown for parallel projection in Eqn. 1.7, the term in the brackets can be recognised as the equation for a projection along lines of constant \( x \):

\[ P_{\theta=0}(t) = \int_{-\infty}^{\infty} \mu(x, y) \, dy \]  (1.13)

Substituting in Eqn. 1.12 results in:

\[ F(u, 0) = \int_{-\infty}^{\infty} P_{\theta=0}(t) e^{-i2\pi ux} \, dx \]  (1.14)

The right-hand side of Eqn. 1.14 represents the 1D Fourier transform of the projection \( P_{\theta=0} \). From Eqn. 1.10, the relationship between the vertical projection and the 2D
Fourier transform of the sample function will be as follows:

\[ F(u, 0) = S_{\theta=0}(u) \]  \hspace{1cm} (1.15)

Equation 1.15 is the simplest form of the Fourier slice theorem. It describes the Fourier transform of the projection of the transmitted parallel X-rays, at vertical axis \( \theta = 0 \), as the Fourier transform of the image at the horizontal radial profile. This relationship can be generalised for different angles of rotation. The Fourier transform, \( F(u, v) \), of a sample function, \( \mu(x, y) \), at an angle, \( \theta \), with respect to the \( x \)-axis in the space domain corresponds to the Fourier transform, \( S_{\theta=0}(u) \), rotating by the same angle with respect to the \( u \)-axis in the frequency domain. This is shown in Fig. 1.10. In this sense, the Fourier transformation of a projection along the X-ray parallel lines, that make an angle \( \theta + 90^\circ \) with respect to the \( x \)-axis reflect the Fourier transform of the image, along the radial line (BB in Fig. 1.10) that makes an angle \( \theta \) with respect to the \( u \)-axis.

![Diagram](image)

Figure 1.10: The Fourier slice theorem relates the Fourier transform of a projection to the Fourier transform of a sample along a radial line [Kak and Slaney 1988].

As shown in Fig. 1.10, the rotated version of \((x, y)\) coordinate in \((t, s)\) system is expressed as:
where a projection along lines of constant \( t \) in \((t, s)\) coordinate system can be written as:

\[
P_{\theta=0}(t) = \int_{-\infty}^{\infty} \mu(t, s) \, ds
\]  

Substituting the projection of Eqn. 1.17 in Eqn. 1.10 the Fourier transform is given by:

\[
S_{\theta}(w) = \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \mu(t, s) \right] e^{-i2\pi wt} \, dt
\]  

Using the coordinate transformation of Eqn. 1.16, the Fourier transform of Eqn. 1.18 can be transformed into the \((x, y)\) coordinate system as follows:

\[
S_{\theta}(w) = \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \mu(x, y) \right] e^{-i2\pi wt(x \cos \theta + y \sin \theta)} \, dx \, dy
\]  

where the right-hand side of Eqn. 1.19 is the 2D Fourier transformation of the image at a spatial frequency of \((u = w \cos \theta, v = w \sin \theta)\). This can be presented as:

\[
S_{\theta}(w) = F(u, v) = F(w \cos \theta + w \sin \theta)
\]  

Equation 1.20 characterises the straight ray tomography and demonstrates the Fourier slice theorem. By taking the projections of a sample function at angles \( \theta_1, \theta_2, ..., \theta_k \) and Fourier transforming each of these, the values of \( F(u, v) \) can be determined on radial lines such as in Fig. 1.10. For an infinite number of projections, \( F(u, v) \) can be verified at all points of the \( uv\)-plane, but practically only a finite number of projections can be taken. In that case, the function \( F(u, v) \) can only be determined along a finite number of radial lines as shown in Fig. 1.11.
1.2.7.3 The filtered back-projection (FBP)

Filtered back-projection (FBP) is an accurate reconstruction algorithm [Kak and Slaney 1988, Herman 1995] that is in use in most of the applications of straight ray tomography. This algorithm is derived from the Fourier slice theorem.

Here, the algorithm is explained using a simple example. The sample in Fig. 1.12 is assumed to have only one point (pixel) with significant attenuation corresponds to a high density material. The 1D projection at three different angles causes a decrease in intensity that corresponds to an increase in the attenuation, as shown in Fig. 1.12.
Figure 1.12: Schematic of 1D projection of a sample at three different angles and the corresponding reconstruction from the obtained projection data (http://bruker-microct.com/home.htm).

Figure 1.12(b) shows that for every projection, the attenuation value is back-projected in the reconstruction area. After back-projection at several angles, the position of the attenuation point (pixel) can be localised in the reconstruction. By increasing the number of back-projections at different angles, this localisation becomes more clear, as shown in Fig. 1.13.

Figure 1.13: The dependency of the quality of the reconstruction image of a point sample on the available projection data from different angles (http://bruker-microct.com/home.htm).
The back-projection from a number of projections reconstructs an image of the attenuation area. For each projection, the attenuation is homogeneously back-distributed along the projection line, for that, the superposition of the attenuation from different angles causes an evident blur in the reconstruction, as shown in Fig. 1.14(a). Pre-filtering can correct this blur by adding some negative attenuation to eliminate the positive blur in the back-projection process (convolution). In this sense, the filtered back-projection algorithm is derived from the Fourier slice theorem. From the inverse Fourier transform, the sample function, \((x, y)\) is:

\[
\mu(x, y) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F(u, v) e^{2\pi i w (ux + vy)} \, du \, dv
\]  

(1.21)

The rectangular coordinate system in the frequency domain, \((u, v)\), can be transformed to a polar coordinate system, \((w, \theta)\), by substituting \((u = w \cos \theta), \quad (v = w \sin \theta)\) and differentials by \((du \, dv = w \, dw \, d\theta)\). Equation (1.21) can be re-written as:

\[
\mu(x, y) = \int_{0}^{2\pi} \int_{0}^{\infty} F(w, \theta) e^{2\pi i w (x \cos \theta + y \sin \theta)} \, w \, dw \, d\theta
\]  

(1.22)
The above integral can be split into two by considering \( \theta \) from 0 to \( \pi \) and from \( \pi \) to \( 2\pi \). By substituting Eqn. 1.6 and using the property of Fourier transformations that \([F(w, \theta + \pi) = F(-w, \theta)]\), Eqn. 1.22 can be expressed as:

\[
\mu(x, y) = \int_0^\pi \left[ \int_{-\infty}^{\infty} F(w, \theta) |w| e^{i2\pi wt} dw \right] d\theta
\] (1.23)

From Eqn. 1.20, the 2D Fourier transform \( F(w, \theta) \) can be substituted with the Fourier transform of the projection at angle \( \theta \), \( S_\theta(w) \), as follows:

\[
\mu(x, y) = \int_0^\pi \left[ \int_{-\infty}^{\infty} S_\theta(w) |w| e^{i2\pi wt} dw \right] d\theta
\] (1.24)

The above integral may be expressed in other format, as follows:

\[
\mu(x, y) = \int_0^\pi Q_\theta(x \cos \theta + y \sin \theta) \ d\theta
\] (1.25)

where

\[
Q_\theta(t) = \int_{-\infty}^{\infty} S_\theta(w) |w| e^{i2\pi wt} dw
\]

\[
= F^{-1}\left\{ S_\theta(w) |w| \right\}
\] (1.26)

Equation 1.26 presents a filtering operation. The frequency response of the filter is given by \( |w| \). By substituting Eqn. 1.10 that shows \( S_\theta(w) \) is the 1D Fourier transformation, Eqn. 1.26 can be re-written as:

\[
Q_\theta(t) = P_\theta(t) \odot h(t)
\] (1.27)

where \( h(t) = F\{|w|\} \) is the filter function.

Therefore \( Q_\theta(t) \) is called a “filtered-projection”. The filtered-projection, \( Q_\theta \), at different angles, \( \theta \), should then be back-projected as in Eqn. 1.25 to form of \( \mu(x, y) \). In this process, every point \((x, y)\) in the image plane corresponds to a value of \( t = x \cos \theta + y \sin \theta \). The filtered-projection, \( Q_\theta \), contributes its value \( t \) to the reconstruction at all of the points (pixels) along a line through the sample \( \mu \). This way in the reconstruction process, each filtered-projection, \( Q_\theta \), is back-projected over the image plane. The filter, \( h(t) = F\{|w|\} \), is an ideal inversion filter in frequency space. As shown in Fig. 1.11, the informations at low frequencies (near the origin) is enhanced compared to the information at high frequencies. The ramp filter, \(|w|\), corrects this effect by putting a linear weight in Fourier space to reduce the low spatial
frequencies and increase the high spatial frequencies. The filter, \( h(t) \), is depicted in spatial and frequency space in Fig. 1.15. Further information can be found in [Kak and Slaney, 1988; Herman, 1995].

**Figure 1.15:** Schematic view of the projection filter, \( h(t) \), in the spatial domain [Kak and Slaney, 1988].

1.2.7.4 **Fan beam**

For the parallel projection, the source-detector system linearly scan over a length of projection, at several angle of rotation with a certain interval. This process takes as long as few seconds [Kak and Slaney, 1988]. Using a fan beam radiation, shown in Fig. 1.16, is a much faster solution to generate these line integrals.

For the fan beam imaging, the simple filtered back-projection presented for parallel projection in section 1.2.7.3 becomes a weighted back-projection that considers the fan beam geometry. An alternative solution is to re-order the fan beam projection into an equivalent parallel beam projection, by applying constraints on the angles at which the fan beam projections should be collected and also on the angles at which projection data should be sampled. To read more about this re-sorting algorithm and the weighted back-projection algorithm, please refer to [Kak and Slaney, 1988].
Figure 1.16: A fan beam projection is collected if all the rays meet in one location [Kak and Slaney 1988].
More recently, high-resolution, inexpensive flat-panel detectors have become available (see section 1.2.4). The configuration of such detectors offers greater dynamic range, however, these detectors require a slightly greater radiation exposure. As shown in imaging geometry of Fig. 1.5 imaging is accomplished by using a rotating sample to which an X-ray source and detector are fixed. A cone-shaped source of radiation can be directed through the sample onto the X-ray detector on the opposite side. During the rotation, multiple sequential planar projection images of the field of view (FOV) are acquired in a complete, or sometimes partial, arc. This procedure varies from a traditional CT, which uses a fan-shaped (see section 1.2.7.4) X-ray beam (e.g., in a helical progression [Hu, 1999]) to acquire individual image slices of the FOV and then stacks the slices to obtain a 3D representation. As such in fan beam geometry, each slice requires a separate scan and separate 2D reconstruction, however, the cone beam radiation incorporates the entire FOV and thus only one rotational sequence of the sample is necessary to acquire enough data for image reconstruction.

Cone beam CT has been used for medical radiotherapy guidances [Cho et al., 1995] and geological applications [Recur et al., 2014a]. The cone-beam geometry was developed as an alternative to conventional CT using either fan-beam, to provide more rapid acquisition of a data set of the entire FOV and it uses a comparatively less expensive radiation detector. Obvious advantages of such a system, which provides a shorter imaging time, include reduction in distortion in the image due to the sample movements, reduction in deformations, and increased X-ray tube efficiency. However, its main disadvantage, especially with larger FOVs, is a limitation in image quality related to noise and contrast resolution because of the detection of large amounts of scattered radiation.

1.3 Conclusion

In this chapter, the basics of tomography were described with special emphasis on: 1) the physics of X-ray, 2) demonstration of the production process of X-ray energy spectrum consisting of continuous (bremstralung) spectrum and characteristic peaks, 3) presenting the full energy dependent form of the X-ray attenuation and 4) the interaction of X-rays with matter at different energies. These concepts form the basis for understanding the image artefacts that are evident in reconstructions, which assume monochromatic X-ray radiation, and the correction techniques of those artefacts. Also, one can go a step further and use the energy dependency of $\mu$CT as a benefit to characterise the sample materials. As such, the main developments of this thesis are the image artefacts correction and material characterisation, using the energy selective techniques. Chapter 2 is a review of the definition of these two problems in $\mu$CT and the description of many available energy selective solution methods.
The applied energy selective techniques, in chapter 3, 4 and 8 for artefacts correction, and in chapter 5, 6 and 7 for material characterisation, are applied on projection images. These projection images are then reconstructed using the filtered back-projection algorithm described in section 1.2.7. There are techniques that are applied on the reconstructed image, e.g., the material characterisation technique of section 6.3.2 in which case an image reconstruction is required at the very early stage of the image processing.

Throughout the thesis, I used flowcharts to illustrate the algorithms, workflows or processes, showing the start and stop steps with red squares, decision-making steps with green ellipses, processing steps with orange squares, input and output data with purple trapezium and logical and mathematical steps and connections with yellow circles, and their orders by connecting them with arrows. These diagrammatic representations are used to accompany with the demonstrations of the solution models in the relevant sections.
Chapter 2

Energy selective techniques

2.1 Introduction

There are two main reasons that motivate undertaking this research on energy selective techniques in μCT. Firstly, one of the most important artefacts while working with CT is beam hardening (BH). This artefact is the result of the polychromatic nature of X-rays used in the μCT systems. When an X-ray beam passes through a sample, the lower energy photons are attenuated more readily, as the attenuation coefficient generally decreases with increasing energy. As such, the X-ray beam that passes through the denser part of the sample includes higher mean energy and is less likely to be attenuated, i.e., the beam becomes harder; for that, this effect is called beam hardening artefact. The transmitted intensity recorded on the detectors corresponds to the attenuation of a polychromatic radiation (Beer-Lamber law in Eqn. [1.3]), however standard tomographic reconstruction algorithms assume monochromatic radiation. Since the transmitted intensity data are not linear with the sample thickness, the reconstruction produces some visual distortions, such as brighter edges and streaking artefacts. These artefacts make subsequent tomogram segmentation and analysis difficult.

Secondly, X-ray μCT imaging enables nondestructive visualisation of the internal structure of samples. In addition, μCT allows quantitative analysis of the composition of the material. In the energy range [1, 120] keV in μCT imaging, the two main interactions of X-rays with matter are photoelectric absorption (PE) and Compton scattering (CS). These effects are subsequently dependent on atomic number and density of the constituent materials of a sample. As such, attenuation coefficient can be represented in from of a two-basis function, that corresponds to the contribution of PE and CS effects in the total attenuation coefficient. These two functions can be used to estimate the atomic number and density distribution of the materials of the sample. This method is applicable for both intensity images (pre-reconstruction) and the reconstructed image (post-reconstruction). The post-reconstruction method is simple, fast and easy to implement, but is prone to be affected by the artefacts in the reconstructed images, especially the beam-hardening artefacts. The pre-reconstruction method can automatically correct the BH and is more accurate.
Section 2.2 starts with a demonstration of the physics of the BH artefacts, and continues with an overview of the existing BH correction methods in tomography, with their advantages and disadvantages. I have also chosen several methods and implemented them in chapter 3 to assess their accuracy and choose the most appropriate model. Afterwards, using the selected model of chapter 3, a method is presented to compensate the BH for the concentric cylindrical samples in chapter 4.

Section 2.3 begins with a brief review of the material characterisation methods and summarises recent advances in this field. Furthermore, I implemented a pre-reconstruction and a post-reconstruction material characterisation technique in µCT in chapter 6 to compare with the results of my work in chapter 5.

2.2 Beam hardening (BH) artefacts and correction techniques in CT

µCT systems in the laboratory use a micro-focus X-ray source (see section 1.2.3.1) that emits polychromatic (bremsstrahlung) radiation (see section 1.2.3). The spectrum of the X-ray source spans many wavelengths (see Fig. 2.2) and attenuation is a function of X-ray energy. Figure 2.1 shows attenuation coefficient plots of silicon and platinum subsequently with lower and higher atomic number. These plots illustrate the nonlinear form of the attenuation coefficient as a function of energy.
2.2 Beam hardening (BH) artefacts and correction techniques in CT

Figure 2.1: Attenuation of a) Silicon and b) Platinum as a function of photon Energy (http://physics.nist.gov/PhysRefData/XrayMassCoef/tab4.html). These plots are presented to show that the nonlinear trend of the attenuation coefficients result in the nonlinearity of the beam hardening artefacts (see Eqn. 1.2). Plots of the attenuation for the energy range of imaging in this thesis, [1, 120] keV, are presented in figure 5.7 for several samples used in the experiments.
When a polychromatic X-ray beam passes through matter, low energy photons are more likely to be attenuated, as the attenuation coefficient generally decreases with increasing energy (see Fig. 2.1). Figure 2.2 shows that as the beam passes through 0.25, 0.5, 1, 2, 4 and 8 mm aluminium filter, the lower energy X-ray is getting attenuated more readily, thus, the mean energy of the beam increases gradually, i.e., beam hardening. The rate at which the beam is attenuated decreases at higher energies, so the harder a beam is, the less it is further attenuated. This means that the total attenuation given by the Beer-Lambert law of Eqn. 1.2 i.e., the logarithm of the ratio of the attenuated and incoming X-ray beam (yellow arrows in Fig. 2.2), is not valid for polychromatic X-ray spectra and attenuation estimated in this way is not a linear function of material thickness. This is specified in the beam hardening curves of section 3.2.2. If this nonlinear effect is not compensated, the reconstructed images will be corrupted by severe edge artefacts and streaks.

Figure 2.2: Effect of beam hardening on reduction of spectra’s photon counts as the beam is passing through the aluminium filters with thickness of 0.25, 0.5, 1, 2, 4, 6 mm shown subsequently in green, blue, red, purple, yellow and black colours. The spectra is recorded using Amptek CdTe spectrum analyser.

Figure 2.3(i) shows a sample made of poly-methylmethacrylate (PMMA), three rods of a high density material (aluminium) and two holes filled with air. Figure 2.3(ii) shows the filtered-back-projection (FBP) reconstruction (see section 1.2.7.3) of the uncorrected (beam hardened) measured projections of the sample. This figure shows significant artefacts around the edges of this image, that is called “cupping artefacts” and streaks between the aluminium rods, that is called “streaking artefacts”. In ad-
dition, the background attenuation in the convex hull of the sample is overestimated in the reconstructed image. Gompel et al. [Van Gompel et al., 2011] applied an iterative BH method, explained in section 2.2.3.2, to correct the BH of this image that is shown in Fig. 2.3(iii). Figure 2.3(iv) depicts the line profiles along horizontal line through the reconstructed image of the sample, in which black and grey lines, shown in Fig. 2.3(ii) and (iii), correspond to the beam hardened and corrected reconstruction respectively.

Figure 2.3: Illustration of BH effect; (i) a sample made of PMMA and aluminium, (ii) reconstruction including BH artefacts, (iii) BH corrected reconstruction and (iv) a line through the reconstructions [Van Gompel et al., 2011].

BH artefacts makes the quantitative interpretation of the \( \mu \)CT images and segmentation very difficult. This also complicates the calibration and resolution measurements. Furthermore, the same materials can result in different intensity-values in projections depending on the surrounding material.

The problem of BH artefact is common between \( \mu \)CT and clinical CT because both systems use polychromatic X-rays, however, the BH artefacts are avoided in the systems that have monochromatic synchrotron radiation. Thus, correction for these artefacts becomes a matter of utmost importance in \( \mu \)CT and clinical CT, to obtain quantitative data, and is reflected in a large number of publications [Paziresh et al.].
This section reviews some of these methods.

There are a number of techniques that can be used to minimise this effect which can be generally categorised as 1) hardware filtration or 2) beam hardening correction software techniques. Typically two types of software BH correction are available: 2a) BH linearisation and 2b) post-reconstruction iterative methods.

2.2.1 Hardware filtering

Hardware filtering is the most common method to narrow the broad spectrum of an X-ray source [Hammersberg and Måns 1998]. By placing a filter between the source and the sample, the low energy X-rays are attenuated. This helps to achieve a beam with higher mean energy and a narrower energy spectrum. Almost all of the commercial systems use hardware filtering in addition to software beam hardening correction. Fig. 2.4 shows the spectrum of the tungsten source normalised over the area with 0.25 mm Al filtering at 60 keV (blue line) and with 0.25 mm Cu filter at 100 keV (red line). Figure 2.2 shows the variations in spectrum’s photon counts at 100 keV X-ray beam as it passes through the 0.25, 0.5, 1, 2, 4 and 8 mm aluminium filters. The figure shows as the spectrum transmitted through the specimen, the effect of SNR varies as well. Without filtering, very soft radiation will not penetrate the specimen and does not contribute to the signal information, but it will reduce the dynamic range. The spectrum that passed through 8mm Al filter shows the highest mean energy in the figure.

Figure 2.4: Hardware Filtering. The spectra imaged at 60 keV with 0.25 mm Al filter and100 keV with 0.25 mm Cu filter, using Amptek CdTe spectrum analyser.
The main disadvantage of this technique is reduction of the photon counts which results in a decrease in the image signal-to-noise ratio (SNR) and increase in the required acquisition time for the same result. Furthermore, this method only partially helps to correct the BH artefacts.

### 2.2.2 Linearisation BH software correction methods

The more commonly applied correction method is based on applying a linearisation procedure on the projection data \cite{Van_de_Castelee_et_al_2002, Herman_1979, Hammersberg_and_Mans_1998}, henceforth called BH linearisation methods in this thesis. The Beer-Lambert law for a homogeneous sample and a monochromatic source is shown in Eqn. 1.2. One can plot the measured attenuation coefficient versus the sample thickness, that is “beam hardening curve” (BH curve), and is expected to reflect a linear function, while the experimental attenuation data has a significant deviation from the linear trend. I measured the BH curves of several material imaged at the ANU \(\mu\)CT facility that is shown in Fig. 3.4. To correct the BH curves, the measured nonlinear relation can be fitted with a model. The inverse of the model should be applied on the BH curve to linearise the data. This method is most applicable for the samples that are composed of only one material.

Several linearisation methods have been developed for BH correction \cite{Herman_1979, Van_de_Castelee_et_al_2002, Kingston_et_al_2012}. Herman \cite{Herman_1979} modelled the BH curve with a polynomial. I implemented the polynomial BH correction method using the projection data obtained at the ANU \(\mu\)CT facility and presented the results in section 3.3.1. Van de Casteele et al., \cite{Van_de_Castelee_et_al_2002} modelled the BH curve based on the physical model. I implemented BH correction using this model in section 3.3.2. These two methods offer acceptable results, however the first requires several parameters to be estimated depending to the order of the polynomial and the second needs some initial information about the attenuation coefficient values or these information should be estimated and doesn’t provide good results for all materials.

Kingston et al., \cite{Kingston_et_al_2012} developed a method to minimise the re-projection distance. This method, that is explained in section 2.2.2.1, provided a good BH artefact correction for the ANU \(\mu\)CT system but was not compatible for cylindrical samples. More than 50\% of samples at the ANU \(\mu\)CT facility have a cylindrical shape, thus, further investigation was required to find a proper BH linearisation model for correction of BH artefacts of cylindrical sample, which is surveyed in chapter 3. I applied the chosen model of chapter 3 on nested-cylinder samples and presented the results in chapter 4. Ketcham and Hanna, presented an iterative optimisation algorithm on the regions-of-interest (ROI)s chosen by an expert user, to find a generalised spline-interpolated transform function for BH correction of heterogeneous specimens. This method is explained in section 2.2.2.2.
I applied a non-iterative procedure using a cubic spline model, on the BH curve of the homogeneous cylindrical specimens imaged at ANU µCT facility, to linearise the data.

### 2.2.2.1 Linearisation BH correction by minimising re-projection distance

This method assumes an average material for the heterogeneous samples and uses a procedure that minimises the re-projection distance to find the best correction curve. Function $B$, that is an eight order polynomial, is used to model the BH curve, as follows:

$$
\begin{aligned}
B_a(x) &= \sum_{i=1}^{8} a_i b_i(x); \\
b(x) &= \sum_{j=1}^{8} m_j x^j
\end{aligned}
$$

(2.1)

Where $a_i$ and $m_i$ are the constants of the eight order polynomials. This process involves eight reconstructions and re-projections of the experiment data. The best BH curve generates a projection set that minimises the re-projection distance, $d_i$, that is the difference between the uncorrected projection $P_u$ and the projection, which is reconstructed and then re-projected, $RR^{-1}P_u$, as follows:

$$
\text{minimise} \left\{ \begin{array}{c}
8 \sum_{i=1}^{8} a_i (RR^{-1} - I) b_i(P_u) \\
8 \sum_{i=1}^{8} a_i b_i(P_u)
\end{array} \right\}
$$

(2.2)

A flowchart for this method is shown in Fig. 2.5. This technique doesn’t require a priori information of the X-ray spectrum or materials. It works well for single-material samples, and also multiple-material samples if the BH curve determined for the average of all the materials of the sample.

The work presented in chapter 4 is complementary to the BH correction method developed by Kingston et al. [Kingston et al., 2012] explained in this section. That method enforces self-consistency in the data but does not work for cylindrical samples. The model can not determine any objective where attenuation is function a function of radius because BH projections still exists in the re-projections [Kingston et al., 2012]. Chapter 4 considers the specimens composed of nested cylinders, e.g., a rock core within a container to correct the BH artefacts in their tomograms. This assumption covers a significant fraction (> 50%) of the specimens currently imaged at ANU µCT facility.
Data acquisition

Intensity images (projections); $P_u$

Down-sampling

Generate and store 8 projection sets $b_1(P_u), b_2(P_u), \ldots, b_8(P_u)$ from Eqn. 2.1

Generate and store 8 re-projection sets $RR^{-1}b_1(P_u), RR^{-1}b_2(P_u), \ldots, RR^{-1}b_8(P_u)$ from Eqn. 2.1

Calculate re-projection differences;

$$d_i = RR^{-1}b_i(P_u) - b_i(P_u) \quad i \in [1, 8]$$

Parameter extraction;

$a_i$ of Eqn. 2.2

Remap the polynomial of Eqn. 2.1 to $P_u$

Corrected intensity images

CT image reconstruction

Figure 2.5: Flowchart of the linearisation BH correction by minimising re-projection distance (Section 2.2.2.1) [Kingston et al., 2012].

Draft Copy – 21 November 2016
2.2.2.2 Linearisation iterative expert-guided BH correction for heterogeneous specimens

This method [Ketcham and Hanna, 2014] requires an expert user to identify and choose some regions-of-interest (ROIs) that most clearly indicate BH artefacts in a reconstructed image. These ROIs ideally should include a single material or void space. These regions are used to construct a transform function, $f$, that transforms each polychromatic projection data, $P$, into the value it should be if the X-ray beam were mono-energetic, $M$, i.e., $M = f(P)$.

A set of uniform (evenly-spaced) nodes of splines are distributed over the range of $P$, with the endpoints of the function fixed to be endpoints of the data values. A cubic spline interpolates between these nodes.

Next, an iterative optimisation procedure, using a simplex method [Press et al., 1988], is used to estimate the the coefficients of the spline. In every iteration, the estimated coefficients are used to generate the transformed projection data, $M$. This projection is then reconstructed using the filtered back-projection algorithm (see section 1.2.7.3) and used to test the correction. The iterative process runs until the BH is minimised. This process is depicted the flowchart of Fig. 2.6.
§2.2 Beam hardening (BH) artefacts and correction techniques in CT

Data acquisition

Intensity images (projections)

CT image reconstruction

Choose ROIs

Re-projection; P

Fit the transform function \( M = f(P) \) with a cubic spline

Parameter extraction; coefficients of the spline

Generate monochromatic data; M

Corrected BH intensity images

CT image reconstruction

If accuracy condition not satisfied

If accuracy condition satisfied

Figure 2.6: Flowchart of the iterative expert-guided BH correction method (Section 2.2.2.2) [Ketcham and Hanna, 2014].

Draft Copy – 21 November 2016
2.2.3 Post-reconstruction iterative BH software correction methods

BH correction for multiple-material samples can be performed using a post-reconstruction iterative (PRI) approach. PRI methods begin with a preliminary reconstruction of the data, which is used to estimate the intersection length of each material with each X-ray path. These methods are mostly using \textit{a priori} information about the sample materials and the X-ray spectrum to start an iterative procedure, that provide an improved estimations of BH correction in each iteration and consequently correct the BH.

Although PRI methods can perform well in BH artefact correction for multiple-material samples, their iterative nature makes these methods computationally intensive.

Krumm et al. [Krumm et al., 2008] and Van Gompel [Van Gompel et al., 2011] improved the IPR method, respectively, by presenting the methods that eliminate the need for prior knowledge of the spectrum or material attenuations, and by an approach based on the physical model in that it’s assumed that spectrum can be represented in the form of small energy bins.

2.2.3.1 Post-reconstruction iterative, reference-less BH correction method

This BH correction method is called “reference-less” because it doesn’t require \textit{a priori} information about the spectrum or the constituent materials of the sample. This information is usually used to compute the mono-energetic and poly-energetic re-projections, instead, this information is obtained by segmenting the reconstructed image. A simple thresholding operation is used to segment the materials of the sample. The segmented maps of materials are then re-projected. Next, one can plot the propagation path lengths of the X-rays within the different materials and their measured intensity. This provides a N-dimensional BH curve for each material, that is fitted with a hyperplane for mono-energetic assumption (See Fig. 2.8a) and with hypersurface for poly-energetic assumption (See Fig. 2.8b). The difference between the mono-energetic and poly-energetic re-projections, \( P_{\text{correction}} \), is the correction that should be added to projection data, \( P_u \), to correct the BH, as follows:

\[
P_c = P_u + P_{\text{correction}}
\]

where \( P_c \) is the corrected projection. The entire correction process has an iterative nature and is shown in Fig. 2.7 [Krumm et al., 2008].
2.2 Beam hardening (BH) artefacts and correction techniques in CT

Data acquisition

Intensity images (projections) ($P_u$)

CT image reconstruction

Segmentation

Material 1
Material 2
Material 3

Re-projection
Re-projection
Re-projection

Plot N-dimensional BH curve; $N$ is the number of materials

Fit the BH curve with mono-energetic model assumption (Hyperplane); Fig. 2.8a
Fit the BH curve with poly-energetic model assumption (Hypersurface); Fig. 2.8b

The correction value ($P_{\text{correction}}$)

Corrected intensity images; Eqn. 2.3 ($P_c = P_u + P_{\text{correction}}$)

CT image reconstruction

If accuracy condition not satisfied

Figure 2.7: Flowchart of the iterative reference-less BH correction (Section 2.2.3.1) [Krumm et al., 2008].

Draft Copy – 21 November 2016
Figure 2.8: (a) shows the polychromatic and (b) the monochromatic approximation of the point cloud propagation path length versus ray sum plot of a two-material specimen, by a two-dimensional plane and surface with 400 nodes. Black dots indicate computed attenuation values [Krumm et al., 2008].
2.2.3.2 Post-reconstruction iterative BH correction based on a physical model

This method is similar to the method in section 2.2.3.1 in using the difference of mono-energetic and poly-energetic data as the correction, but requires \textit{a priori} information about the number of materials and number of spectrum energy bins. The spectrum can be represented with a small and predefined number of energy bins. The sample consists of a known number of different materials. The procedure includes segmenting the sample and assigning each pixel to one of the materials, assigning the energy bin and estimating the X-ray attenuation for each material for each of the energy bins. The parameter estimation is treated as an optimisation problem, minimising the difference between the observed measurements and the estimated projections. This process is iterative and is charted in Fig. 2.9 [Van Gompel et al., 2011].
Energy selective techniques

Data acquisition

Intensity images (projections) \((P_u)\)

CT image reconstruction

If accuracy condition not satisfied

Segmentation

Number of materials \((N)\)

Material \(\{1, 2, \ldots N\}\)

Simulate the projections

Number of energy bins \((E)\)

Mono-energetic simulated projections

Poly-energetic simulated projections

The correction value \((P_{\text{correction}})\)

Corrected intensity images; Eqn. 2.3 \((P_c = P_u + P_{\text{correction}})\)

If accuracy condition satisfied

Figure 2.9: Flowchart of the iterative physical energy distribution BH correction (Section 2.2.3.2) [Van Gompel et al., 2011].
2.3 Material characterisation in CT

The aim of this part of the research in this thesis, is to find an effective model to characterise the constituent materials of a sample, i.e., estimate the effective atomic number \( Z \) and density \( \rho \) of samples such as porous and complex material rocks from oil reservoir, using X-ray computed tomography.

Currently there are three main methods to estimate \( Z \) and \( \rho \) of sample materials; physical model, gamma absorption and dual-energy computed tomography. In this thesis, I used the dual-energy X-ray \( \mu \text{CT} \) imaging to estimate \( Z \) and \( \rho \) of materials. This method is more accurate and environmental condition doesn’t affect the results as much as other methods.

The identified approaches are based on dual-energy imaging, i.e., recording a sample twice by illuminating low-energy and high energy photons separately. Section 5.3.3 demonstrates modelling a dual-energy spectra. When performing dual-energy imaging, the attenuation coefficient should be accommodated accordingly. The attenuation coefficient can be presented as a linear combination of the basis functions and coefficients which are functions of energy.

As described in section 1.2.6, there are two main mechanisms by which X-rays interact with matter in a typical \( \mu \text{CT} \) X-ray energy range of \([10, 120]\) keV. The photoelectric absorption (PE; see section 1.2.5.1) is dominant at lower energies (e.g., less than 30 keV for biological materials but increases with atomic number) while Compton scattering (CS; see section 1.2.5.2) is more prevalent at higher energies. Alvarez and Macovski [Alvarez and Macovski, 1976] modelled the attenuation coefficient of a material as a two-basis function that characterises PE and CS. The material discrimination capability of dual-energy CT relies on the fact that PE depends strongly on \( Z \) and CS is proportional to \( \rho \). I calibrated and applied the full Alvarez and Macovski (AM) model in chapter 5.

The AM model has been used in various simplified forms [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi, 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2010; Kaewkhao et al., 2008]. The simplified form have been applied on either projection (see section 5.4.1) and reconstruction images (see section 5.4.2). Alvarez and Macovski [Alvarez and Macovski, 1976] presented the full intensity model but didn’t use it, instead, they simplified the model to polynomials to estimate \( \rho \) and \( Z \) values. Siddiqui and Khamees [Siddiqui et al., 2004] (SK) simplified the Alvarez and Macovski attenuation coefficient model (AMAC; see section 5.1) by assuming the data is collected at two monochromatic energies as follows:

\[
\mu_E = a_p^F \mu_p + a_c^E \mu_c, \quad E \in \{E_p, E_c\}
\]  

(2.4)
where $\mu_p$ and $\mu_c$ are the contribution of PE and CS to the total attenuation coefficient at their dominant energies, $E_p$ and $E_c$, respectively. I implemented the Alvarez and Macovski polynomial model (AMP) and SK models, subsequently, in section 6.2 and 6.3 to compare their results with that of the full model in chapter 5.

The SK model includes less computation, however, the estimated results using the SK model have significant deviation from the expected $\rho$ and $Z$ values. Derzhi et al., [Derzhi, 2012] presented a post-correction method for the SK model. Heismann et al. [Heismann et al., 2003] presented a source-weighting method for dual-energy material characterisation. These two methods are, respectively, studied in section 2.3.1 and 2.3.2.

Estimating the density and effective atomic number of a sample using the simplified forms doesn’t provide applicable information about the sample materials in an acceptable range of accuracy. One objective of this thesis is to use a full model, that consider the energy range of X-ray spectrum, to produce reasonable $Z$ and $\rho$ estimations of the rock sample materials and avoid the the long process of post-correction. Following this aim, the full Alvarez and Macovski model is used in chapter 5, along with a new method that is demonstrated in chapter 7.

### 2.3.1 Correction on Siddiqui and Khamees (SK) method

Derzhi et al., [Derzhi, 2012] applied a post-correction technique for the SK method using reference materials. Derzhi estimated the relative and absolute errors, $\epsilon$ and $\delta$, between the $\rho$ estimation provided by the SK method [Siddiqui et al., 2004] and the physical calculations. Next, he determined a functional relationship between the estimated $Z$ from the SK method and the estimated $\epsilon$ and $\delta$ values, to estimate the coefficients of that function for the system of reference materials. This is demonstrated in the flowchart of Fig. 2.10. Next, they applied these corrections to correct the $Z$ and $\rho$ estimations of target materials provide by the SK method, as shown in the flowchart of Fig. 2.11.
Data Acquisition; µCT imaging at $E_{1}^{max}$

Projections of reference material ($\omega = \{1,2,3\}$) at $E_{1}^{max}$

CT image reconstruction at $E_{1}$

SK model; Eqn. 2.4

Fit SK model on reconstruction images

Calibration parameter estimation

Calibrated SK model

Parameter estimation; $\rho$ and $Z$ reconstructed images

Estimated $\rho$ reconstructed images

Calculate $\rho = \frac{mass}{volume}$

Estimated $Z$ reconstructed images

Estimate $\epsilon$ and $\delta$ for $\rho$

$\epsilon$ and $\delta$

Estimate $Z$ as a linear function of $\epsilon$ and $\delta$

Coefficients of linear function

Go to Fig. 2.11(*)

Figure 2.10: Flowchart of estimation of the corrections to be applied on the SK method; with $\epsilon$ being the relative error and $\delta$ being the absolute error (Section 2.3.1) [Derzhi, 2012].

Draft Copy – 21 November 2016
Energy selective techniques

Data Acquisition; µCT imaging at $E_{1}^{\text{max}}$

Projections of reference material ($\omega = \{1, 2, 3\}$) at $E_{1}^{\text{max}}$

CT image reconstruction at $E_{1}$

SK model; Eqn. 2.4

Fit SK model on reconstruction images

Calibration parameter estimation

Calibrated SK model

Parameter estimation; $\rho$ and $Z$ reconstructed images

Estimated $\rho$ reconstructed images

Estimated $Z$ reconstructed images

Apply corrections

Corrected $\rho$ and $Z$ intensity images

Theoretical $\rho$ and $Z$ values of reference materials

Figure 2.11: Flowchart of applying the corrections of Fig. 2.10 on the SK method (Section 2.3.1) [Derzhi, 2012].

Draft Copy – 21 November 2016
2.3.2 Source-weighting method

Heismann et al., [Heismann et al. 2003] used the projection images recorded at two energy levels to quantitatively estimate $Z$ and $\rho$ of the materials of a sample such that:

$$
\begin{pmatrix}
\mu_1(\rho, Z) \\
\mu_2(\rho, Z)
\end{pmatrix}
\rightarrow
\begin{pmatrix}
\rho(\mu_1, \mu_2) \\
Z(\mu_1, \mu_2)
\end{pmatrix}
\tag{2.5}
$$

Substituting Eqn. 1.4 in the above equation, one can obtain:

$$
\begin{pmatrix}
\mu_1(\rho, Z) \\
\mu_2(\rho, Z)
\end{pmatrix}
= 
\begin{pmatrix}
K_1 \\
K_2
\end{pmatrix}
\begin{pmatrix}
g_1 \\
g_2
\end{pmatrix}
\cdot
\begin{pmatrix}
\rho \\
\rho Z^n
\end{pmatrix}
\tag{2.6}
$$

where $g_\epsilon = K_1 \int \frac{S_\epsilon(E) dE}{E^{\mu}}$. From there $\rho$ and $Z$ are calculated as the weighted difference of $\mu_1$ and $\mu_2$, and $Z$ as a non-linear function of the ratio of the $\mu_1$ as follows:

$$
\begin{align*}
\rho &= \frac{1}{K_2} \frac{g_2 \mu_1 - g_1 \mu_2}{g_2 - g_1} \\
Z &= \left( K_2 \left( \frac{1 - \frac{\mu_1}{\mu_2}}{\frac{g_2}{g_1} - \frac{g_1}{g_2}} \right) \right)^{\frac{1}{n}}
\end{align*}
\tag{2.7}
$$

Figure 2.12 (a) shows $Z$ as a nonlinear function of the ratio of dual-energy attenuation coefficients and Fig. 2.12 (b) shows $\rho$ as a weighted difference of attenuation coefficients at two energy spectra.
Figure 2.12: Plots of the numerical results of $Z$ and $\rho$ projections: a) shows a function, $F(Z) = \frac{\mu_1}{\rho}$, and b) shows $\rho(\mu_1, \mu_2)$ for recorded images at 80 and 140 keV ($\mu_1$ and $\mu_2$ are normalised to CT values $C$; where $C = 1000 \times \frac{\mu - \mu_{\text{water}}}{\mu_{\text{water}}}$. [Heismann et al., 2003].
2.4 Conclusion

This chapter described the two main energy related issues in μCT: 1) BH and 2) material characterisation. Several energy selective techniques have been surveyed, that lies in this two main categories. These methods should consider the polychromatic nature of the X-ray source and energy dependency of attenuation coefficient.

Standard tomographic reconstruction algorithms assume monochromatic radiation. Ignoring the polychromatic nature of the radiation in reconstruction produces inconsistent attenuation coefficient values in the tomogram which is identifiable in the form of cupping and streaking artefacts. Section 2.2 reviewed the description of the BH artefact and many available techniques for its correction.

Section 2.3 included the energy selective methods to characterise the constituent materials of a sample. X-ray interactions with matter and lower and higher energies occur in form of PE and CS (see section 1.2.6). As a consequence, imaging a sample at two energy spectra provides information relevant to PE and CS effects, which in turn, correspond to atomic number and density of sample materials, thus, making material characterisation possible. Both approaches improve images such that segmentation is possible.

In future chapters of this thesis, I implemented several mentioned methods of this chapter. The results of these implementation are compared with the results of the developed methods in this thesis, to assess the accuracy and applicability of the methods. For BH correction, chapter 3 includes implementation of several linearisation BH correction models including some models mentioned in this chapter. In chapter 4, I am using the most appropriate model of chapter 3 to correct the BH of nested-cylinders. For material characterisation methods, I have implemented AMP and SK models of this chapter, in chapter 6. As previously discussed, all the previous application of AM model were using a simplified form that because of its limitations and the considerable computation required. I have calibrated and used the full AM model in chapter 5. The results of this chapter is compared with the results of SK and AMP model in section 6.
Assessment of several linearisation X-ray beam hardening correction methods

3.1 Introduction

Micrometer-scale computed tomography (µCT) systems (see section 1.2) in the laboratory use a micro-focus X-ray source (see section 1.2.3.1) that emits polychromatic (Bremsstrahlung) radiation (see section 1.2.3). As mentioned in section 2.2, low-energy X-rays are attenuated more readily as the X-ray beam passes through a sample, causing the resulting X-ray beam to have a higher proportion of high-energy X-rays, i.e., X-ray beam-hardening (BH). Therefore the total attenuation, given by Beer-Lamber law in Eqn. 1.2 is no longer a linear function of material thickness. This effect can produce severe BH artefacts, including cupping and streaking artefacts, in the reconstructed images. Apart from these visual aspects, quantitative problems may arise, thus, these artefacts make subsequent tomogram segmentation and analysis difficult.

There are a number of techniques that can be used to correct this artefacts (see section 2.2). BH can be reduced by physically filtering the beam, effectively pre-hardening the beam (see section 2.2.1). However, sometimes sufficient filtering is not used or may not be feasible due to reduced X-ray flux. In these cases, the use of some form of software correction method is required. Several correction methods have been developed that apply a linearisation curve (see section 1.2.6.1), called BH curve. The BH curve is the nonlinear relationship between sample thickness and the measured intensity. It can be measured or estimated and fitted using a BH model, e.g., a polynomial [Herman, 1979]. The inverse of the BH curve is applied to remap the measured intensity. In order to directly measure the curve, one can image some kind of wedge phantom [Van de Casteele et al., 2002; Herman, 1979]. Methods to estimate the curve without imaging phantom are typically iterative and computationally intensive (see section 2.2.3), therefore, I chose to work with BH curves to correct the data captured using ANU µCT facility [Sakellariou et al., 2004].
In this work, I considered using cylindrical specimens, e.g., brines that are imaged in a cylindrical container. This assumption covers a significant fraction (> 50%) of the specimens currently imaged at ANU µCT facility. Section 3.2.1 describes how to generate BH curves directly from the projection data of a homogeneous cylindrical specimen, similar to that obtained by imaging wedge phantoms. Section 3.2 plots the BH curves of several frequently used samples at the ANU µCT facility to view the nonlinear trend of beam hardened data versus the sample thickness. The BH curve is applied in linearisation methods to correct the BH artefacts. An overview of the existing linearisation BH correction methods in tomography is presented in section 1.2.6.1. Here I am implementing two of the mentioned non-iterative linearisation methods: the polynomial model [Herman, 1979] in section 3.3.1 and the bimodal energy model [Van de Casteele et al., 2002] in section 3.3.2. This is followed by a study of three further BH models including the power law model in section 3.3.3 [Paziresh et al., 2013], the cubic spline model [Ketcham and Hanna, 2014] (see section 2.2.2.2) in a non-iterative form for the homogeneous samples of this chapter in section 3.3.4, and finally a linear spline model in section 3.3.5 that is an extension of the bimodal model [Van de Casteele et al., 2002]. These techniques will be investigated to determine the most appropriate model to be used at the ANU µCT facility for correction of artefacts caused by beam hardening. Section 3.4 covers the performance assessment of the reviewed methods.

This research has been carried out within the “Computed Tomography” group of the Applied Mathematics Department at the Australian National University (ANU). I applied the linearisation models and performed the assessment to find out the most appropriate model for BH correction of cylindrical samples at ANU µCT facility. A survey of the applied models in this chapter is in preparation for publication with the title and author list as follows:


The linearisation BH correction only is applicable for homogeneous samples because different materials attenuate X-rays differently and thus have different BH curves. From the five models described in this chapter, I have chosen one with the lowest error and least number of parameters to estimate to correct the BH of the heterogeneous (concentric) cylinders in chapter 4. That research was presented at the International Conference on Tomography of Materials and Structures 2013 (ICTM 2013). As explained in section 3.2.2, the brine containers used in the department are mostly made of polyoxymethylene, which is a low density material. However, if a container is made of a high density material, because X-rays pass through more material at the edges than the centre of the container, in a fan beam radiation, an inverse BH effect is evident in the tomogram, that intensifies the difficulties in segmentation. For the correction of
this effect, we refer to:


3.2 Measuring beam hardening curves

This section includes demonstration of imaging the wedge phantoms in section 3.2.1 and plotting the BH curves of the most commonly used samples at the ANU µCT facility in section 3.2.2.

3.2.1 Wedge and cylinder phantoms

Generally, for linearisation a wedge (or step wedge) phantom is used as the sample, i.e., a series of contiguous, uniformly shaded rectangles, arranged progressively from smallest to largest thickness. This process is used to test the characterisation of the X-ray beam. When X-rays are passing through the wedge, the recorded intensity is consequently growing progressively darker from white (or light grey) at the thinnest end to black (or dark grey) at the thickest end of the wedge. In this sense, the recorded intensity of a wedge phantom is proportional to the thickness of the sample, thus it can directly measure the BH curve. A cylinder can be considered as a combination of two wedge phantoms, one growing from one edge of the cross-section of the cylinder (circle) to the maximum thickness that is centre of the circle and the second from the centre to the other edge. Figure 3.1 shows that the softer part of the X-ray spectrum is becoming more attenuated as the beam passes through more thickness of sample. This means that the beam is more hardened, thus, the recorded projections on the detector using this arrangement shows the effect of BH (see section 2.2) and can directly produce the BH curve (the dashed blue line). This figure also shows the expected projection of the cross-section of the cylindrical sample without BH (the black line). Note that since this research involves imaging the cylindrical samples, the measured projections can directly provide the BH curve.
Assessment of several linearisation X-ray beam hardening correction methods

3.2.2 Beam hardening curves of common materials at the ANU µCT facility

This research includes imaging several solid materials and several fluids (oil/water) with different salinity concentrations in cylindrical containers. These samples are most commonly used in the department. As explained in section 3.2.1, the BH curves can be directly measured from the cylindrical samples. These BH curves were used for BH correction using the five different BH linearisation models in section 3.3 to determine the most appropriate model for ANU µCT facility [Sakellariou et al., 2004] based on the accuracy of the BH corrections.

For the imaging involved in this research, I used a system that consists of the “X-tek system limited RTR 225 keV” X-ray tube that has 2 µm tungsten target material and 0.5 mm beryllium window. The detector was a Perkin Elmer “XRD 1621 scintillator-based area detector” [PerkinElmer, 2012] with 2048 × 2048 (width × height) pixels with square pixel width 0.2 mm. The camera length, i.e., source to detector distance (CL) was 1000 mm and sample to detector distance, i.e., sample distance (SD) was 20 mm for our imaging geometry (shown in Fig. 1.5). I imaged the samples at 80 keVp tube voltage with X-ray current of 100 mA and exposure time of 4 seconds for all cases. The tube container used for all samples was polyoxymethylene with the chemical structure of \((CH_2O)_n\) with 0.5 mm wall thickness and 6 mm radius inside the container.

Figure 3.1: Illustration of the BH (i) the quantitative measurement of source with different filters corresponding to the thickness of the shown sample \(S_1 = 0.5\) mm and \(S_2 = 2\) mm Al filter), and (ii) schematics drawing of beam hardened and the ideal projection.
Samples with different salinities have been chosen for imaging to compare the changes in BH curves with the change of the salinity concentration of the samples. The BH curves visualise the nonlinear BH effect versus sample thickness for these materials (see Fig. 3.4). The samples are CsI, NaI and CsCl with 0.1, 0.19, 0.25, 0.357, 0.5, 0.75, 1, 1.5, 2 molarity (M), BrC8 in oil with 2.5, 5, 10, 20 and 100 M of BrC8, 100 M of BrC10, 100 M of BrC11, 100 M of BrC14, and diodomethane (C2H2I2) with different salinities (IC6, IC8, IC10).

The BH curve required calculation of the attenuation of samples (Beer-Lambert law; see section 1.2.6). As shown in the Beer-Lambert law in Eqn. 1.2, the attenuation of an X-ray is defined as $-\ln\left(\frac{I}{I_0}\right)$ where $I$ is the intensity of a beam with the sample present, and $I_0$ is the intensity of the beam with no sample present, known as the clear field, i.e., $-\ln\left(\frac{I-I_{DF}}{I_{CF}-I_{DF}}\right)$. I measured dark field, clear field and the projections of the samples. Images needed to be registered before linearisation. The sample projection image were centred and the clear field image, that contains the projection of the container which is common to all measurements, were scaled to match the sample projection image. The brine image is scaled in both horizontal and vertical directions for better match of the images. Next, I fitted the measured projection data, $P$, with an ideal projection of a cylinder to estimate the radius, $R$, centre of the images as follows:

$$\minimise \sum_{\omega} \| P^\omega - \alpha \times \sqrt{(R^2 - (x - x_c)^2 - y_c)^2} \|^2. \quad (3.1)$$

where $P$ is the projection of the sample, $\omega$, [see figure 3.1(ii) dashed blue line] and $x$ and $y$ are the horizontal and depth axes of the cross-section of cylinder samples (the projected circle), $x_c$ and $y_c$ are the distance to centre in horizontal and depth axes if the sample is not aligned and $\alpha = 1$ for a circular cylinder. Using the estimated $R$, the images are shifted by $x_c$ to centre them.

I imaged the container tube in the clear field image. Since linearisation BH correction method is only possible for homogeneous samples, the BH curve should only plot the intensity relevant to the sample inside the container and thus I removed the information around the fitted sample cylinder. The linearisation of Eqn. 1.5 removes the direct effect of container on the sample projection image, since identical container tube or filtering is present for $I$ and $I_0$. However, the indirect effect on intensity by altering the beam spectrum, i.e., hardening the beam, is still present.

Figure 3.3 shows a fan beam arrangement with three different types of filtering and the variations that occurred on the spectra of X-rays. If we place a cylindrical sample in-line with these filters in the imaging geometry of Fig. 1.5, the beam that passes through the edges of a cross-section of a cylindrical sample (a 1D circular projection shown in Fig. 3.1(ii)) is more attenuated than the beam that passes through the centre of the sample, i.e., an inverse cupping artefact. Container tubes can have a simi-
lar effect as seen in Fig. 3.3 ii, though the degree to which the cupping and inverse cupping effects influence the sample is dependent on the attenuation, thickness and fan angle. The inverse cupping effect is not as dramatic for the flat sheet filtering (see Fig. 3.3 ii) as it is for the cylindrical containers (see Fig. 3.3 iii) because the X-ray path lengths show less variation for flat sheet filters. Within this chapter, to better view the BH effect, a hardware filter has not been used. Also this chapter uses the most common container tube in the department, polyoxymethylene, which is a low-attenuating material. There is a slight distortion in the edges of the projection of the brine/rock data that I cropped and extrapolated. For further information about the samples consisting of a high density containers, please refer to [Holt et al., 2014].

After alignment, the linearised intensity images are calculated as in Eqn. 1.5. To form a BH curve directly from the cylindrical sample (see section 3.2.1), I calculated the thickness \( s \) of the cylindrical samples, as the beam is passing through; from one edge of the cross-section of the cylinder (circle) to the centre (maximum thickness; \( 2R \)) and from the centre to the other edge (as shown in Fig. 3.2) as follows:

\[
\begin{align*}
B &= \arctan\left( \frac{x}{CL} \right), \\
h &= SD \times \sin(B),
\end{align*}
\]

therefore,

\[
\begin{align*}
s &= 2 \times \sqrt{R^2 - h^2}; & h < R, \\
s &= 0; & h > R.
\end{align*}
\]

Figure 3.2: Schematic of plotting the BH curve, i.e., the intensity of the projection versus the path length of X-ray (s) for a cylindrical sample.

This allowed a table of the recorded projection of a cylinder on the detector with relevant thickness to serve as the BH curve as shown in Fig. 3.4. This figure shows that the higher attenuating material with higher density produces more BH compared with the lower molarity and less dense (lower effective Z) materials. In section 3.3, I used the BH curve of CsI calculated in this section and applied several linearisation models on the beam hardened data. The inverse of the models were remapped on the data to correct the BH artefact.
Figure 3.3: The attenuation of the X-ray spectra using different filters or container, as the beam is passing through the sample. This plots are quantitative measurement of source with different filters corresponding to the thickness of the shown sample: (i) $S_1 = 0.5\text{mm}$ and $S_2 = 0.5\text{mm Al filter}$, (ii) $S_1 = 0.5\text{mm Al}$ and $S_2 = 1\text{mm Al filter}$, (iii) $S_1 = 0.5\text{mm Al}$ and $S_2 = 2\text{mm Al filter}$. 
Figure 3.4: BH curve of (i) NaI, (ii) CsI, (iii) CsCl, (iv) 100 per BrC, (v) BrC₈ in oil, and (vi) IC₉ with different salinities.
3.3 Fitting BH curve models and performing BH correction

As mentioned in section 2.2, the softer beam that passes through the edges of a cylindrical sample is attenuated more as its travels through the denser part of the cylinder, i.e., the centre (see Fig. 2.2). This forms a concave shape in cylindrical samples, and thus is called cupping artefact. It is clear that the BH artefact becomes more severe for higher attenuating materials, such as 2M CsI. For that, from the available samples for which I plotted the BH curves in section 3.2.2, I chose to show the plot of the 2M CsI brine in a cylindrical container to demonstrate of the model fits on the BH curve and the BH corrections, in this section, although all of the samples mentioned in section 3.2.2 have been considered for the assessment of the models.

Figure 3.5 shows the 2D reconstruction of the uncorrected 2M CsI projection using the filtered back-projection. The horizontal profile though the centre of image (dashed blue line) shows the cupping artefact. All the reconstructions of this chapter are from one symmetrical radiograph and so are very noisy. Due to lack of experimental data at the time of this study, a single radiograph used. Since the same noise is copied to the all projection angles, the ring artefacts are evident in the cross-sectional reconstructed image as shown in figure 3.5. However, to assess the accuracy of the BH methods in section 3.4, the average root-mean-square error of the images are calculated. Similar to Fig. 3.5, within all the reconstructions of this chapter, the dashed blue line gives the location of a profile though the uncorrected reconstructed image of the sample, to be compared with the corrected reconstructions.

<table>
<thead>
<tr>
<th>(i)</th>
<th>(ii)</th>
</tr>
</thead>
</table>

![Image](image.png)

Figure 3.5: A cross-sectional reconstructed uncorrected image of 2M CsI in cylindrical container.

Section 3.3 covers a study of five different models that have been fitted on the BH
Assessment of several linearisation X-ray beam hardening correction methods

curve including 1) polynomial [Herman, 1979], 2) bimodal [Van de Casteele et al., 2002], 3) power law behaviour [Paziresh et al., 2013], 4) cubic spline [Ketcham and Hanna, 2014], and 5) linear spline in sections 3.3.1 to 3.3.5 respectively. These models are fitted on the estimated BH curves of the samples of section 3.2.2. If the inverse of these models are applied to the beam hardened data, the resultant BH curve should find a linear trend, as expected in the monochromatic case, which means the BH artefacts are corrected. Figure 3.6 shows a general picture of the linearisation BH correction process.

Figure 3.6: Flowchart of linearisation BH correction. The BH curve of samples can be obtained having prior knowledge of sample shape, i.e., wedge or cylindrical specimens of uniform composition, i.e., homogeneous samples (see section 3.2.1 and Fig. 3.1 and 3.2).
3.3.1 Polynomial model

Herman et al., [Herman, 1979] modelled $P = \mu(s)ds = -\ln\left(\frac{l-l_{DF}}{I_{CF}-l_{DF}}\right)$, as a polynomial function of $s$, the X-ray path length from one-edge of the cylinder to the centre and from the centre to the other edge through the thickness of the sample material, as follows:

$$P(s) = \sum_{i=0}^{n} a_i s^i$$

(3.4)

The attenuation of air is negligible. For small beam hardening artefacts, a lower-order polynomial is sufficient [Herman, 1979]. However, for more severe artefacts as in denser materials, polynomial degrees of four, six, or eight are required [Hammersberg and Måns, 1998]. In this process, the coefficients can be estimated by simply using a least square fit between the polynomial model, $P(s)$ in Eqn. 3.4, and the measured data, $P$, as follows:

$$\min_{\{a_i\}} \sum_{j=-R}^{R} \| P(s) - P \|^2.$$  

(3.5)

where $R$ is the radius and $j$ is the variable of summation. Once the polynomial coefficients are calculated, it is also easy to correct the BH effect by applying the inverse of the polynomial model to the measured data. The corrected projections are reconstructed using filtered back-projection (see section 1.2.7.3). Figure 3.7 shows the BH curve of the 2M CsI sample and a polynomial of order eight fit on the measured data. Figure 3.8 shows the reconstructed image after applying the polynomial model of degrees four, six and eight and a line through it to show the correction. The fitting results has almost equal root-mean-square (RMS) error between the corrected images and a smooth disc with an average attenuation value for the prediction, $\mu_{avg}$, for degree four and six, but a slightly lower error for degree eight. The RMS error is calculated as $\sqrt{\frac{1}{n} \sum_{j=1}^{n} (\mu_j - \mu_{avg})^2}$ where $n$ is the number of image pixels of the cross-section of the cylinder.

![Figure 3.7: Plot of the uncorrected (main) data, polynomial of order eight fit and the corrected (linearised) data](image-url)
Figure 3.8: (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the polynomial model of order (a-four, b-six, c-eight), (ii) profile through the centre of the uncorrected (blue line) and corrected (red line) images.
3.3.2 Bimodal energy model

The bimodal model [Van de Casteele, 2004] has taken the physical photoelectric absorption (PE) and Compton scattering (CS) phenomena (see section 1.2.5) into consideration for the two energy regions, \(E_1\) and \(E_2\). Having Eqn. 1.3 and considering a dual-monochromatic radiation at PE and CS energy regions, Eqn. 1.2 can be re-written as:

\[ -\ln\left(\frac{I}{I_0}\right) = -\ln\left(\frac{AE_1e^{-\mu_p\tilde{s}} + AE_2e^{-\mu_c\tilde{s}}}{A_{E_1} + A_{E_2}}\right) \]  

(3.6)

where \(\mu_p = \mu(E_1)\), \(\mu_c = \mu(E_2)\). Because this model assumes a dual-monochromatic radiation, \(A_{E_1}\) and \(A_{E_2}\) are constants. Where in this thesis the polychromatic nature of spectrum, is considered, it's introduced by \(S(E)\) that is the incident X-ray energy spectrum modulated by detector quantum efficiency and attenuated by the non-sample materials between source and detector (see section 5.3). As mentioned in this section, \(A\) is monochromatic assumption of radiation at a specific energy and therefore is a constant. Having \(\alpha = \frac{A_{E_1}}{A_{E_2}}\), Eqn. 3.6 can be written as:

\[ -\ln\left(\frac{I}{I_0}\right) = -\ln\left(\frac{\alpha e^{-\mu_p\tilde{s}} + e^{-\mu_c\tilde{s}}}{\alpha + 1}\right) \]  

(3.7)

Using basic rules of logarithmic equations, Eqn. 3.7 can be re-written as:

\[ P(s) = -\ln\left(\frac{I}{I_0}\right) = \mu_c\tilde{s} + \ln\left(\frac{1 + \alpha}{1 + \frac{1}{\alpha}e^{-\left(\mu_p - \mu_c\right)\tilde{s}}}\right) \]  

(3.8)

This equation shows that for the small thicknesses, the equation between the measured data and the sample thickness is linear. PE is dominant at lower energies so the first section of Eqn. 3.8 is valid for the lower energy beam. CS is dominant at higher energies where the beam is more attenuated and the second section of the Eqn. 3.8 is valid for the higher energy beam. I used the model in Eqn. 3.8 to fit on the BH curve of 2M Csl in a least square manner of Eqn. 3.5 to estimate \(\mu_p\), \(\mu_c\) and \(\alpha\). Figure 3.9 shows the bimodal model fit to the measured data and Fig. 3.10 shows the corrected reconstruction after applying the inverse of the bimodal model to the measured data and a line through the corrected reconstruction.
Assessment of several linearisation X-ray beam hardening correction methods

Figure 3.9: Plot of the uncorrected (main) data, bimodal fit and the corrected (linearised) data

Figure 3.10: (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the bimodal model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.
3.3.3 Power law model

Figure 3.11 shows the BH curve of aluminium and glass imaged at 80 keV. The linear nature of the log-log plot in Fig. 3.11 shows that a simple power law behaviour can indeed serve as an appropriate BH model. Therefore the measured projection data can be modelled as a power law relation with the thickness of the sample, as follows:

\[ P(s) = as^k \]  

(3.9)

The least square fit between the measured data and the power law model optimises the \( a \) and \( k \) values for a single cylinder. I applied the inverse of the power law fit to remap the data and achieve the linearised data. Figure 3.12 illustrates how well the power law model corrected the cupping artefacts with only two parameters to be estimated. The RMS error of the applied power law BH correction method compared to a smooth disc is estimated to be \( 0.642 \times 10^{-1}\% \). Figure 3.13 shows the BH correction using the bimodal model.
Figure 3.12: Plot of the uncorrected (main) data, power law fit and the corrected (linearised) data

Figure 3.13: (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the power law model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.
3.3.4 Cubic spline model

A spline possesses a high degree of smoothness where the polynomial-pieces connect (nodes) and is popular because of their accuracy of evaluation and capacity to approximate complex shapes through curve fitting. Ketcham and Hanna [Ketcham and Hanna, 2014] introduced a method that applied cubic spline interpolation of a set of uniform nodes over the data range to correct the BH of heterogeneous samples (see section 2.2.2.2).

This chapter includes the BH correction of homogeneous cylinders, thus, a non-iterative linearisation would be sufficient for BH correction of these samples. We aim to apply the chosen model of this chapter and apply it for correction of nested-cylinders in the next chapter. As such, the BH curve is modelled with piecewise polynomials $P_1, P_2, ..., P_k$ as follows:

$$
\begin{align*}
P(s) &= P_1(s), \quad s_0 < t < s_1; \\
P(s) &= P_2(s), \quad s_1 < t < s_2; \\
& \quad \vdots \\
P(s) &= P_k(s), \quad s_{k-1} < s < s_k
\end{align*}
$$

(3.10)

Figure 3.14: Plot of the uncorrected (main) data, spline fit and the corrected (linearised) data.

I used a cubic spline with the number of nodes that can varied from one to the value that provides smoothness. Splines with few nodes are generally smoother than splines with many nodes, however, increasing the number of nodes usually increases the fit of the spline function to the data. I used non-uniform nodes to give the
curve freedom to bend where required. Figure 3.14 shows the spline fit to 2M CsI BH curve. The inverse of the model is numerically remapped to linearise the data. Fig. 3.15 shows the reconstruction of the BH corrected data. Similar to previous sections, the corrected projection is reconstructed using filtered back-projection and the RMS error of the reconstructed image compared to a disc with an average value of corrected image is calculated to be $6.36 \times 10^{-1}\%$ RMS error.

![Figure 3.15](image)

Figure 3.15: (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the spline model, (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.

### 3.3.5 Linear spline model

This is the approximation and extension of the bimodal mode. I segmented the BH curve into number of non-uniform, linear spline using with the first and end values borrowed from the uncorrected measurements. I applied a brute-force search on the model-data fit to find the optimal connecting point (nodes) through the length of the data, and modelled the data as follows:

$$
\begin{align*}
  P(s) &= a_1(s) + b_1, & s_0 < s < s_1, \\
  P(s) &= a_2(s) + b_2, & s_1 < s < s_2, \\
  &\vdots \\
  P(s) &= a_k(s) + b_k, & s_{k-1} < s < s_k
\end{align*}
$$

(3.11)
Figure 3.16: (i) A cross-sectional reconstruction of 2M CsI in a cylindrical container corrected by applying the linear spline model with (a-2_lines, b-3_lines), and (ii) profile through the centre of the uncorrected image (blue line) and the corrected image (red line) image.
Bimodal model consider the dual-monochromatic radiation for PE at lower energies (e.g., less than 30 keV for biological materials but increases with atomic number) and CS at higher energies. The PE and CS have an overlap in energy range [30, 80] keV. Here, I decided to fit a linear spline on the data in three regions and see how the tri-linear piecewise functions fitting model responded for BH correction as shown in Fig. 3.16(a) and 3.16(b). This model still has reserved its linear trend and better results are expected by dividing the energy range into more bins. Figure 3.16 shows the BH correction using this model (red line) and the uncorrected data (blue line).

The next section compares the reconstruction of the corrected and uncorrected data to determine the efficiency of the above mentioned linearisation BH correction models to identify the most suitable BH linearisation model for the ANU μCT facility.

3.4 Performance assessment of the applied linearisation BH correction models

After investigating five different models for BH correction I found that the spline model, has the lowest error, followed by the eight order polynomial model, then power law model with very slight differences. The overall models mentioned have compensated the BH effect well, which is expected since this is a single material. Figure 3.17 shows the RMS error chart of the applied models.

![RMS Error Chart](image)

Figure 3.17: The average RMS error of corrected images compared with uniform disc.

Using the BH linearisation method produced a good correction method but the majority of them i.e., polynomial, power law and spline models, had no physical background. Furthermore, higher degree polynomials produce better fit, but also caused an increase in the number of parameters to be estimated. Bimodal considered PE and CS energy region and fitted the BH curve differently for in the BH curve but the
results were found to be noise sensitive. Even though spline and power law models don’t have a defined physical background, the correction result was superior. The polynomial of degree eight requires estimation of nine parameters and cubic spline require four parameters for each spline, while power law has the least number of parameters to be estimated, only two. Considering the small difference in the applied BH correction, power law is performing as a good, simple model for ANU μCT system.

3.5 Conclusion

As mentioned in chapter 2.2, there are three main methods for BH correction. Firstly, hardware filtering that only offers a reduction of the problem. Secondly, iterative software correction methods that are computationally unfeasible, therefore, the main procedure under investigation in this chapter is linearisation technique from which I chose five different BH correction models including: 1) bimodal, and 2) polynomial, 3) power law behaviour, 4) cubic spline, and 4) linear spline models. Every value on the models is corrected towards the linear trend line, which is expected in the monochromatic case.

To prepare the data, several solid materials and several fluids (oil/water) with different salinity concentrations as well as other materials has been imaged at the ANU μCT facility. Materials which have the most usage in our imaging system have been used as samples. Higher salinity, and thus higher effective atomic number, leads to more severe hardening of a beam as it passes though the sample material. Different materials and salinity levels have been chosen for imaging to visualise their BH effect. CsI , NaI and CsCl with 0.1, 0.19, 0.25, 0.357, 0.5, 0.75, 1, 1.5, 2 M, BrC₈ in Oil with 2.5, 5, 10, 20, and 100M of BrC₈, 100M of BrC₁₀, 100M of BrC₁₁, 100M of BrC₁₄, and IC₆, IC₈, IC₁₀ have been imaged at the ANU μCT facility separately. This chapter included measurement the BH curves of cylinder samples directly from their projections versus thickness of the cylinder and fit the BH curves with the five mentioned models. Next, the inverse of the model remapped to linearise the data. Finally, this section determined the model which has average lowest error for all the materials and salinities that used in this chapter.

I acknowledge the existence of ring artefacts that was introduced in section 3.3 in the RMS error estimations of table 3.17 however these errors are estimated using the same images for all applied BH models. Also the measured errors are already small. Furthermore, the main focus of this study about assessing the accuracy of the applied models could be presented in section 3.4 Therefore in this case, the ring artefacts can be ignored.

For the assessment of the applied BH model, we note that the bimodal model is
the only model that has a physical background by considering the PE and CS energy regions, and so the bimodal model fit the BH curve with different models in PE and CS energy regions. The linear spline model was introduced as the approximation and extension of the bimodal model. These models were found to be noise sensitive. Even though the spline, power law, and polynomial models don’t have a defined physical origin, they were found to have the lowest RMS errors, respectively, $6.36 \times 10^{-1}\%$, $6.24 \times 10^{-1}\%$, and $6.41 \times 10^{-1}\%$ on average for all the materials and densities that I investigated (see Fig. 3.17). Considering that only two parameters must be estimated in the power law model, and the small difference in error when using the power law model when compared to the spline and polynomial models, supports the statement that the power law model is a good and simple model for the ANU μCT system. However, spline is the most accurate model for complicated and heterogeneous specimens.
4.1 Introduction

As described in section 2.2, X-ray beam-hardening (BH) effect produces artefacts in form of cupping or streaking artefacts in the reconstructed images. As a result, the quantitative analysis and specifically segmentation will be very difficult. The amount of BH varies depending on the material composition of the specimen and the incident X-ray spectrum. In section 3.2.2, I measured the BH curve of several single-material cylindrical specimens, using ANU μCT facility [Sakellariou et al., 2004], and plotted their BH curves. Next, in section 3.3, I used five BH linearisation models to linearise the data and assessed the accuracy and applicability of the models for ANU μCT in section 3.4.

This chapter considers the specimens composed of nested-cylinders, e.g., a rock core within a container and uses the chosen model of chapter 3 to correct the BH artefacts of these specimens. As mentioned in section 3.1, this assumption covers a significant fraction (> 50%) of the specimens currently imaged at ANU μCT facility. By assuming a uniform material for each cylinder, one can generate BH curves directly from the projection data in a manner similar to that obtained by imaging wedge phantoms described in section 3.2.1. Here, I demonstrate the principle for concentric multi-component cylinders using the power law model (see section 3.3.3). The work presented here is complementary to the BH correction method previously developed by Kingston et al., [Kingston et al., 2012] in our group at ANU, that minimises re-projection distance (see section 1.2.6.1). That method enforces self-consistency in the data but does not work for objects where attenuation is a function of radius.

This chapter shows 1) how to determine the centre and radius of the cylinders of nested-cylinders in section 4.2, 2) generate BH curves using these cylinder parameter values in section 4.3, and 3) how to linearise the projection data of the nested-
cylinders by fitting a power law model to the BH curves in section 4.4. Section 3.5 demonstrate that the BH artefacts are significantly reduced in the tomographic reconstructions resulting from these corrected projections.

This research has been carried out within the “Computed Tomography” group of the Applied Mathematics Department at the Australian National University (ANU). I am the first author of a conference proceeding publication in the “Proceeding of the 1st International Conference on Tomography of Materials and Structures (ICTMS 2013)”. I have applied the beam hardening corrections on the samples and prepared the manuscript. In relation to estimation of the radii of cylinders that are used in beam hardening correction of multiple nested-cylinder specimens, I sought the advice of Dr Shane Latham. This research is published with the title and author list as follows:


4.2 Fitting the cylinder (or circles)

Here, we are considering specimens consisting of nested-cylinders. This could, for example, simply be a single cylindrical rock core, or a three cylinder system such as a rock core encased in a cylindrical container filled with high contrast fluid.

For the proposed method to work, the cylinder edges must be accurately determined. The circles are nested into each other, however, we don’t expect an ideal concentric form. To discover the centres $c_i$ and radii $R_i$ defining the edges, a minimisation problem is solved, where the cost function is defined as the sum of the dot products of the reconstructed-image gradient with the circle normals divided by the distance to the circle perimeter as follows:

$$C_{circ}(R, c) = \frac{G(i). (i - c)}{\|i - c\| \left(\|i - c\| - R\right)^2}. \quad (4.1)$$

Here $G(i)$ is the reconstructed-image gradient vector at pixel $i = (i_0, i_1)$. Powell minimisation was used to discover local minima of this cost function, employing multiple starts, where the starting radii were varied from 10% of the image width to 50% of the image width. The starting centre coordinate for the Powell optimisation was the centre coordinate of the reconstructed-image. From the multiple local minima, the best $n$ circles are chosen as those that have the lowest associated cost values and are also non-coincident (i.e. radius and centre coordinate differ by more than one pixel).
4.3 Fitting material attenuation

The projection of $n$ nested-cylinders is modelled by $2n - 1$ solid cylinders. A hollow cylinder can be modelled as the projection of a cylinder with its outer radius and attenuation $\mu$ along with the projection of a cylinder with its inner radius and attenuation $-\mu$.

An initial estimate for $\mu_i$ can be considered as the mean attenuation value in the reconstructed image of the $i^{th}$ cylinder region. An improved estimate of the attenuations can be obtained by optimising the match between the true-specimen projections and the nested-cylinder projections. One could potentially use the same minimisation approach to additionally fit the circle parameters and avoid the need for the reconstructed image (gradient) in the cost function, as in Eqn. (4.1). However, true-sample non-uniformity, particularly at the inner true-sample boundary, tend to bias the solution and result in poor circle fits for porous samples.

4.4 Fitting the beam hardening correction model

As outlined in the introduction, the BH curve is modelled as a linear combination of $n$ power laws for $n$ cylinders as follows:

$$P_{bh} = a_0P_{k0}^0 + a_1P_{k1}^1 + ..., \quad (4.2)$$

where $P_i$ are the estimated linear projection data per-cylinder/material and $P_{bh}$ is the beam hardened projection produced by the curve. The $(a_i, k_i)$ parameters are fit by minimising the least square error of measured projections and the uniform-attenuation nested-cylinder model beam hardened projections. This model works from the outside of the nested-cylinder where I progressively identify the exponents and attenuation for each cylinder and then subtract its attenuation from the projections. This allows the next inner cylinder to be analysed in isolation. The subtraction and subsequent addition is done in linearised projection space which makes the calculation of Eqn. (4.2) valid.
4.5 Applying the beam hardening correction

This section applies the model of section 4.4 for BH correction of two single cylinder specimens with non-uniform texture in section 4.5.1 and a nested-cylinder specimen in section 4.5.2.

The specimens of this section are imaged at 80 kVp with X-ray current of 100 μA with exposure time of 4 seconds, using the source and detector set-up described in section 3.2.2. The projections were imaged at 2880 angles. I linearised the projection data and applied alignment [Kingston et al., 2011], auto-focus [Kingston et al., 2010], drift correction [Myers et al., 2011]. The reconstructions were applied using Katsevich filtered back-projection reconstruction method [Katsevich, 2002; Varslot et al., 2010].

4.5.1 Single cylinder

For a single cylinder, the beam-hardened corrected estimated linear projections are calculated as the inverse of the BH curve, as shown in Eqn. (4.2).

Figure 4.1 and 4.2 shows the cupping and streaking artefacts for two single cylinder examples. Despite the objects showing quite non-uniform texture, assuming an average attenuation coefficient over the cylinders to produce BH correction curves seems to have been successful with both types of artefacts significantly reduced in both cases.

4.5.2 Nested-cylinders

For multiple materials, the inversion of the power law (see section 3.3.3) is performed per-cylinder/material with the corrected projection calculated as the sum of per-material corrected projections. The per-material inversion requires the calculation of the per-material contributions to the measured projections. These contributions are estimated from simulated-projections (Radon transform) of the per-material (per-annulus) masked reconstructed image (i.e. the image reconstructed from the measured projections). The procedure is depicted in Fig. 4.3.

Figure 4.4 shows the cupping artefacts around the specimen container and around the edge of the rock core specimen have been reduced for the 2 cylinder system using the assumed BH model (4.2) and the proposed correction.
Fig. 4.1: Horizontal slices through two single cylinder specimens (a). (i) reconstructions with beam-hardening artefacts, (ii) reconstructions after correction, and (iii) profile through the centre of images as indicated by dashed lines.
Figure 4.2: Horizontal slices through two single cylinder specimens (b). (i) reconstructions with beam-hardening artefacts, (ii) reconstructions after correction, and (iii) profile through the centre of images as indicated by dashed lines.
§4.5 Applying the beam hardening correction

Data acquisition

Intensity images (projections)

CT image reconstruction

Segmentation by fitting the cylinders; Eqn. 4.1

Cylinder 1  Cylinder 2  Cylinder 3

Simulated projections of each cylinder

Fit power law per cylinder

Parameter extraction; \((a_i,k_i)s\)

Estimate corrected projection; Eqn. 4.2

Corrected intensity images

CT image reconstruction

Figure 4.3: Flowchart of the BH correction of nested-cylinders.
Figure 4.4: A horizontal slice through a three cylinder specimen including the rock, fluid and the holder. (i) reconstructed using measured attenuation, (ii) reconstructed using corrected attenuation, and (iii) profile through the centre of images as indicated by dashed lines.
4.6 Conclusion

A simple beam-hardening correction method has been demonstrated for single and multiple nested-cylinder specimens. The method essentially turns the projection of cylinders into the image of a wedge phantom to directly measure the beam-hardening curve. Several examples have been included to demonstrate that the method does indeed reduce cupping and streaking artefacts. This method is complementary to the method previously developed in our group and presented at SPIE 2012 [Kingston et al., 2012] method which works on any specimen by cylinders. Future work could include developing an automatic method to determine the execution of cylindrical and non-cylindrical beam hardening correction code.

Equation 4.1 estimated the centres and radii of the nested-cylinders of the specimen. In this chapter, if two of nested-cylinders sample have similar grey values, beam hardening may affect that and they may be treated as one object. The sample holder in this chapter is polyoxymethylene, which is a low attenuating material. Apart from beam hardening artefacts that make subsequent tomogram segmentation and analysis difficult, for samples including a high density holder or nested-cylinder, the beam will be more attenuated around the edges as shown in figure 3.3 and therefore an effect which called inverse cupping artefact will happen which cause further complexity in segmentation. This effect is further explained in [Holt et al., 2014].
Beam hardening correction of concentric cylindrical specimens using power law model
Chapter 5

Material characterisation using dual-energy imaging and the AM attenuation model

5.1 Introduction

Imaging with two X-ray energy spectra, henceforth referred to as dual-energy imaging, and the Alvarez and Macovski [Alvarez and Macovski, 1976] transmitted intensity (AMTI) model were used in this study to estimate the maps of density ($\rho$) and atomic number ($Z$) of mineralogical samples. Dual-energy computed-tomography (CT) is being adopted for material discrimination [Siddiqui et al., 2004; Derzhi, 2012] and provides more information than conventional CT. Dual-energy material discrimination has found applications in the fields of medical imaging [Johnson et al., 2007], luggage screening [Ying et al., 2007] and the petrochemical/mineral reservoir industry [Siddiqui et al., 2004].

Single-energy micro-CT ($\mu$CT) can provide micron resolution spatial structure images with a high signal-to-noise ratio for determining the structure of samples but doesn’t provide compositional information. In contrast, dual-energy imaging can provide three-dimensional (3D) maps of density and atomic number of constituent materials in a sample. Although single-energy CT may be used to discriminate between materials that have very different attenuation coefficients, some samples such as rocks, can contain materials that have similar attenuation coefficients while their physical or transport properties are different. Atomic number and density mapping of a rock sample provides valuable input towards identifying the minerals present and their 3D distribution. This mineralogical and structural information is, in turn, essential to geological classification of sedimentary rock texture and subsequent alterations by diagenetic processes during burial. The information is also essential for predicting the mechanical and transport properties of the rock and its pores using digital images. One of the main applications is the extraction of oil and gas from reservoir rocks, since the minerals and their distribution strongly affect properties such as wettability, which is highly relevant to recovery from conventional reservoirs by waterflooding, or brittleness, which dictates whether an unconventional reservoir
is amenable to hydraulic fracturing. Single-energy imaging has limited ability to distinguish minerals such as quartz from feldspars or calcite from dolomite, which leads to uncertainties in modelling of geomechanical and transport properties [Golab et al., 2010]. If the attenuation coefficients vary differently with energy, dual-energy imaging can aid material discrimination.

Alvarez and Macovski [Alvarez and Macovski, 1976] (AM) presented attenuation coefficient (see section 1.2.6) as a two basis model to account for the two forms of the interaction of X-rays with matter, i.e., photoelectric absorption (PE) (see section 1.2.5.1) and Compton scattering (CS) (see section 1.2.5.2). These effects are, subsequently, dependent on atomic number and density of sample materials. As explained in section 2.3, this model has been used in several simplified forms. [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi, 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2010; Kaewkhao et al., 2008]. The model requires calibration and has several limitations, i.e., the model doesn’t account for K-edges and there’s no agreed value upon some parameters of the model. For this reason, Alvarez and Macovski simplified the model to polynomials to estimate the PE and CS images, after they presented the full model. In this sense, they did not use the full AM model (the full Beer-Lambert formulae) for determination of the $\rho$ and $Z$ as is done in our work in chapter 5. I have implemented the Alvarez and macovski polynomial model (AMP) [Alvarez and Macovski, 1976] (see section 6.2) and Siddiqui and Khamees model (SK) [Alvarez and Macovski, 1976] (see section 6.3) in the next chapter to compare with the results of this chapter.

In this chapter, I calibrated and applied the model in its full un-simplified form, for material discrimination in rock samples. Section 5.2 covers the theoretical background of dual-energy imaging, adapting the attenuation coefficient model for dual-energy imaging and presented the Alvarez and Macovski attenuation coefficient (AMAC) and AMTI models that can be used for material discrimination. These models require a priori spectral information. Section 5.3 describes the simulation of X-ray energy spectrum. Section 5.4 calibrates the AMAC model using the simulation and establishes a benchmark for the model in terms of accuracy. Section 5.4.1 describes the parameter estimation for a given setup applying the attenuation coefficient data of a set of reference materials obtained from the National Institute of Standards and Technology (NIST). Section 5.4.2 demonstrates the AMTI model calibration using the simulated projections of cylinders applying the same attenuation coefficients of the reference materials as in section 5.4.1. For the experimental protocol, section 5.4.3 applies the collective calibration and spectral information to model the measured intensity. The relative error between this AMTI model and the sample images captured at the Australian National University (ANU) $\mu$CT facility [Sakellariou et al., 2004] is minimised to estimate the density and atomic number of each of the sample constituent materials, and section 5.5 covers the estimation, segmentation and analysis of $\rho$ and $Z$ maps of three rock samples: two sandstone and a carbonate.
As mentioned in section 2.2, the conventional reconstruction algorithms, that is mostly in use, assume monochromatic radiation although the X-ray radiation is often polychromatic and therefore the reconstructions will include visible evidences in the form of cupping artefacts (in cylindrical sample images) or streaking artefacts (between high density materials). The attenuation coefficient model used for dual-energy analysis is a function of energy and inherently accounts for beam hardening. This is described and shown in section 5.5.1.

This research has been carried out within the “Computed Tomography” group of the Applied Mathematics Department at the Australian National University (ANU). The theory of material characterisation using dual-energy imaging was first presented in 1976 in [Alvarez and Macovski 1976]. As mentioned, the model has been used in several simplified forms [Alvarez and Macovski 1976; Siddiqui et al. 2004; Derzhi 2012; Heismann et al. 2003; Park and Kim 2011; Abudurexiti et al. 2010; Kaewkhao et al. 2008] but has not previously been used in its full form. The implementation of the full model requires calibration, exact knowledge of the spectra, expensive computation and consideration of the inadequacy of the model described in section 5.4.1. In this sense, this chapter is novel work for using the full AMTI model (the full Beer-Lambert formulae) for determination of the $\rho$ and $Z$ of materials. I am the first author of a published paper based on the contents of this chapter in “Journal of Applied Physics”. Within this chapter, I applied the AMAC and AMTI models in their full forms. I measured and simulated the projections of sample materials and used them to calibrated the AMTI model. I used the calibrated model to estimate $\rho$ and $Z$ of simulated and measured projection to establish the accuracy benchmarks. Finally, I measured the projections of rock samples and estimated their $\rho$ and $Z$ maps. I also simulated and measured the spectra and corrected the spectra measurements. While this is my own work, to successfully carry it out I received support from members of the “Computed Tomography” group. In relation to the simulation of the spectra, I sought advice from Dr Wilfred Fullagar. I carried out simulation of section 5.4.1 to investigate the limitations of the model and sought the advice of Dr Andrew Kingston on this topic. To ensure the sample preparation method was best-practice for the application, I sought the advice of Dr Michael Turner and Dr Andrew Fogden on preparation of the samples. Dr Shane Latham and I together worked on the segmentation parts of this chapter. I prepared the manuscript of this research that has been published in “Journal of Applied Physics” with the title and author list as follows:


The initial application of the full model is published in the “Proceedings of the 2nd International Conference on Tomography of Materials and Structure (ICTMS2015)” with the title and author list as follows:

The algorithm used in this research for estimation of the $\rho$ and $Z$ of the samples is applied along with a library of materials to match with the $\rho$ and $Z$ values to identify the sample materials in an iterative process. This idea has been patented and described, subsequently, with the titles and author lists as follows:


### 5.2 Alvarez and Macovski attenuation coefficient (AMAC) and transmitted intensity (AMTI) models

The Beer-Lambert law in Eqn. 1.2 describes the attenuation of monochromatic radiation [Beer, 1852]. As explained in section 1.2.6 the Beer-Lambert law is adapted to account for the polychromatic nature of X-rays because the attenuation coefficient ($\mu$) and X-ray radiation ($S_\epsilon(E)$) are functions of energy ($E$), therefore, the transmitted intensity ($I$) as a function of $E$ is represented in Eqn. 1.3.

It is also explained in section 1.2.6 in the X-ray radiation energy range [10, 120] keV, the two most important interactions of X-ray photons with matter are the photoelectric absorption and Compton scattering. Alvarez and Macovski [Alvarez and Macovski, 1976] modelled the attenuation coefficient, $\mu(E)$, as an energy-dependent linear combination of photoelectric absorption [$p(s, E)$] and Compton scattering [$c(s, E)$]. Equation (5.1) specifies the energy dependency of $p(s, E)$ and $c(s, E)$ and their contribution to the total linear attenuation coefficients $\mu(s, E)$. In Eqn. (5.1), classically $m = 3$ while for numerical fits to experimental data, $m$ lies between 3 and 3.5 [Cho et al., 1975].

$$\mu(s, E) = \frac{p(s, E)}{E^m} + c(s, E) f_{KN}(E), \quad (5.1)$$

where $f_{KN}$ is the Klein-Nishina function [Klein and Nishina, 1928], i.e.,
\[ f_{KN}(E) = \frac{1 + a}{a^2} \left[ \frac{2(1 + a)}{1 + 2a} \right] + \frac{1}{2a} \ln(a + 2a) - \frac{1 + 3a}{(1 + 2a)^2}; \quad a = \frac{E}{510.975} \text{ keV}. \]  

(5.2)

Henceforth, the Alvarez and Macovski attenuation coefficient model in Eqn. (5.1) is referred to as the AMAC model.

The photoelectric effect, \( p(s, E) \), increases approximately with the cube of atomic number \( (Z^n; n - 1 \approx 3) \) and Compton scattering, \( c(s, E) \), is proportional to density \( (\rho) \). The exponent \( (n - 1) \) can be in the interval \([3, 4]\) for numerical fits to experimental data [Cho et al., 1975]. Equation (5.3) shows how the photoelectric and Compton absorbances vary with the \( \rho \) and \( Z \) of the sample material.

\[ p(s, E) = K_1 \frac{Z}{A} \rho Z^{n-1}; \quad c(s, E) = K_2 \frac{Z}{A} \rho. \]  

(5.3)

Here, \( K_1 \) and \( K_2 \) are constants, \( A \) is atomic weight of material, \( Z = Z(s) \) and \( \rho = \rho(s) \) are the atomic number and density of the 3D sample. Based on the comment of a referees while publishing the paper of this chapter, the image of \( Z \) and \( \rho \) are written in bold to show the vector form of them, otherwise the final results of \( Z \) and \( \rho \), which are scalar values (the average over the image) are written in normal font, e.g., table 5.2 and 5.3.

For compound sample materials, the effective atomic number \( (Z_{\text{eff}}) \) can be derived as follows:

\[ Z_{\text{eff}} = \sqrt[3]{\sum_j f_j Z_j^n} \]  

(5.4)

where \( f_j \) is the fraction of the electrons associated with each element \( j \), that is, the fraction of number of atoms of element \( j \) multiplied by its atomic number over the total number of electrons of the molecule. The molecular weight \( (A_{\text{eff}}) \) is taken from NIST where \( (\frac{Z_{\text{eff}}}{A_{\text{eff}}} \approx 0.5) \) in Eqn. 5.3. The \( Z_j \) is the atomic number and \( A_j \) is the atomic weight of each element.

By substituting the AMAC model into Eqn. (1.3), one can estimate \( \int p(s, E) \) and \( \int c(s, E) \) and so reconstruct and segment the \( Z \) and \( \rho \) maps of constituent sample materials. This requires capturing the transmitted intensity image \( (I_\varepsilon) \) at photoelectric absorption and Compton scattering dominant energies with energy labels \( \varepsilon \in \{\varepsilon_1, \varepsilon_2\} \). The mentioned intensity measurements, henceforth called Alvarez and Macovski transmitted intensity (AMTI) model, is according to the following equa-
Material characterisation using dual-energy imaging and the AM attenuation model

\[ I_{\varepsilon} = \int_{E=0}^{\varepsilon} S_{\varepsilon}(E) \exp \left[ - \frac{\int L(s, E) \, ds}{E^m} - \int c(s, E) \, ds \, f_{KN}(E) \right] dE \quad (5.5) \]

5.3 Modelling the physics of X-ray energy spectrum \([S_{\varepsilon}(E)]\)

In this section, I characterise the spectrum \(S_{\varepsilon}(E)\) by modelling X-ray generation at the source-target materials and subsequent propagation to the detector. It was simulated as follows: Bremsstrahlung was simulated using Kramer’s law [Kramers, 1923] and characteristic emission lines were added to approximate the spectrum from the tungsten target. This spectrum was then modulated by the spectral transmission of each non-sample absorbing material between the source and the detector. The X-ray tube was an “X-tek system limited RTR 225 keV” with 2 \(\mu\)m tungsten target material and 0.5 mm beryllium window. The detector was a Perkin Elmer “XRD 1621 scintillator-based area detector” [PerkinElmer, 2012] with 2048 \(\times\) 2048 (width \(\times\) height) pixels with square pixel width 0.2 mm. The camera to detector distance (CL) was 1000 mm for our imaging geometry. Consequently, the absorbing materials between source and detector were: 2 \(\mu\)m tungsten on 500 \(\mu\)m beryllium window on the X-ray source, 1000 mm air and sensor protection materials (0.75 mm of Aluminium and 0.75 mm of carbon fiber). Transmission due to the materials was modelled as [Spangenberg, 1948] \(\prod_{i} e^{-\mu_{i}(E) s_{i}}\), where \(\mu_{i}(E)\) is the energy dependent attenuation coefficient of absorbing materials taken from NIST and \(s_{i}\) is the thickness of the \(i^{th}\) material. X-rays were further modulated by the attenuation of the detector’s 650 \(\mu\)m caesium iodide scintillator \((1 - e^{-\mu_{sci}(E) s_{sci}})\). An energy proportional detector (Flat Panel Perkin Elmer XRD 1621) was used, so the energy absorbed by the detector was modelled as:

\[
S_{\varepsilon}(E) = E \times \left[ \frac{K}{2\pi c} \left( \frac{E_{\max}}{E} - 1 \right) \sum_{i} k_{ji}(E - E_{i}) \right] \times \prod_{i} e^{-\mu_{i}(E) s_{i}} \times (1 - e^{-\mu_{sci}(E) s_{sci}}) \quad (5.6)
\]

The relative magnitude of Kramer’s constant, \(K\), and the emission line intensities, \(k_{ji}\), were adjusted based on attenuation corrected observation of source spectra, using a cadmium telluride (CdTe) detector (XR-100T-CdTe Amptek spectrum analyser) after applying a stripping algorithm [Redus et al., 2009] as shown consequently in section 5.3.1 and 5.3.1.1. This procedure is depicted in Fig. 5.1.
§5.3 Modelling the physics of X-ray energy spectrum $[S_\varepsilon(E)]$

- Data acquisition; using Amptek XR-100T-CdTe spectrum analyser detector
- Measure the spectrum; section 5.3.1
- Correct partial registry; section 5.3.1.1
- Apply stripping algorithm
- Corrected measurement

Simulate the spectrum; section 5.3
- Simulated spectrum
- Fit simulated spectrum on measurement
- Parameter extraction; $(K_i,k_j)$ in section 5.3.1.1
- Corrected spectrum $[S_\varepsilon(E)]$
- Model dual-energy spectra at $E_{\varepsilon}^{\text{max}}$; $\varepsilon \in \{\varepsilon_1, \varepsilon_2\}$ keV
- $S_{\varepsilon_1}(E)$
- $S_{\varepsilon_2}(E)$

* to Fig. 5.8 & 5.10 & 5.12 & 5.13

Figure 5.1: Flowchart of the Modelling the physics of X-ray energy spectrum $[S_\varepsilon(E)]$, with $\varepsilon$ being the energy label.
Figure 5.2: Simulated spectrum at 100 maximum energy; modified to match that seen for our experimental protocol, meaning that the spectrum is modified to be as measured by the detector with CsI scintillator. The plot shows a jump at 33.169 keV that relates to the K-edge of Iodine.

Figure 5.3 shows the mass attenuation coefficient, $\mu / \rho$, and the mass energy absorption, $\mu_{en} / \rho$, of the scintillator material (CsI). The mass energy absorption coefficients include the further emission of radiation by the charged particle when traveling through the matter. It is defined as $\mu_{en} / \rho = (1 - g) \mu / \rho$ where $g$ is the average fraction of the kinetic energy of secondary charged particles that is subsequently lost in radiative energy-loss processes as the particles slow to rest in the matter. For energy range less than 100 keV, the numerical values of $g$ are relatively small and $\mu_{en} / \rho$ and $\mu / \rho$ are almost similar. Here I note that I used the attenuation coefficient of the scintillator material (CsI), $\mu_{sci}$, for the absorbed energy in place of $\mu_{en,sci}$ in Eqn. 5.6 which is reasonable in [1, 120] keV energy range.
5.3 Modelling the physics of X-ray energy spectrum \[ S(\varepsilon) \]

Figure 5.3: Attenuation of CsI as a function of photon Energy (http://physics.nist.gov/PhysRefData/XrayMassCoef/tab4.html).

5.3.1 Measuring the X-ray energy spectrum

I used the Amptek XR-100T-CdTe spectrum analyser detector which has a 3 x 3 x 1 mm Cadmium Telluride (CdTe) diode detector to measure X-ray photons. The XR-100T-CdTe is capable of detecting energies from a few keV to several hundreds of keV, with an efficiency that peaks from 10 to 100 keV [Redus et al., 2009]. The detector was connected to the Amptek PX4 digital pulse processor including digital pulse shaping amplifier, integrated multichannel analyser and power supplies. The multichannel analyser provided the histogram of photon counts versus their energies (spectrum). This was sent to the installed Amptek software (ADMCA) on the computer to display the measured spectrum. Figure 1.3 shows the normalised measured spectrum using the Amptek spectrum analyser at 100 keV.

5.3.1.1 Correction of the partial registry of the measured X-ray spectra on the detector

The simulated spectrum of section [5.3 Fig. 5.2] is fitted to measured spectrum (Fig. 1.3) to match the energy channels using the characteristic peaks and maximum voltage \( E_{\text{max}} \) as reference energies.
Both Cd and Te have two X-ray fluorescent (XRF) characteristic peaks. Some XRFs produced in the detector by the interaction with Cd or Te escape the detector and thus reduce the measured energy, what is termed “partial registry”. In CdTe, the characteristic energies are 23.2 and 26.1 keV for the Cd $K_\alpha$ and $K_\beta$, and 27.5 and 31.0 keV for $K_\alpha$ and $K_\beta$ of the Te. Thus in CdTe detector there are four characteristic energies associated with a “partial registry” of the spectrum signal. The escaped of the X-ray fluorescence and consequent “partial registry” of the parent signal means that the observable energy is registered at a lower value than normal. The blue line in Fig. 5.4 (b), (c) and (d) are the spectra measured at 60, 100 and 120 keV using Amptek CdTe spectrum analyser, including the partial registry.

To correct the partial registry of spectra, a “stripping” developed by [Redus et al., 2009] was applied. The difference ($N_\delta$) between the true number of photons of energy ($N_t(E)$) and the number of photons detected ($N_d(E)$) at energy (E) is shown in the Eqn. (5.7).

\[ N_\delta = \sum_j f_j(E + E_j)N_t(E + E_j) - \sum_j f_j(E - E_j)N_t(E) \]  

(5.7)

Here, $f_j$ is the probability of characteristic photon $j$ escaping at energy E. The term $\sum_j f_j(E + E_j)N_t(E + E_j)$ includes added photon counts to $N_t(E)$ for interaction of photons at higher energies $(E + E_j)$ and $\sum_j f_j(E - E_j)N_t(E)$ and reduced photon counts due to interaction at lower energies $(E - E_j)$.

I applied the “stripping” algorithm from the highest energy channel and proceeded to the lowest energy channel. At the highest energy channel, I assumed there were no excess counts from higher energy photons. The ratio of counts in each escape peak to the photopeak was fit with a fifth order polynomial to obtain the escape peak yield versus energy [Redus et al., 2009]. The four terms of $f_j(E)$ are modelled according to the following:

\[ f_j(E) = a_0 + a_1E + a_2E^2 + a_3E^3 + a_4E^4 + a_5E^5. \]  

(5.8)

The values of the six coefficients ($a_0, a_1, a_2, a_3, a_4, a_5$) were obtained by fitting the measured data points in [Redus et al., 2009] with Eqn. 5.8. The four term $f_j(E - E_j)N_d(E)$ of Eqn. 5.7 correspondence to partial registry due to the four XRF mechanisms (shown in Fig. 5.4 yellow line) of the CdTe detector is estimated. These values are subtracted that from the escape channel $N_d(E - E_j)$ and added back to the parent channel $N_d(E)$. Figure 5.4 shows the corrected measured spectrum in purple line. Figure 5.4 (a) depicts our implementation of the “stripping” algorithm correction on the 80 keV spectrum data obtained from [Redus et al., 2009].
§5.3 Modelling the physics of X-ray energy spectrum \[S_e(E)\]

5.3.2 Correction of the characteristic peaks of the simulated X-ray spectra

The spectrum of Fig. 5.2 was simulated as seen by the CsI flat-panel detector (see section 1.2.4) of the ANU \(\mu\)CT system [Sakellariou et al., 2004]. After applying the “stripping” algorithm in section 5.3.1.1 I modified the corrected measured spectrum of Fig. 5.4 as \(1 - \frac{e^{-\mu_{sci}(E)} s_{sci}}{1 - e^{-\mu_{CdTe}(E)} s_{CdTe}}\) to match that seen by CsI detector with \(s_{CsI}\) and \(s_{CdTe}\) being the thickness of the ANU flat-panel CsI and the Amptek CdTe detectors respectively.

The corrected measured spectra has been used to fit the simulated spectra and estimate the values of \(K\) and \(k_j\) in Eqn. 5.6. Figure 5.5 shows the modelled X-ray spectra after applying the estimated \(K\) and \(k_j\). Figure 5.5(c) red line (simulated spectrum at
100 keV maximum energy) is the same figure as figure 5.2. This figure shows both the simulation and measurement of the spectrum at 100 keV to compare them after estimation of the constants $K$ and $k_j$ of Eqn. 5.6.

![Figure 5.5](image1.png)

(a) ![Figure 5.5](image2.png)

(b) ![Figure 5.5](image3.png)

(c) ![Figure 5.5](image4.png)

(d) Figure 5.5: Plot of the partial registry corrected measured spectrum fitted to simulated spectrum to match the XRFs amplitude for: a) 80 ([Redus et al., 2009]), b) 60, c) 100 and d) 120 keV

### 5.3.3 X-ray dual-spectra

Solving the AMTI model (5.5) requires a model for $S_E(E)$ which is simulated in section 5.3. In this research, the dual-energy spectra were simulated approximately as follows: 1) spectrum $\epsilon_1$ with maximum energy of 60 keV and 0.5 mm Al filtering for which the photoelectric absorption effect is dominant, and 2) spectrum $\epsilon_2$ with maximum energy of 120 keV and 0.35 mm Cu filtering, for which the Compton scattering dominates for $Z \lesssim 13$ as shown in Fig. 5.6. In an ideal case, the spectra should be chosen such that they distinctly correspond to photoelectric and Compton attenuation basis within the AMAC model. However, the polychromatic nature of the illuminated X-ray is less than ideal because the two spectra overlap in energy
range between 30 to 60 keV. Within this thesis, I measured several spectra with maximum energy ranging between 40 to 130 keV and different filters, e.g., Al, Cu, lead and glass with Al ranging from 0.25 to 5 mm and Cu ranging from 0.1 to 2 mm to find the dual-energy spectra as distinct as possible such that their effective energy associate with photoelectric absorption and Compton scattering energy regions.

Figure 5.6: Simulated dual-energy spectra at 60 (red line) and 120 keV (blue line) maximum energies; modified to match that seen for our experimental protocol (section 5.3), and the spectra weight (dashed cyan line) that is the absolute difference of the dual-energy spectra. This weight is added to the AMAC model in section 5.4.1

5.4 Simulation: Validating and calibrating the model

I calibrated the AMAC model for our experimental setup using several readily available materials that span the Z and ρ ranges of interest for rocks. One can choose to have different number and range of reference materials for calibration. These are carbon (C), acrylic (C₃O₂H₈), teflon (C₂F₄), glass (SiO₂), aluminium (Al), marble (CaCO₃) and titanium (Ti). I analyse radiographs of cylindrical samples of these materials to find optimal values for $K_1, K_2, m$ and $n$. The estimation of $K_1, K_2, m$ and $n$ is partly motivated by the experimental setup. The choice of reference materials and the spectral weight function affects the estimation of $K_1, K_2, m$ and $n$. First, in section 5.4.1 I have calibrated the AMAC model using our simulated spectra.
and attenuation coefficient data $[\mu(E)/\rho]$ from NIST. This gives an estimate of parameter values, demonstrates the adequacy of the AMAC model (5.1), and establishes a benchmark on the attainable accuracy of $\rho$ and $Z_{\text{eff}}$. In section 5.4.2, I then simulate the experiments to be used for calibration of the AMTI model (5.5) to show that our proposed method both a) gives similar parameter values, and b) can attain the comparable accuracy. Finally, in section 5.4.3, I calibrate the AMTI model using the measured radiographs to demonstrate that our simulated spectra is accurate since again the parameter values and accuracy are comparable.

## 5.4.1 AMAC model calibration using NIST data

I was required to estimate the photoelectric absorption coefficient, $K_1$, Compton scattering coefficient, $K_2$, energy exponent constant, $m$, and atomic number exponent constant, $n$, for the AMAC model (5.1) using the selected reference materials and the two simulated spectra. $K_1$ and $K_2$ constants estimate the contribution of PE and CS effects to the model. The numerical fits to NIST data for $m$ and $n$, subsequently, lies in the range [3, 3.5] and [3, 4] [Cho et al., 1975].

The attenuation coefficients ($\mu$) of the reference materials ($\omega$) were obtained from the NIST database in the energy range [1, 120] keV for the simulations. I fit (in a least square sense) the AMAC model (5.1) with the NIST data to calibrate the model for our reference materials as shown in Eqn. 5.9.

\[
\text{minimise} \sum_{E,\omega,i} W_i(E) \| \mu_{\text{fit}}(s, E) - \mu^{\text{NIST}}(s, E) - \epsilon_s(E) f_K(E) \|^2. \quad (5.9)
\]

Initially titanium dominated the fits therefore, to prevent excessive influence of materials with higher atomic number, the error calculation was modified to minimise the relative error i.e., $\text{min}(\epsilon_s^2)^2$ over all pixels, $i$. The estimated parameters are $K_1 = 13.96 \quad (\text{keV}^3/\text{cm}^2)$, $K_2 = 0.30 \quad (\text{cm}^2/\text{gr})$, $m = 3.00$ and $n = 3.20$. Figure 5.7 shows a plot of attenuation coefficients according to NIST data (red line) and the model (dashed blue line) fits applying the estimated $K_1$, $K_2$, $m$ and $n$ constants for glass, acrylic, titanium and marble to be discussed in this section.

To improve the calibration I decided to apply the spectra influence, so I weighted Eqn. 5.9 with the absolute difference of the spectra $[W(E)]$ as shown in Fig. 5.6 (dashed cyan line). This gives lower weight to the overlapping energy region between lower and higher energy spectra than the effective PE and CS regions (Fig. 5.6). Adding the spectra weight also means the maximum K-edge in our reference materials (Ti; approximately 5 keV) is avoided through applying spectra weight. For these simulations shown in Fig. 5.6 that model our experimental setup, the spectra start at about 10 keV so the K-edges do not impact the results when I apply the spectra
weight to AMAC model calibration. I used different spectral weights, e.g., absolute difference, squared difference and square root of the absolute difference of the dual spectra and to assess the accuracy of results compare to no weight. The average relative error of $\rho$ and $Z$ estimation showed the absolute difference spectra is lowest with around 0.6% lower error compared to no spectral weight.

I note here that the AMAC model does not account for increased absorption above the K-edges of materials. Within our range of reference materials, Ti has the highest K-edge at 4.99 keV and marble the next highest K-edge at 2.48 keV (see Fig. 5.7c and d). Figure 5.7b shows a plot of the fitting results for glass, which was one of the reference materials. Glass and aluminium have K-edges at 1.84 and 1.56 keV, respectively, which are well below the transmission energies in our setup. The average relative error between the AMAC model estimated attenuation coefficients and the NIST attenuation coefficients in the energy range [1, 120] keV is 16.50%, however the relative error in energy range [10, 120] keV is 1.96% as shown in table 5.1. As noted, the inaccuracy is mostly because the model does not account for K-edge absorption of titanium and marble, therefore, our selected spectra (Fig. 5.6) reduced calibration error, due to K-edges, by approximately 14%.

I also note that using the attenuation coefficient values of AMAC model for calibration will result in totally compatible $\mu$ values with that of the model, however using NIST attenuation coefficients for calibration (even after avoiding K-edges; energy range of [10, 120] keV) shows 1.96% average relative error between NIST and the model attenuation coefficients. In this case the inaccuracy is mostly due to inadequacy of the AMAC model. A noticeable error of 5% in energy range of [10, 120] keV shown in table 5.1 for acrylic is because it does not match the Alvarez and Macovski model. Acrylic doesn’t have a K-edge in [10, 120] keV energy range. In the absence of any spectral information corresponding to the mismatch between the acrylic attenuation with the AMAC model, we can mention that acrylic has a very low attenuation that possibly cause this error. The estimated atomic number is a mathematical model to best reflect the observed attenuation measurements, rather than an actual physical reality (e.g., there is no fractional atomic number elements). Figure 5.8 is the flowchart of the procedure of the AMAC model calibration explained in this section.
Material characterisation using dual-energy imaging and the AM attenuation model

Figure 5.7: Plot of \( \ln(\mu) \) versus \((E = [1, 120] \text{keV})\) of NIST data (red line) and AMAC model (blue dashed line) fits applying the the estimated \( K_1, K_2, m \) and \( n \) constants in section 5.4.1 for a) glass, b) acrylic, c) titanium and d) marble.

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated model-data relative error in [1, 120] keV</th>
<th>Estimated model-data relative error in [10, 120] keV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>18.75 %</td>
<td>1.29 %</td>
</tr>
<tr>
<td>C</td>
<td>2.98 %</td>
<td>2.79 %</td>
</tr>
<tr>
<td>Marble</td>
<td>25.71 %</td>
<td>0.85 %</td>
</tr>
<tr>
<td>Acr</td>
<td>5.52 %</td>
<td>5.00 %</td>
</tr>
<tr>
<td>Teflon</td>
<td>1.81 %</td>
<td>1.23 %</td>
</tr>
<tr>
<td>Glass</td>
<td>5.80 %</td>
<td>1.26 %</td>
</tr>
<tr>
<td>Ti</td>
<td>54.98 %</td>
<td>1.29 %</td>
</tr>
<tr>
<td>Average</td>
<td>16.50 %</td>
<td>1.96 %</td>
</tr>
</tbody>
</table>

Table 5.1: Relative error between NIST attenuation coefficient and AMAC model for reference materials using AMAC model (Section 5.4.1).
5.4 Simulation: Validating and calibrating the model

5.4.1 Data Acquisition; from NIST

Attenuation coefficient \([\mu(E)]\) of 7 reference material (\(\omega\))

Theoretical \(\rho\) and \(Z\) values of material \(\omega\)

Fit \(\mu(E)\) on AMAC model; Eqn. 5.9

Weight of Dual-energy spectra; \(*\) from Fig. 5.1

Parameter estimation; \((K_1, K_2, m, n)\)

\(\diamond\) to Fig. 5.10 & 5.12

Calibrate the AMAC model

Calibrated AMAC model

Figure 5.8: Flowchart of the AMAC model calibration (Section 5.4.1).

5.4.2 AMTI model calibration using simulated cylinder images

I simulated radiographs \((P_{\omega \epsilon (sim)}^{\omega})\) of aluminium, carbon, marble, acrylic, carbon, glass and titanium with 10.00, 6.08, 10.00, 9.90, 19.56, 10.00, 6.09 mm diameter cylinders of each reference material (with cylinder sizes and materials matching the physical experiments of section 5.5). The source to sample distances (SD) are 33.8, 17.3, 33.8, 34.5, 71, 35.2, 17.8 mm subsequently and camera length (CL) is 1000 mm for all cases. The attenuation coefficient values of materials are taken from the NIST attenuation coefficient curves. The samples were imaged using the cone beam X-ray radiation in a circle trajectory (shown in Fig. 1.5) at two different energies: 60 keV with 0.5mm Al filter \((S_{\epsilon_1})\) and 120 keV with 0.35mm Cu filter \((S_{\epsilon_2})\) (Fig. 5.6) with 1440 angles of projections.

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Material characterisation using dual-energy imaging and the AM attenuation model

I simulated $\rho$ and $Z_{\text{eff}}$ (5.4) projections of reference materials to build $\int p(s, E) \, ds$ and $\int c(s, E) \, ds$ projections (5.3). The atomic number and energy exponent values ($m$ and $n$) are taken from section 5.4.1 and applied to the AMTI model (5.10) to estimate $K_1$ and $K_2$ and validate the estimation of calibration parameters in section 5.4.1. $K_1$ and $K_2$ were obtained with a least-square fit using the relative error as follows:

$$\text{minimise} \sum_{i} \left| \frac{P_{\text{sim}}^i}{S_i(E)} \right|^2 = \sum_{E=0}^{\infty} \left| \frac{\int L p(s, E) \, ds}{E^m} + \int L c(s, E) \, ds f_{KN}(E) \right|^2.$$

(5.10)

This equation minimises the sum of squares of the errors over all the pixels in the $\int p(s, E) \, ds$ and $\int c(s, E) \, ds$ projections. PE and CS constants estimations are $K_1 = 13.94 \, (\text{keV}^3 \text{cm}^2 \text{gr})$ and $K_2 = 0.30 \, (\text{cm}^2 \text{gr})$ which shows AMTI model calibration is compatible with the AMAC model calibration using the simulated attenuation coefficient data from NIST and validates our proposed experimental calibration technique using cylinders of reference materials. Figure 5.9 shows a horizontal line through the simulated projection image of glass cylinder and the AMTI model fit on that. I have chosen to show the plots of material glass and marble because they are respectively close in atomic structure to quartz in sandstones and calcite in carbonate rocks which will be examined in section 5.5.

![Glass sample simulated at 60 & 120 keV spectra](image1.png)

![Marble sample simulated at 60 & 120 keV spectra](image2.png)

Figure 5.9: A line through a simulated projection cylinder and the AMTI model fit: at 60 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a)glass and b) marble
To calculate density and atomic number of reference materials, the calibrated AMTI model (5.5) is matched with simulated projections of reference materials using Newton-Raphson optimisation method [Ryaben’kii and Tsynkov 2006] to estimate photoelectric ($\int p(s,E) \, ds$) and Compton($\int c(s,E) \, ds$) projections of materials. The $\frac{Z}{\rho} \rho Z^{n-1}$ and $\frac{Z}{\rho}$ images have been reconstructed by filtered back-projection and used to calculate the density and atomic number of each pixel of the image which may contain an element or a compound or a mixture of materials. In the case of compound or mixture materials the effective atomic number can be derived using Eqn. (5.4). The above density and atomic number mapping procedure, using the simulation of reference materials, is shown in Fig. 5.10.

I note here that there are several material dependent parameters ($\mu$, $Z_{\text{eff}}$ and $\frac{Z}{\rho}$) in the AMTI model which may affect both calibration and $\rho$ and $Z$ estimation using the model. Although the general structure of compound and mixture materials of our reference materials are known, I acknowledge some material composition uncertainty in our estimations. For instance, glass or borosilicate with the chemical structure of 80.60% silica (SiO$_2$), 12.60% boric oxide (B$_2$O$_3$), 4.20% sodium oxide (Na$_2$O) and 2.20% aluminium oxide (Al$_2$O$_3$), and 3.00% mixed of (Fe$_2$O$_3$, CaO, MgO, Cl) according to the NIST database. I matched the chemical composition of our reference materials such that the avg($\frac{\delta \rho}{\rho}$) and avg($\frac{\delta Z}{Z}$) were as low as 0.61% and 0.77%, however, using the same calibration on experimental data resulted in increases of $\rho$ and $Z$ estimation average relative error to 4.28% and 2.75% for all reference materials. Therefore I decided to retain the simulations close to experimental data. This way the average of material uncertainty error for all reference materials of experimental and simulated results are compatible.

Table 5.2 shows the average estimated density and their atomic numbers of the reference materials using simulated projections of cylinders of these materials data and their relevant theoretical $\rho$ and $Z$ values. The estimated results show errors as follows: avg($\frac{\delta \rho}{\rho}$) = 2.19%, avg($\frac{\delta Z}{Z}$) = 0.88%, [min, max]($\frac{\delta \rho}{\rho}$) = [0.8%, 5.73%] and [min, max]($\frac{\delta Z}{Z}$) = [0.28%, 1.82%]. The calibrated AMAC model itself has about 1.96% average error for all materials in energy range of [10, 120] keV because of the inadequacy of the model. The average relative errors of estimated $\rho$ and $Z$ in this case are comparable. I have applied the estimated $m$ and $n$ values of this section for our experimental protocol in the next two sections. In the next section, I apply the calibrated model to experimental data of the same set of materials to estimate $\rho$ and $Z$ and compare the experimental results and simulated results. I then analyse three types of rock cores using the method.
Data Acquisition; from NIST for $[1, E_{\epsilon_1}^{\text{max}}]$, of dual-energy spectra $\star$ from Fig. 5.1

Attenuation coefficient $[\mu(E)]$ of 7 reference material ($\omega$) in $[1, E_{\epsilon_1}^{\text{max}}]$

Simulate projections of materials $\omega$ for $[1, E_{\epsilon_1}^{\text{max}}]$

Theoretical $\rho$ and $Z$ values of material $\omega$

Fit intensity images on AMTI model; Eqn. 5.10

Parameter estimation; $(K_1, K_2)$

Calibrate the AMTI model

Calibrated AMTI model

Estimated $\rho$ intensity images of 7 materials

Parameter estimation; $\mathcal{P}$ and $\mathcal{C}$ intensity images

Estimated $Z$ intensity images of 7 materials

CT image reconstruction of $\rho_{\text{material}}$

CT image reconstruction of $Z_{\text{material}}$

Figure 5.10: Flowchart of the AMTI model calibration and $\rho$ and $Z$ estimation, using simulated projections of cylinders of 7 reference materials (Section 5.4.2), with $\epsilon$ being the energy label and pre-processing step explained in section 5.5.

$\mathcal{C} = \int L \, c(s, E)$ from Eq. 5.3

Draft Copy – 21 November 2016
5.4.3 Testing the AMTI model calibration using the real cylinder images

I imaged the cylindrical samples of aluminium (Al), carbon (C), acrylic (C₅O₂H₈), marble (CaCO₃), teflon (C₂F₄), glass (SiO₂), titanium (Ti) using the parameters of the experiment as described in section 5.4.2 with the exposure time of 2 seconds and X-ray current of 100 μA for all cases.

In this section also, first I calibrate the AMTI model (5.5) using experimental images to compare with the calibration of the simulated data in section 5.4.1 and 5.4.2. The $K_1$ and $K_2$ values are estimated to be 13.50 (keV cm$^2$ gr$^{-1}$) and 0.29 (cm$^2$ gr$^{-1}$) subsequently which are comparable with the $K_1$ and $K_2$ estimations in section 5.4.1 and 5.4.2. This shows that the calibration of the AMAC model using NIST attenuation coefficients of reference materials (section 5.4.1), or calibration of the AMTI model using the simulated images of reference materials (section 5.4.2) has almost the same estimated values as in this section where I calibrated the AMTI model using the experimental images of reference materials. It also shows that I can calibrate the model for a set of reference materials and then compute the density and atomic number for one of the materials as shown in next paragraph, or even other materials as I will show in section 5.5.1 for rocks.

To estimate projections of $ρZ/A$ and $ρZ$, I have used the Newton-Raphson method to minimise the absolute error between the calibrated model (5.5) and experimental radiographs of the material samples. Using a priori information of materials, $Z/A$, I can obtain the $ρ$ and $Z$ projections. Figure 5.11 shows a horizontal line through the projection image of the glass sample and the model fit to that. This can be reconstructed using standard filtered back-projection to generate a two-channel ($ρ, Z$) volume image of the sample. This procedure is illustrated using the flowchart of Fig. 5.12.

Table 5.2 shows average $ρ$ and $Z$ estimation applying the real data in this section. It also shows average $ρ$ and $Z$ estimation of section 5.4.2 using simulated cylinder images and the theoretical values for comparison. The density and atomic number error intervals are [0.97%, 7.85%] and [0.45%, 2.64%] respectively with an average relative error of 2.87% and 1.26%. The results using the real data is comparable with the results of simulations in sections 5.4.1 and 5.4.2. This means that the $ρ$ and $Z$ estimations of a sample constituent materials using the calibrated full model (5.5) can be used to identify the materials by comparing to a database of theoretical $ρ$ and $Z$ values of materials (future work).
Material characterisation using dual-energy imaging and the AM attenuation model

Figure 5.11: A line through an imaged projection cylinder and the AMTI model fit: at 60 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a) glass and b) marble.

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$ using simulated data</th>
<th>Estimated $\rho$ using real data</th>
<th>Theoretical $\rho$</th>
<th>Estimated $Z$ using simulated data</th>
<th>Estimated $Z$ using real data</th>
<th>Theoretical $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>2.64</td>
<td>2.64</td>
<td>2.70</td>
<td>13.14</td>
<td>13.34</td>
<td>13.00</td>
</tr>
<tr>
<td>C</td>
<td>1.43</td>
<td>1.43</td>
<td>1.46</td>
<td>5.89</td>
<td>5.95</td>
<td>6.00</td>
</tr>
<tr>
<td>Marble</td>
<td>2.67</td>
<td>2.75</td>
<td>2.70</td>
<td>15.44</td>
<td>15.57</td>
<td>15.35</td>
</tr>
<tr>
<td>Acr</td>
<td>1.25</td>
<td>1.28</td>
<td>1.18</td>
<td>6.45</td>
<td>6.42</td>
<td>6.51</td>
</tr>
<tr>
<td>Teflon</td>
<td>2.13</td>
<td>2.08</td>
<td>2.15</td>
<td>8.43</td>
<td>8.50</td>
<td>8.45</td>
</tr>
<tr>
<td>Glass</td>
<td>2.19</td>
<td>2.20</td>
<td>2.23</td>
<td>11.77</td>
<td>11.48</td>
<td>11.65</td>
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<tr>
<td>Ti</td>
<td>4.38</td>
<td>4.38</td>
<td>4.50</td>
<td>21.90</td>
<td>21.90</td>
<td>22.00</td>
</tr>
</tbody>
</table>

Table 5.2: Estimated effective atomic number and bulk density of reference materials using AMTI model (Section 5.4.2 and 5.4.3).
Figure 5.12: Flowchart of the AMTI model calibration and \( \rho \) and \( Z \) estimation, using real intensity images of cylinders of 7 reference materials (Section 5.4.3), with \( \epsilon \) being the energy label and pre-processing step explained in section 5.5. \( P = \int p(s, E) \) and \( C = \int c(s, E) \) from Eq. 5.3.
5.5 Experimental analysis

In this section, I apply the same method as in section 5.4.3 to calculate density and atomic number distributions in several rock samples including Bentheimer and Berea sandstones and a carbonate. I imaged the radiographs \( P_{\omega}^{\text{sim}} \) of material \( \omega \), that is Bentheimer sandstone, Berea sandstones or the carbonate cylinders, with 10 mm diameter. The source to sample distance (SD) are 35 mm for Bentheimer and Berea sandstones and 13 mm for the carbonate sample. Camera length (CL) is 1000 mm for all cases. The samples were imaged at two different energies: 60 keV with 0.5 mm Al filter \( S_{\epsilon_1} \) and 120 keV with 0.35 mm Cu filter \( S_{\epsilon_2} \) (Fig. 5.6). The X-ray current was the same at both 60 and 120 keV, but was varied depending on the material: Berea was imaged at 80 mA, whilst Bentheimer and the carbonate were imaged at 100 \( \mu \)A. The X-ray exposure time for Bentheimer, Berea and the carbonate samples respectively were 3.2, 4 and 3.2 seconds for 60 keV radiation and 2, 2.5 and 2 seconds for 120 keV radiation. The total number of projections were imaged within one circle trajectory (shown in Fig. 1.5) at 1440 angles for Bentheimer and Berea sandstones and at 2880 angles for the carbonate sample. I linearised the projection data and applied alignment [Kingston et al., 2011], auto-focus [Kingston et al., 2010], drift correction [Myers et al., 2011]. The projection data also masked for the region outside the sample cylinder. Where the estimated atomic number and density using AMTI model were less than or equal to zero, I regularised \( \rho \) and \( Z \) values with \( 1 \times 10^{-3} \) and \( 12 \times 10^{-5} \) (using 12 as the rounded up average atomic number of reference materials). These steps are called pre-processing in Fig. 5.12 and 5.13.

I used parameters \( K_1 \) and \( K_2 \) from section 5.4.3 and \( m \) and \( n \) from section 5.4.1 in the model (5.5). \( I_\epsilon \) are radiographs of rock samples \( I_{\epsilon_1} \) and \( I_{\epsilon_2} \). The absolute error between the calibrated model and \( I_\epsilon \) is minimised using Newton-Raphson method to estimate the projections of \( \rho Z A^{-1} \) and \( Z A \). The atomic number and density 3D images of Bentheimer, Berea and Carbonate were reconstructed using Katsevich filtered back-projection reconstruction method [Katsevich, 2002; Varslot et al., 2010]. Shane and I applied the single-phase (quartz) segmentation of \( \rho \) and \( Z \) tomograms in Bentheimer and Berea sandstones and dual-phase segmentation (calcite and dolomite) in carbonate. I determined the average of each segment for \( \rho \) and \( Z \) as shown in Fig. 5.15a-iii and 5.15b-iii. Figure 5.13 depicts the density and atomic number estimation of rock samples explained in this section.
§5.5  Experimental analysis

Data Acquisition; µCT imaging using $S_{\varepsilon_1}$; of dual-energy spectra * from Fig. 5.1

3D projections of rocks imaged using $S_{\varepsilon_1}$

Pre-processing

Parameter estimation; $P$ and $C$ intensity images

Calibrated AMTI model; ‡ from Fig. 5.12

Estimated $\rho$ intensity images

CT image reconstruction of $\rho$

Segmentation (see section 5.5.1)

Material 1

map of $\rho_{\text{material}1}$

map of $Z_{\text{material}1}$

map of $\rho_{\text{material}2}$

map of $Z_{\text{material}2}$

Material 2

map of $\rho_{\text{material}3}$

map of $Z_{\text{material}3}$

Material 3

Data Acquisition; µCT imaging using $S_{\varepsilon_2}$; of dual-energy spectra * from Fig. 5.1

3D projections of rocks imaged using $S_{\varepsilon_2}$

Pre-processing

Dual-energy spectra; * from Fig. 5.1

Estimated $Z$ intensity images

CT image reconstruction of $Z$

Figure 5.13: Flowchart of $\rho$ and $Z$ estimation using real intensity images of cylinders of rocks and the calibrated AMTI model (Section 5.5), with $\varepsilon$ being the energy label and pre-processing step explained in section 5.5. $P = \int p(s, E)$ and $C = \int c(s, E)$ from Eq. 5.3.
5.5.1 Material discrimination of rock using AMTI model

The main component of sandstones is quartz so I apply a single-phase segmentation for Bentheimer and Berea sandstones. For each of the $\rho$ and $Z$ reconstructed images a 2D histogram of neighbourhood-mean versus neighbourhood standard-deviation is calculated. The standard-deviation value where the 2D histogram forms peaks is used as an estimate of the image noise, $\hat{\sigma}_\rho$ and $\hat{\sigma}_Z$. The neighbourhood standard-deviation images (one for $\rho$ tomogram and one for $Z$ tomogram) are thresholded ($< 1.25 \times \hat{\sigma}_\rho$ and $< 1.25 \times \hat{\sigma}_Z$, respectively). The pair of image masks are combined into a single image mask via logical-and operation. The $\rho$ and $Z$ images are masked, and a Gaussian distribution is fit to the truncated histogram (truncated around the relevant quartz $\rho$ (or $Z$) value).

For the Bentheimer sandstone the mean of the segmented quartz density and atomic number map using the above mentioned method, shown in table 5.3, have relative error of 2.64% and 1.44% respectively.

The segmented quartz in Berea sandstone, shows the mean $\rho = 2.64$ with $\hat{\sigma}_\rho = 0.23$ and $Z = 11.79$ with $\hat{\sigma}_Z = 0.48$ which include a relative error of 0.37% and 0.08% respectively. A slice through reconstruction of $\rho$ and $Z$ image of Berea is shown in Fig. 5.14a-ii and b-ii. The estimated relative errors show the estimated results using the full model (5.5) provides good indication of the segmented material.

The sample material of rocks are unknown so I considered the constituent material $Z/A$ value to be i.e., 0.5 because the $Z/A$ of quartz is about 0.499. The $Z$ values can still be estimated independent of $Z/A$ value.

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$</th>
<th>Theoretical $\rho$</th>
<th>Estimated $Z$</th>
<th>Theoretical $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bentheimer (quartz)</td>
<td>2.72</td>
<td>2.65</td>
<td>11.61</td>
<td>11.78</td>
</tr>
<tr>
<td>Berea (quartz)</td>
<td>2.64</td>
<td>2.65</td>
<td>11.79</td>
<td>11.78</td>
</tr>
<tr>
<td>Carbonate (Calcite)</td>
<td>2.57</td>
<td>2.71</td>
<td>15.23</td>
<td>15.71</td>
</tr>
<tr>
<td>Carbonate (Dolomite)</td>
<td>2.81</td>
<td>2.87</td>
<td>13.41</td>
<td>13.74</td>
</tr>
</tbody>
</table>

Table 5.3: Estimated effective atomic number and bulk density of rocks using AMTI model (Section 5.5.1).
Figure 5.14: a-i) reconstructed slice of Berea sandstone at $E_{\text{max}} = 60\text{keV}$, b-i) reconstructed slice Berea sandstone at $E_{\text{max}} = 120\text{keV}$, a-ii) reconstructed slice of the estimated $Z$ using the AMTI model and b-ii) reconstructed slice of the estimated $\rho$ using the AMTI model. The cupping artefacts are evident around the edges in a-i, while a-ii and b-ii don’t have the BH artefacts. The image contrast in enhanced to illustrate the existence of the cupping artefact in a-i and no visible BH in b-i, however the a-ii and b-ii images shows the original grey scales of the images.
The third sample rock is carbonate which consists of calcite and dolomite. For dual-phase segmentation of the carbonate, the masking process is the same but fitting the mixture model is more involved. First a mixture model of two Gaussians is fit to the Z image (parameters are two weights, two means, one standard deviation). A two-Gaussian mixture is also fit to the masked $\rho$ image histogram but with only one parameter (the standard deviation). The weights from the Z mixture module fit are used for the $\rho$ mixture model. The mean values for the $\rho$ mixture model are calculated by further masking the $\rho$ image. The first and second $\rho$ mean is calculated, respectively, by masking +/- one standard deviation of the first and second Z-mean.

Calcite and dolomite have very similar attenuation coefficients which make it difficult to distinguish in a single-energy imaging (see the reconstruction of carbonate sample imaged at 120 keV in Fig. 5.15a-i compared to segmented image in Fig. 5.15b-i). The atomic number of calcite is estimated to be 13.41 with $\sigma_Z = 0.55$ and dolomite is 15.23 with $\sigma_Z = 0.55$ which shows relative error of 5.16% and 2.09% respectively. The calcite and dolomite density estimation using the full AMTI model is 2.57 (gr/cm$^3$) and dolomite density is 2.81 (gr/cm$^3$) which contains 3.05% and 2.40% relative error, respectively. The calcite density relative error shows higher value than the maximum estimated relative error for reference materials. This is due to 1) the carbonate sample tilted between the two scans. This causes the rotation axis to pass through the rock at a different angle and makes accurate registration of projections impossible. The reconstruction is consequently poor at edges (as can be seen in Fig. 5.15b-ii). The segmentation/analysis method described above accounts for this as much as possible; 2) the fact that calcite is the predominant phase of the carbonate sample as shown in segmentation Fig. 5.15b-i and the segmented calcite may contain micro-scale air pores and clay which reduce the accuracy of our estimations; and 3) the heavy filtering of 0.35 mm Cu used for $\varepsilon_2 = 120$ keV spectra which reduce signal-to-noise (SNR) ratio. Since the dominant physical interaction of X-ray with matter in the range of $\varepsilon_2$ is Compton scattering which is dependent on $\rho$, the $\rho$ image are consequently noisy. Calcite and dolomite have similar density values. In this case, atomic number estimations enables materials discrimination and even identification well, as shown in Fig. 5.15b-ii, dolomite is clearly visible as dark patches in the slice through the estimated atomic number reconstruction, compatible with the segmented dolomite regions of Fig. 5.15b-i.

About the tilt in the carbonate reconstruction of image 5.15, I note that the dual-energy experiment started in the first year of my PhD. The experiments include spectrum characterisation and calibration, object scanning and rock scanning. The samples include seven reference materials (aluminium, carbon, marble, acrylic, Teflon, glass and titanium) and the rock samples include Bentheimer and Berea sandstones and a carbonate. These measurements done at ANU1 $\mu$CT system was later upgraded with different components. Also dual energy tomography is a slow process, particularly for high-energy scanning because of the low SNR and long measurement time required to capture the the signal, as mentioned in this thesis. The only titled
image is the carbonate imaged at 120 keV. Therefore, it was not feasible or necessary to re-do the whole process.

The estimation of material properties via the full model are accurate with average relative error of 2.15% for the above mentioned rock samples which make material discrimination possible but the \( \rho \) images are noisy due to heavy filtering. This can be seen (along with the effect of the sample movement) in the results of the Carbonate presented in Fig. 5.15b-ii.

### 5.5.2 Beam hardening correction in AMTI model

As mentioned in section 2.2, conventional reconstruction algorithms assume monochromatic radiation while the X-ray is a function of energy as shown in spectra simulation of Fig. 5.6. This causes inconsistent values in the reconstructed images because physically the lower energy radiation is being attenuated as it passes through the material which leaves harder X-rays. This appears in the form of cupping and/or streaking artefacts in the reconstructed images. Figure 5.14i shows cupping artefacts around the edges of the a slice through the reconstructed image of Berea sandstone captured at 60 keV. An indication of the performance of the model can be seen in the lack of the beam-hardening artefacts in the reconstructions of \( \rho \) and \( Z \) volumes. The AMTI model (5.5) in its full form is a function of energy and should model beam hardening effect. The beam hardening correction is analytical over the broad spectra, and thus inherently superior to single-energy approximate correction methods. This is a direct benefit of the full model that inherently accounts for the beam-hardening in the projections of \( (\frac{0.5}{\pi})\rho Z^{m-1} \) and \( (\frac{0.5}{\pi})\rho \left( (\frac{0.5}{\pi}) \simeq 1 \right) \). The beam hardening artefact shown in Fig. 5.14a-i is corrected in the \( Z \) and \( \rho \) reconstructions in Fig. 5.14a-ii and 5.14b-ii.
Material characterisation using dual-energy imaging and the AM attenuation model

Figure 5.15: a-i) reconstructed slice of the carbonate masked $Z$, b-i) reconstructed slice of the carbonate masked $\rho$, a-ii) reconstructed slice of the estimated $Z$ using the AMTI model 5.5, b-ii) reconstructed slice of the estimated $\rho$ using the AMTI model, a-iii) the plot of fitted Gaussian to histogram of masked $Z$ and b-iii) the plot of fitted Gaussian to histogram of masked $\rho$. 

Draft Copy – 21 November 2016
5.6 Conclusion

The Alvarez and Macovski model has been used broadly for material discrimination purposes in a simplified form (e.g., [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi, 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2010; Kaewkhao et al., 2008]). Here, I have applied the Alvarez and Macovski model in its full form. I calibrated the photoelectric absorption coefficient ($K_1$), Compton scattering coefficient ($K_2$), energy exponent ($m$) and atomic number exponent ($n$) by fitting the full AMAC model and the NIST attenuation coefficient data for a particular setup of reference materials. The relative error between the AMAC model and the NIST attenuation coefficient data shows 1.92% and 5.00% of average and maximum error. This shows an inherent error in the model.

The maximum error occurs for acrylic which doesn’t fit the model well. The relative error in the estimated density of acrylic using the simulated cores in section 5.4.2 and real imaged cylinders in section 5.4.3 subsequently are 5.73% and 7.85% which exceeds the average relative error by 3.81% and 2.85%.

I also calibrated the AMTI model using the simulated projections of cylinders of the reference materials. I applied the calibrated AMTI model to estimate the $\rho$ and $Z$ projections of materials which are later reconstructed to $\rho$ and $Z$ images. The accuracy benchmark shows the AMTI model has 1.96% and 5.00% average and maximum relative error for $\rho$ estimation and 0.88% and 1.82% average and maximum relative error for $Z$ estimation.

I also applied the calibrated the AMTI model to estimate $\rho$ and $Z$ projections of three rocks (Bentheimer and Berea sandstone and a carbonate). I reconstructed 3D projections using filtered back-projection. To obtain the $\rho$ and $Z$ maps of the main components of rocks (quartz in sandstones and calcite and dolomite in carbonate), the $\rho$ and $Z$ tomograms were masked to exclude “material-boundary” voxels determined by standard deviation of local grey levels and fitted Gaussians to the histograms of the masked images. The segmented $\rho$ and $Z$ regions includes 2.80% and 1.50% relative average density and atomic number estimation error.

The error tolerances of $Z$ and for material characterisation purpose are very material dependent. For instance, where the two constituent materials in a sample are very different, e.g., $>1$, with the average 2% error, the material discrimination is still possible. However, similar chemical structure of two materials, e.g., when they only differ in one substance make the material discrimination difficult and obviously the error should be very low.

In this chapter, I showed that given precise knowledge of spectra (see section 5.3.3), the AMTI model is able to differentiate and identify materials via the $\rho$ and $Z$ mapping even if the constituent materials have similar attenuation coefficients in one en-
nergy spectra, provided their $\rho$ and/or $Z$ values vary. However the proposed model calculations requires precise knowledge of spectra and reference materials including $\bar{Z}$ value for the unknown rock sample, it has some benefits such as: 1) The model reasonably corrected beam hardening effect in reconstructed $\rho$ and $Z$ images. 2) it can yield a good average estimated $\rho$ and $Z$ material properties with average of 2.62% and 1.19% with maximum of 7.85% and 2.64% of expected values respectively, and 3) the materials are still identifiable through $Z$ estimation even if the $\rho$ of two constituent materials of sample having similar values and $Z$ is not dependent on $\bar{Z}$. Also, $Z$ estimations are 1.43% more accurate in average than $\rho$ estimations because the images captured at 120 keV suffer from low SNR due to the heavy filtering at high voltage.

The cross-sectional reconstruction images presented figure 5.14 and 5.15 in this chapter and the following chapters are from the mid-plane of the cone beam shown in figure 1.5, therefore it is effectively a fan beam and the effective thickness of the slices are about one voxel, or perhaps slightly more if the point spread function is slightly larger than the voxel size. As a result the SNR are not affected because of the cone beam imaging.

For further improvement, we plan to apply an iterative modification of the density and atomic number estimations on material matching with a material dictionary. In the reconstruction algorithm, we include an iterative update on the initial $\rho$ and $Z$ estimations of materials through the full model and a probabilistic classification to manage the materials distributions based on the material library [Recur et al., 2014b].
Assessment of the full AM model in comparison with two simplified forms

6.1 Introduction

Chapter 5 demonstrated how I used dual-energy imaging and the full Alvarez and Macovski transmitted intensity (AMTI) model to estimate the density ($\rho$) and atomic number ($Z$) of reference materials and rock samples. This model requires exact knowledge of spectra and calibration. The model include considerable computations over the energy range of the spectra. This model also has limitations, e.g., it doesn’t account for K-edges. For that, to date, researchers have applied only simplified forms of the model in various ways [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi, 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2010; Kaewkhao et al., 2008]. Some of these methods are surveyed in section 2.3, as mentioned in section 5.1. Alvarez and Macovski presented the full AMTI model in [Alvarez and Macovski, 1976], however, they used a polynomial simplification of it to estimate $\rho$ and $Z$ of the samples.

This chapter calibrates and uses two of these simplified models including: 1) the Alvarez and Macovski polynomial (AMP) model [Alvarez and Macovski, 1976], that is a simplified form of the AMTI model (see section 5.5) in section 6.2.1, and 2) the Siddiqui and Khames (SK) [Siddiqui et al., 2004] model, that assumes dual-monochromatic approximation of the Alvarez and Macovski attenuation coefficient (AMAC) model (see section 5.1) in section 6.3.

This research was carried out in the “Computed Tomography” group of the Applied Mathematics Department at the Australian National University. I measured the projections of seven reference materials and and three rock samples including Bentheimer and Berea sandstones and a carbonate using the ANU $\mu$CT facility [Sakellariou et al., 2004]. Next, I calibrated the AMP transmitted intensity model in section 6.2.1 and the SK attenuation coefficient model in section 6.3.1 I used the cal-

Draft Copy – 21 November 2016
ibrated models to estimate the \( \rho \) and \( Z \) 3D projections of the sample materials. In relation to segmentation of the 3D tomograms of the rocks, I worked together with Dr Shane Latham. I estimated the mean \( \rho \) and \( Z \) values for the reference materials and the segmented rocks to compared with those of the full AMTI model from sections 5.4.3 and 5.5.1. I am preparing the manuscript of this research for publication with the title and author list as follows:


### 6.2 Alvarez and Macovski Polynomial (AMP) transmitted intensity model

As mentioned in 6.1, Alvarez and Macovski presented the full AMTI model in [Alvarez and Macovski, 1976], however, they mentioned that exact analytic forms of the spectra \( S_i(E) \) (see section 5.3) were not known, thus, they introduced a polynomial approximation of the AMTI model (Eqn. 5.5) to estimate the density and atomic number of materials. Using the power series

\[
\ln(I_E) = b_{E\ell}^E \mathcal{P} + b_{E1}^E \mathcal{C} + b_{E2}^E \mathcal{P}^2 + b_{E3}^E \mathcal{C}^2 + b_{E4}^E \mathcal{P} \mathcal{C} + b_{E5}^E \mathcal{P}^3 + b_{E6}^E \mathcal{C}^3 \tag{6.1}
\]

where

\( I_E \) is the transmitted intensity imaged with maximum tube energy, \( E \); \( E \in \{E_1 = 60\text{keV}, E_2 = 120\text{keV}\} \). \( p(s, E) \) and \( c(s, E) \) are the contributions of photoelectric absorption (PE) and Compton scattering (CS) to the total attenuation coefficient, that are subsequently dependent on \( Z \) and \( \rho \) of the sample materials. For details, please refer to section 5.2.

To be able to use the AMP model, one needs to calibrate the model by estimating the eight coefficients of the model, \( b_{E0}^E, b_{E1}^E, \ldots b_{E7}^E \), having the \( \mathcal{P} \) and \( \mathcal{C} \) images of the reference materials.

#### 6.2.1 The AMP model calibration using the real cylinder images

I used the images of the cylindrical samples of aluminium (Al), carbon (C), acrylic (C\(_5\)H\(_8\)O\(_2\)), marble (CaCO\(_3\)), teflon (C\(_2\)F\(_4\)), glass (SiO\(_2\)), titanium (Ti), as in section 5.4.3, to be able to compare the results of the AMP and AMTI models. The samples were imaged using the cone beam X-ray radiation in a circle trajectory (shown in Fig. 1.5) at 60 keV with 0.5 mm Al filter and 120 keV with 0.35 mm Cu filter (Fig. 5.6).
with 1440 angles of projection with the exposure time of 2 seconds and X-ray current of 100 μA for all cases. The samples were 10.00, 6.08, 10.00, 9.90, 19.56, 10.00, and 6.09 mm in diameter. The source to sample distances (SD) were subsequently 33.8, 17.3, 33.8, 34.5, 71, 35.2, and 17.8 mm, respectively and the camera length (CL) was 1000 mm for all cases.

I simulated the projections, $P$ and $C$ of the cylinders of the mentioned seven reference materials, having their a priori information, $\rho$ and $Z_{\text{eff}}$ (see Eqn. 5.4). The value of the exponent of the atomic number is estimated be $n = 3.20$ (see section 5.4.1). Next, I applied the AMP model (Eqn. 6.1) on the experimental images, $P_{\omega}^E$, of the reference materials, $\omega$, to estimate the calibration parameters, $b_0^E$, $b_1^E$, ... $b_7^E$, in a least-square manner using the relative error as follows:

$$\text{minimise} \sum_{\{b_0^E, b_1^E, ..., b_7^E\}, \omega, \mu, \lambda} \| P_{\omega}^E - (b_0^E + b_1^E P + b_2^E C + b_3^E P^2 + b_4^E C^2 + b_5^E P C + b_6^E P^3 + b_7^E C^3) \|^2.$$

(6.2)

<table>
<thead>
<tr>
<th>Calibration parameters</th>
<th>estimated value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b_0^E$</td>
<td>$-1.82 \times 10^{-1}$</td>
</tr>
<tr>
<td>$b_1^E$</td>
<td>$1.39 \times 10^{-2}$</td>
</tr>
<tr>
<td>$b_2^E$</td>
<td>$6.01 \times 10$</td>
</tr>
<tr>
<td>$b_3^E$</td>
<td>$-3.44 \times 10^{-5}$</td>
</tr>
<tr>
<td>$b_4^E$</td>
<td>$-1.72 \times 10^{3}$</td>
</tr>
<tr>
<td>$b_5^E$</td>
<td>$1.42 \times 10^{-1}$</td>
</tr>
<tr>
<td>$b_6^E$</td>
<td>$3.52 \times 10^{-8}$</td>
</tr>
<tr>
<td>$b_7^E$</td>
<td>$1.86 \times 10^{4}$</td>
</tr>
</tbody>
</table>

Table 6.1: Estimated calibration parameters for AMP model (Eqn. 6.1).
A flowchart of the AMP model calibration and $\rho$ and $Z$ estimation procedure is shown in Fig 6.1. Table 6.1 shows the calibration parameters, $b_0^E$, $b_1^E$, ... $b_7^E$. The calibrated AMP equations, $I_{E_i}$ and $I_{E_j}$, can now be used simultaneously to estimate the $P$ and $C$ projections of the reference materials. I used the Newton-Raphson method to minimise the absolute error over all pixels, $i$ between the calibrated model (6.1) and experimental radiographs of the samples. The $P$ and $C$ projections were reconstructed using filtered back-reconstruction and the average density and atomic number were estimated. Table 6.2 is the accuracy benchmark of $\rho$ and $Z$ estimations using the AMP model (6.1). The average relative error for all the reference materials are $\text{avg}(\frac{\delta \rho}{\rho}) = 4.00\%$, $\text{avg}(\frac{\delta Z}{Z}) = 5.36\%$, with minimum and maximum relative error for density and atomic number equal to $[\text{min, max}](\frac{\delta \rho}{\rho}) = [0.90\%, 9.09\%]$ and $[\text{min, max}](\frac{\delta Z}{Z}) = [0.17\%, 15.24\%]$.

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$ using real data</th>
<th>Relative error of estimated $\rho$</th>
<th>Estimated $Z$ using real data</th>
<th>Relative error of estimated $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>2.56</td>
<td>5.32 %</td>
<td>13.48</td>
<td>3.71 %</td>
</tr>
<tr>
<td>C</td>
<td>1.45</td>
<td>0.90%</td>
<td>6.70</td>
<td>11.72 %</td>
</tr>
<tr>
<td>Marble</td>
<td>2.75</td>
<td>1.92%</td>
<td>15.32</td>
<td>0.17 %</td>
</tr>
<tr>
<td>Acr</td>
<td>1.30</td>
<td>9.09%</td>
<td>5.52</td>
<td>15.24%</td>
</tr>
<tr>
<td>Teflon</td>
<td>2.13</td>
<td>0.92%</td>
<td>8.47</td>
<td>0.22%</td>
</tr>
<tr>
<td>Glass</td>
<td>2.17</td>
<td>2.81%</td>
<td>12.05</td>
<td>3.39%</td>
</tr>
<tr>
<td>Ti</td>
<td>4.82</td>
<td>7.05%</td>
<td>21.32</td>
<td>3.08%</td>
</tr>
</tbody>
</table>

Table 6.2: Estimated effective atomic number and bulk density of reference materials using AMP model (Eqn. 6.1).
§6.2  Alvarez and Macovski Polynomial (AMP) transmitted intensity model

Data Acquisition; μCT imaging using $S_{\varepsilon_1}$; of dual-energy spectra * from Fig. 5.1

Projections of 7 reference materials ($\omega$) imaged using $S_{\varepsilon_1}$

Pre-processing

Theoretical $\rho$ and $Z$ values of material $\omega$

Fit intensity images on AMP model for monochromatic ($E_1, E_2$); Eqn. 6.1

Parameter estimation; ($b_{E_0}, b_{E_1}, ..., b_{E_7}$); Eqn. 6.2

Calibrate the AMP model

Calibrated AMTI model

Parameter estimation; $P$ and $C$ intensity images

Estimated $\rho$ intensity images

CT image reconstruction of $\rho$

Estimated $Z$ intensity images

CT image reconstruction of $Z$

Figure 6.1: Flowchart of the AMP model calibration and $\rho$ and $Z$ estimation, using real intensity images of cylinders of 7 reference materials (Section §6.2), with $\varepsilon$ being the energy label and pre-processing step explained in section §5.5. $P = \int L p(s, E)$ and $C = \int L c(s, E)$ from Eq. 5.3.

Draft Copy – 21 November 2016
6.2.2 Material discrimination of rock using AMP model

In this section, I applied the calibrated AMP model on the rock samples used in section 5.5 which are Bentheimer and Berea sandstones and a carbonate, to calculate their \( \rho \) and \( Z \) distributions. Similarly to the reference materials, first the rock samples were imaged at two different energies: 60 keV with 0.5 mm Al filter and 120 keV with 0.35 mm Cu filter (Fig. 5.6). The experimental set-up are as follows: the rock samples were 10 mm in diameter. The source to sample distances (SD) are 35 mm for Bentheimer and Berea sandstones and 13 mm for the carbonate sample. Camera length (CL) is 1000 mm for all cases. The X-ray current was the same at both 60 and 120 keV, but was varied depending on the material: Berea was imaged at 80 \( \mu \)A, whilst Bentheimer and the carbonate were imaged at 100 \( \mu \)A. The X-ray exposure times for Bentheimer, Berea and the carbonate samples respectively were 3.2, 4 and 3.2 seconds for 60 keV radiation and 2, 2.5 and 2 seconds for 120 keV radiation. The total number of projections were imaged within one circle trajectory (shown in Fig. 1.5) at 1440 angles for Bentheimer and Berea sandstones and at 2880 angles for the carbonate sample. I linearised the projection data (see section 1.2.6.1) and applied alignment [Kingston et al., 2011], auto-focus [Kingston et al., 2010], and drift correction [Myers et al., 2011]. The projection data also masked for the region outside the sample cylinder. Where the estimated atomic number and density using AMTI model were less than or equal to zero, I regularised \( \rho \) and \( Z \) values with \( 1 \times 10^{-3} \) and \( 12 \times 10^{-5} \) (using 12 as the rounded up average atomic number of reference materials).

Having the calibration parameters, \( b_0^E, b_1^E, \ldots, b_7^E \) from table. 6.1, I minimised the absolute error between the calibrated AMP model (6.1) and the measured projections, using the Newton-Raphson method. The estimated \( P \) and \( C \) projections from the mentioned optimisation procedure were reconstructed using Katsevich filtered back-projection reconstruction method [Katsevich, 2002; Varslot et al., 2010], to form the atomic number and density 3D images of Bentheimer, Berea and the carbonate. A single-phase (quartz) segmentation of \( \rho \) and \( Z \) tomograms in Bentheimer and Berea sandstones and dual-phase segmentation (calcite and dolomite) in carbonate were applied to segment the maps of materials.

Figures 6.2a-i and 6.2b-i show a cross-section of 3D reconstructed \( Z \) and \( \rho \) images of Berea and Fig. 6.3a-i and 6.3b-i show a cross-section of 3D reconstructed \( Z \) and \( \rho \) images of carbonate sample. Similar to section 5.5.1 a 2D histogram of neighborhood-mean versus neighborhood-standard-deviation are calculated for \( \rho \) and \( Z \) images of rock samples. The noise of the image, \( \hat{\sigma}_\rho \) and \( \hat{\sigma}_Z \) are calculated as the standard-deviation value at the 2D histogram peaks. The neighborhood standard-deviation images (one each for \( \rho \) and \( Z \) tomograms) are thresholded (< 1.25 * \( \hat{\sigma}_\rho \) and < 1.25 * \( \hat{\sigma}_Z \), respectively). The pair of image masks are combined into a single image mask via logical-and operation. The \( \rho \) and \( Z \) images are masked, and a Gaussian distribution is fitted to the truncated histogram of the relevant quartz \( \rho \) or \( Z \) value. For dual-phase segmentation of the carbonate, the same masking process is the same.
but fitting the mixture model is more involved. First a mixture model of two Gaussians is fit to the Z image (parameters are two weights, two means, one standard deviation). A two-Gaussian mixture is also fit to the masked $\rho$ image histogram but with only one parameter (the standard deviation). The weights from the Z mixture module fit are used for the $\rho$ mixture model. The mean values for the $\rho$ mixture model are calculated by further masking the $\rho$ image. The first and second $\rho$ mean is calculated, respectively, by masking +/- one standard deviation of the first and second Z-mean.

Table 6.3 shows the determined average value and relative errors of $\rho$ and Z for the segmented block of quartz in Bentheimer and Berea sandstones and calcite and dolomite in the carbonate sample. For the Bentheimer sandstone, the mean of the segmented quartz density and atomic number maps, using the above mentioned method, shows the mean $\rho = 2.82 (gr/cm^3)$ with $\sigma_\rho = 0.34$ and $Z = 11.35$ with $\sigma_Z = 0.74$ with relative error of 6.41% and 3.65% respectively. The segmented quartz in Berea sandstone, shows the mean $\rho = 2.79 (gr/cm^3)$ with $\sigma_\rho = 0.31$ and $Z = 11.48$ with $\sigma_Z = 0.70$ which include a relative error of 5.28% and 2.55% respectively. The carbonate sample shows the mean values of $\rho_{\text{calcite}} = 2.30 (gr/cm^3)$ with $\sigma_\rho = 0.31$, $\rho_{\text{dolomite}} = 2.57 (gr/cm^3)$ with $\sigma_\rho = 0.31$, $Z_{\text{calcite}} = 16.81$ with $\sigma_Z = 0.85$ and $Z_{\text{dolomite}} = 15.22$ with $\sigma_Z = 0.85$. The relative error of density of calcite and dolomite are 10.45% and 15.12% respectively and the relative error of atomic number of calcite and dolomite are 7.00% and 9.42% respectively. The above estimations are obtained from comparing the results of this section with the theoretical average $\rho$ and Z values of table 5.3.

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$</th>
<th>Relative error of estimated $\rho$</th>
<th>Estimated Z</th>
<th>Relative error of estimated Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bentheimer (quartz)</td>
<td>2.82</td>
<td>6.41 %</td>
<td>11.35</td>
<td>3.65 %</td>
</tr>
<tr>
<td>Berea (quartz)</td>
<td>2.79</td>
<td>5.28 %</td>
<td>11.48</td>
<td>2.55 %</td>
</tr>
<tr>
<td>Carbonate (Calcite)</td>
<td>2.30</td>
<td>10.45 %</td>
<td>16.81</td>
<td>7.00 %</td>
</tr>
<tr>
<td>Carbonate (Dolomite)</td>
<td>2.57</td>
<td>15.12 %</td>
<td>15.22</td>
<td>9.42 %</td>
</tr>
</tbody>
</table>

Table 6.3: Effective atomic number and bulk density of rocks using AMP model.
Assessment of the full AM model in comparison with two simplified forms

Figure 6.2: a-i) reconstructed slice of the estimated Z of Berea sandstone, using the AMP model (6.1), b-i) reconstructed slice of the estimated $\rho$ of Berea sandstone using the AMP model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$, and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.14b-ii and b-ii for reconstruction slice of Berea sandstone imaged at $E_{\text{max}} = 60$ and 120 keV).
§6.2  *Alvarez and Macovski Polynomial (AMP) transmitted intensity model*  

The AMP model doesn’t require *a priori* information about the dual-energy spectra. The model also doesn’t consider attenuation as a function of energy. As mentioned in section 2.2, ignoring the polychromatic nature of X-rays will produce inconsistent values in the reconstructed image in the form of cupping artefacts around the cylinder edges and streaking between high density materials. This is mostly evident in Z images because Z images are derived from the images that captured at lower energy, e.g., $E_1 = 60$ keV in this set-up, and BH is happening for soft or low-energy X-rays when passes through a sample. Please refer to section 2.2 for more details. As such, the BH artefacts are evident in the cross-section of a 3D reconstruction of Berea sandstone and the carbonate sample in Fig. 6.2(a-i) and 6.3(a-i). However, the estimated $\rho$
reconstructions in Fig. 6.2(b-i) and 6.3(b-i) are lacking BH artefacts because \( \rho \) images are derived from the images captured at higher energy, e.g., \( E_1 = 120 \) keV in this set-up, where the X-ray beam has already higher mean energy.

### 6.3 Siddiqui and Khamees (SK) attenuation model

As mentioned in section 2.3, Siddiqui and Khamees [Siddiqui et al., 2004] (SK) simplified the Alvarez and Macovski attenuation coefficient model (AMAC; see section 5.1) by assuming two monochromatic radiation, as follows:

\[
\mu_E = a_{E_1} \rho(s,E) + a_{E_2} c(s,E). \tag{6.3}
\]

where \( \mu_E \) is the attenuation coefficient of the sample, imaged with monochromatic X-ray radiation of energy, \( E \in \{ E_1 = 60 \) keV, \( E_2 = 120 \) keV\}, where lower and higher energies account for PE and CS energy regions, and \( a_{E_1} \) and \( a_{E_2} \) are undetermined PE and CS coefficients. I also note that the two monochromatic radiation energies are chosen to be an effective energy rather than the peak energy. As mentioned in section 5.3.3, we measured several energy spectra and filters at the very early stage of this research, to find the proper combination of the dual-energy before we used them for measurement of the samples.

The SK model is a post-reconstruction model, thus, uses the reconstructed image to estimate the density and atomic number images. As shown in Eqn. 5.3, \( p(s,E) \propto \rho Z^{n-1} \) and \( c(s,E) \propto \rho, \) thus having \( \mu_{E_1} \) and \( \mu_{E_2} \), density and atomic number images can be calculated as follows:

\[
\rho = \frac{a_{E_2} \mu_{E_1} - a_{E_1} \mu_{E_2}}{a_{E_1} a_{E_2} - a_{E_1} a_{E_2}}, \quad Z = \sqrt[3]{\frac{a_{E_2} \mu_{E_1} - a_{E_1} \mu_{E_2}}{a_{E_1} \mu_{E_2} - a_{E_2} \mu_{E_1}}} \tag{6.4}
\]

For the AMTI (see section 5.4.3) and AMP (see section 6.2) models, I estimated and reconstructed the \( \mathcal{P} \) and \( \mathcal{C} \) projections. From those, I then extracted the \( \rho \) and \( Z \) images and segmented the maps of materials in the sample. However, the SK model directly estimates \( \rho \) and \( Z \) images from the reconstructed image. The SK requires calibration for \( a_{E_1}, a_{E_1}^2, a_{E_2} \) and \( a_{E_2}^2 \). The Sk model is calibrated in section 6.3.1 and used in section 6.3.2 to estimate the \( \rho \) and \( Z \) images of the sample materials. Figure 6.4 depicts a flowchart of these processes.
§6.3 Siddiqui and Khamees (SK) attenuation model

Data Acquisition;μCT imaging at $E_{\text{max}}^1$

Projections of reference material ($\omega$) at $E_{\text{max}}^1$

CT image reconstruction at $E_1$

Data Acquisition;μCT imaging at $E_{\text{max}}^2$

Projections of reference material ($\omega$) at $E_{\text{max}}^2$

CT image reconstruction at $E_2$

Fit SK model for monochromatic ($E_1$, $E_2$) on reconstruction images

Parameter estimation; $(a_{E_1}, a_{E_2}, a_{E_1}, a_{E_2})$; Eqn. 6.4

Calibrate the SK model; Eqn. 6.3

Calibrated AMTI model

Parameter estimation; $\rho$ and $Z$ reconstructions

Theoretical $\rho$ and $Z$ values of reference materials

Estimated $\rho$ reconstructed images

Estimated $Z$ reconstructed images

Figure 6.4: Flowchart of the SK model calibration and $\rho$ and $Z$ estimation, using reconstructed images of cylinders of reference materials (Section 6.3). One can choose to have different number of reference materials, $\omega$. We have chosen 7 reference materials, commonly used at the Anu $\mu$CT facility, for the calibration of the models in chapter 5 to 8. This materials are over a range of atomic number and density.
Assessment of the full AM model in comparison with two simplified forms

6.3.1 The SK model calibration using the real cylinder images

To calibrate the SK model, the 3D projections of the seven reference materials were recorded at two energies: 60 keV with 0.5 mm Al filter and 120 keV with 0.35 mm Cu filter with the experimental set-up explained in section 6.2.1. The projections imaged at the lower energy $E_1 = 60$ keV includes the BH artefacts (see section 2.2 for more details). To corrects the BH artefacts, I applied the power law BH linearisation method (see chapter 4). The exponent of the power law is varied to achieve an optimised BH correction. This corrects the cupping artefacts in the reconstructed image, as shown in the image of the cross-section of the Berea sandstone and the carbonate in Fig. 6.5(a-i) and 6.6(a-i). The BH correction changes the intensity values and hinders the accurate reconstruction of $\mu$. This will reduce the accuracy of the estimation of $p(s, E)$ and $c(s, E)$ from Eqn. 6.3 and consequently the estimation of $Z$ and $\rho$ from Eqn. 6.4.

I fitted the tomograms of reference materials with the SK model (6.4) in a least square manner, as shown in Eqn. 6.5 and estimated the calibration parameters, $a_{E_1}^{E_1}$, $a_{E_2}^{E_1}$, $a_{E_2}^{E_1}$ and $a_{E_2}^{E_2}$, that are shown in table 6.4.

$$\text{minimise} \sum_{E, \omega, i} \| \mu^{\omega}(s, E) - [a_{E_1}^{E_1} p(s, E) + a_{E_2}^{E_1} c(s, E)] \|^2. \quad (6.5)$$

<table>
<thead>
<tr>
<th>Calibration parameters</th>
<th>estimated value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{E_1}^{E_1}$</td>
<td>$4.02 \times 10^{-5}$</td>
</tr>
<tr>
<td>$a_{E_2}^{E_1}$</td>
<td>$1.22 \times 10^{-2}$</td>
</tr>
<tr>
<td>$a_{E_1}^{E_2}$</td>
<td>$5.31 \times 10^{-6}$</td>
</tr>
<tr>
<td>$a_{E_2}^{E_2}$</td>
<td>$1.57 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 6.4: Estimated calibration parameters for SK model (Eqn. 6.4).

The estimated calibration parameters of the SK model, $a_{E_1}^{E_1}$, $a_{E_2}^{E_1}$, $a_{E_2}^{E_1}$ and $a_{E_2}^{E_2}$, can be used in Eqn 6.4 to estimate the density and atomic number tomograms of the seven reference materials. Table 6.5 shows the accuracy benchmark of calibration of the SK model using the experimental images of reference materials. The average relative error for all the reference materials are $\text{avg}(\delta_\rho/\rho) = 6.63\%$, $\text{avg}(\delta_Z/Z) = 7.44\%$, with minimum and maximum relative error for density and atomic number equal to $[\text{min}, \text{max}] (\delta_\rho/\rho) = [0.67\%, 14.07\%]$ and $[\text{min}, \text{max}] (\delta_Z/Z) = [0.22\%, 14.00\%]$. 

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Material names | Estimated $\rho$ using real data | Relative error of estimated $\rho$ | Estimated Z using real data | Relative error of estimated Z
---|---|---|---|---
Al | 2.80 | 3.70 % | 12.36 | 7.31 %
C | 1.37 | 6.16 % | 6.84 | 14.00 %
Marble | 3.08 | 14.07 % | 14.38 | 6.25 %
Acr | 1.18 | 0.67 % | 7.35 | 13.58 %
Teflon | 1.93 | 10.23 % | 8.80 | 4.14 %
Glass | 2.33 | 4.48 % | 10.88 | 6.60 %
Ti | 4.18 | 7.11 % | 21.95 | 0.22 %

Table 6.5: Estimated effective atomic number and bulk density of reference materials using SK model (Eqn. 6.3).

### 6.3.2 Material discrimination of rock using SK model

In this section, I applied the same method as in section 6.3.1 to calculate density and atomic number distributions in several rock samples including Bentheimer and Berea sandstones and a carbonate. I used the experimental images of rock samples used in section 6.3.2. The recorded 3D projections were first reconstructed using the Katsevich filtered back-projection reconstruction method [Katsevich, 2002; Varslot et al., 2010] after the pre-processing (linearisation, alignment [Kingston et al., 2011], auto-focus [Kingston et al., 2010] and drift correction [Myers et al., 2011]) and BH correction (see section 4). Next, I applied the calibrated SK model (see section 6.3.1) to estimate the atomic number and density 3D reconstructions and segmented the rocks, as described in section 6.3.2. Figure 6.5a-i and Fig. 6.6a-i show a cross-section of the 3D reconstructed of Z of the Berea sandstone and the carbonate, respectively and Fig. 6.5b-i and Fig. 6.6b-i show a cross-section of the 3D reconstruction of the $\rho$ of the Berea sandstone and the carbonate respectively. Table 6.6 shows the average value and relative errors of the segmented materials in the Z and $\rho$ reconstructions.

The atomic number of quartz in Bentheimer is estimated to be 8.67 with $\sigma_Z = 0.18$ and density is estimated to be 3.34 (gr/cm$^3$) with $\sigma_\rho = 0.15$ (gr/cm$^3$) showing relative error of 26.04% and 26.48% respectively. The atomic number of quartz in Berea is estimated to be 8.41 with $\sigma_Z = 0.22$ and the density is estimated to be 3.37 (gr/cm$^3$) with $\sigma_\rho = 0.15$ showing relative error of 28.56% and 27.36% respectively. For the carbonate sample, the atomic number is estimated to be 11.30 with $\sigma_Z = 0.23$ for calcite and 10.54 with $\sigma_Z = 0.22$ for dolomite, showing a relative error of 23.29% and 32.90% respectively. The calcite and dolomite density estimation using the SK model is 3.39 (gr/cm$^3$) with $\sigma_\rho = 0.22$ and dolomite density is 3.41 (gr/cm$^3$) with $\sigma_\rho = 0.23$, showing 25.20% and 18.81% relative error respectively.
Assessment of the full AM model in comparison with two simplified forms

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$</th>
<th>Relative error of estimated $\rho$</th>
<th>Estimated $Z$</th>
<th>Relative error of estimated $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bentheimer (quartz)</td>
<td>3.34</td>
<td>26.04 %</td>
<td>8.67</td>
<td>26.48 %</td>
</tr>
<tr>
<td>Berea (quartz)</td>
<td>3.37</td>
<td>27.36 %</td>
<td>8.41</td>
<td>28.56 %</td>
</tr>
<tr>
<td>Carbonate (Calcite)</td>
<td>3.39</td>
<td>25.20 %</td>
<td>11.30</td>
<td>23.29 %</td>
</tr>
<tr>
<td>Carbonate (Dolomite)</td>
<td>3.41</td>
<td>18.81 %</td>
<td>10.54</td>
<td>32.90 %</td>
</tr>
</tbody>
</table>

Table 6.6: Effective atomic number and bulk density of materials

Figure 6.5: a-i) reconstructed slice the estimated $Z$ of the Berea sandstone, using the SK model 6.3, b-i) reconstructed slice of the estimated $\rho$ of the Berea sandstone using the SK model, a-ii) the plot of fitted Gaussian to the histogram of masked $Z$ and b-ii) the plot of fitted Gaussian to the histogram of masked $\rho$ (see Fig. 5.14a-ii and b-ii for reconstruction slice of Berea sandstone images at $E_{\text{max}} = 60$ and 120 keV).
§6.4 Assessing the atomic number and density estimations of AMP and SK models in comparison with the results of the full AMTI model (from chapter 5)

The accuracy benchmark of the AMTI (table 5.2), AMP (table 6.2) and SK (table 6.5) models show the average error, $\text{avg}(\delta Z)$, of the estimated atomic number for all reference materials using these models, respectively, are 1.26%, 5.36% and 7.44%. The average error of the estimated density values, $\text{avg}(\delta \rho)$, for all reference materials,
Assessment of the full AM model in comparison with two simplified forms respectively, are 2.87%, 4.00% and 6.63%. This shows that the atomic number estimation of reference materials using the AMTI model is 4.10% and 6.18% more accurate than the AMP and SK models respectively. Similarly, the density estimation of reference materials using the AMTI model is 1.13% and 3.76% more accurate than the AMP and SK models respectively.

The atomic number and density estimations include the minimum and maximum relative errors, $[\min, \max](\delta Z)$ and $[\min, \max](\delta \rho)$, of [0.45%, 2.64%] and [0.97%, 7.85%] for the AMTI model, [0.17%, 15.24%] and [0.90%, 9.09%] for the AMP model, and [0.22%, 14.00%] and [0.67%, 14.07%] for the SK model, respectively. These results show that the AMTI model delivers more consistent results and lower maximum errors than the AMP and SK models results. The maximum error in the AMP and SK model results were 12.60% and 11.36% in atomic number estimation and 1.24% and 6.22% in density estimation, respectively. These results show that $Z$ and $\rho$ estimations using the full AMTI model (5.5) provide a good indication of the segmented material, i.e., the average $Z$ estimations are at least 11.00% more accurate than the two simplified models examined in this section.

The segmented quartz of the Bentheimer and Berea sandstones and the segmented dolomite and calcite of the carbonate sample have average atomic number errors, $\text{avg}(\delta Z)$, $\text{avg}(\delta \rho)$, 2.19%, 2.11% for the AMTI model, 13.71%, 9.31% for the AMP model and 27.81%, 24.35% for the SK model. The atomic number and density estimations include the minimum and maximum relative errors, $[\min, \max](\delta Z)$ and $[\min, \max](\delta \rho)$, of [0.08%, 5.16%] and [0.37%, 3.05%] for the AMTI model, [2.55%, 9.42%], [5.28%, 15.12%] for AMP model and [23.29%, 32.90%], [18.81%, 27.36%] for the SK model, respectively. The results show that AMTI model when compared to the AMP and SK models, has 11.52% and 25.62% more accurate results for atomic number and is also 7.2% and 22.24% more precise for density values, respectively.

As shown above, the atomic number and density estimation using the AMTI model provides a more accurate indication of the materials making material discrimination possible. The higher errors of the simplified models hinder the possibility of material characterisation, specifically for materials that have close material properties. The estimated atomic number and density using the AMTI model are at least 7.2% and 11.52% more accurate in rock samples than those of the AMP and SK models.
6.5 Conclusion

In this chapter, I calibrated and used two simplified forms of the Alvarez and Macovski model [Alvarez and Macovski, 1976] for estimation of density and atomic number of samples: 1) Alvarez and Macovski applied a polynomial model (AMP) to estimated density and atomic numbers after they presented the full model in [Alvarez and Macovski, 1976], and 2) Siddiqui and Khamees [Siddiqui et al., 2004] (SK) in which the attenuation coefficient is modelled as a contribution of PE and CS recorded at two monochromatic radiation. The AMP and SK models required calibration before they could be applied. I calibrated these two models using the images of seven reference materials. I built an accuracy benchmark for the estimated Z and $\rho$ values using the AMP and SK models to compare with the theoretical values of the materials and the results of the AMTI model in section 5.4.3. These show that the results of the AMTI model are more consistent, and have lower maximum error compared to the results of the AMP and SK models, i.e., 12.60% and 11.36% in atomic number estimation and 1.24% and 6.22% in density estimation, respectively. The AMP model performs the analyses on projections, while the SK model is applied on the reconstructed images.

I also imaged three rock samples, Bentheimer and Berea sandstones and a carbonate, and applied the calibrated the AMP and SK models to them to estimate the density and atomic number images and compare with the results of the AMTI model in section 5.5. This showed that, the results of the AMTI model when compared to the AMP and SK models, are more accurate by 11.52% and 25.62% in atomic number and 7.2% and 22.24% in density, respectively.

As explained in section 4.6, the $\rho$ images are noisy due to heavy filtering of 0.35 mm Cu used for 120 keV spectra that reduces the signal-to-noise (SNR) ratio, along with the effect of the sample movement shown in Fig. 5.15b-ii, and the requirement of a priori information ($\frac{Z}{A}$). Calcite and dolomite have similar density values. In this case, given the more reliable results for atomic number, I compared the images of a cross-section of the atomic number obtained by using these three methods. For the Z estimation using the AMTI model in Fig. 5.15a-ii, the image shows dolomite is clearly visible as dark patches in the slice through the estimated atomic number reconstruction, compatible with the segmented dolomite regions of Fig. 5.15b-i. However, the reconstruction of the estimated Z using the AMP model shown in Fig. 6.3 are distorted by BH artefacts. Figure 6.6a-ii shows the Z reconstruction using the SK model, and there dolomite and calcite are not clearly distinguishable.

As mentioned above, the AMP model, similar to the AMTI model, performs the analyses on the projections, however unlike the AMTI mode, the AMP model doesn’t account for the energy dependency of attenuation coefficients and doesn’t consider the X-ray spectrum of energy, thus, the image captured at $E_{\text{max}} = 60$ keV includes
BH artefacts (see section 2.2) that are clearly visible in Z reconstructions, Fig. 5.15a-i and 6.2h-i.

The results from the SK method are more stable since analysis is performed directly on the tomogram. However, since BH correction (see chapter 3) must be performed on the low-energy reconstructions, this hinders any accurate estimation of $\rho$ and $Z$. The full AMTI model, by contrast, analyses the projection images directly and inherently accounts for BH. It is therefore more accurate in estimation of material properties but less stable, i.e., more noisy. This can be seen in the results of the carbonate presented in Fig. 5.15.

Although applying the full model requires precise knowledge of the spectra, the full model yields, on average, 7.81% and 15.9% for atomic estimation and 4.73% and 13.00% for density estimation more accurate results than AMP and SK respectively. Reference materials are require for calibration of both full and simplified forms of the Alvarez and macovski model. The full model is able to identify calcite from dolomite even though they have similar attenuation coefficients. Finally, the full model accounts for BH reasonably well.
Chapter 7

Material characterisation using single-energy imaging and statistical variance

7.1 Introduction

In this chapter, a method is presented to estimate the density ($\rho$) and atomic number ($Z$) of sample materials from measurements of the X-ray transmitted intensity and its statistical variance. This method requires single-energy imaging, and thus, eliminates the requirements of dual-energy imaging of the AMTI model (see chapter 5) and its simplified forms (see chapter 6). The registered X-ray transmitted intensity on the detector and, similarly, a Poissonian variation of it in repeated measurements, are dependent to the “average” energy of detected quanta of the X-ray spectra. As such, the measurement of Fano factor yields the information of average energy. The variance of the registered intensity images from repeated measurements delivers similar information to the higher energy information required in dual-energy imaging. I modified the AMTI model (see section 5.2) and presented the transmitted intensity and statistical variance (TIV) model and applied several spectra with different filters to examine the effect of energy and spectra on $\rho$ and $Z$ calculations. More registered photons and a higher number of images for statistical variance estimation results in less relative error in $\rho$ and $Z$ estimations.

Section 7.2 reviews the definition of Fano factor and the correlation of transmitted intensity and variance in X-ray µCT. Section 7.3 develops the theory of tomography of $\rho$ and $Z$ of materials using single-energy imaging and statistical variance and presents the TIV model. Section 7.4 calibrates the TIV model using the simulation of X-ray transmitted intensity images and estimation of mean and statistical variance images for a given setup using the attenuation coefficient data of a set of reference materials obtained from the National Institute of Science and Technology (NIST), then applies the calibrated TIV model to estimate the $\rho$ and $Z$ images. Section 7.5 demonstrates the simulation of X-ray transmitted intensity images using the simulated projections of the cylinders of materials generated randomly in a Gaussian distribution, and their statistical variance. This works as a simulation of noise seen in experimental
Material characterisation using single-energy imaging and statistical variance

In this chapter, I applied the above mentioned proportionality (Eqn 7.7) in \( \mu\)CT for material characterisation. I sought the advice of Dr Andrew Kingston about using this proportionality as the required higher energy information in dual-energy. From applying this proportionality, Andrew and I discovered that the \( \sigma^2 \) projections can replace the higher energy requirements of the dual-energy imaging (5.3.3) and modified the AMTI model and presented the TIV model that requires imaging only at a single-energy spectra. I then simulated the projections of reference materials and calibrated the TIV model using those projections. Next, I used the calibrated TIV model to estimate the \( \rho \) and \( Z \) of sample materials. The theory and implementation of this research is in preparation for publication with the title and author list as follows:

7.2 The correlation of Transmitted Intensity and Variance

Fano noise, first described by Ugo Fano in 1947 [Fano, 1947], when he measured the fluctuation of an electric charge obtained in a detector. The Fano factor is defined as:

\[ F = \frac{\sigma^2}{I_0} \]  

(7.1)

where Fano factor, \( F \), is the coefficient of fluctuations or measurement of the dispersion of a probability distribution due to Fano noise, \( \sigma^2 \) is variance and \( I_0 \) is the mean of random processes in a time window, \( \varepsilon \).

The Fano factor (\( \frac{\sigma^2}{I_0} \)) has been used in different instances to derive quantum information. It is important in electronics, telecommunications, optical detection, and fundamental physics [Schottky, 1918; Hull and Williams, 1925; Fullagar et al., 2008; Uhlig et al., 2011]. When the finite number of particles that carry energy (such as electrons in an electronic circuit or photons in an optical device) is sufficiently small, the fluctuations, which are the occurrence of independent random events, are significant. Schottky in 1918 [Schottky, 1918] studied the fluctuations of current in vacuum tubes. In electronics [Schottky, 1918; Hull and Williams, 1925], this noise consists of random fluctuations of the electric current in a DC current that originate due to fact that current actually consists of a flow of discrete charges (electrons).

By monitoring how the fluctuations vary with the mean signal, one can estimate the contribution of a single occurrence, even if that contribution is too small to be detected directly. For example, the charge \( (e) \) on an electron can be estimated by correlating the magnitude of an electric current, \( I \), with its noise. If \( N \) electrons pass a point in a given time, \( \varepsilon \), on the average, the mean current is \( I = \frac{eN}{\varepsilon} \). Since the current fluctuations should be of the order \( \sigma_I = \frac{e\sqrt{N}}{\varepsilon} \) (i.e., the standard deviation of the Poisson process), the charge \( e \) can be estimated from the ratio \( \frac{e\sigma^2}{I^2} \). The Poisson noise is modelled as follows:

\[ P = \frac{\lambda^k e^{-\lambda}}{k!} \]  

(7.2)

where \( k \) is the number of occurrences, \( \lambda \) is the expected value or average number of events in a time window \( \varepsilon \) and \( k! \) is the \( k \) factorial.

In optics, Poisson noise describes the fluctuations of the number of photons detected due to their occurrence independent of each other. The correlation of \( \sigma^2 \) and \( I_0 \) of Eqn. [7.1] is neglected in X-ray CT imaging. In \( \mu \)CT, the mean of random process, \( I_0 \) of Eqn. [7.1] is the mean of the X-ray transmitted intensity in repeated measurements. The detected X-ray transmitted intensity on the detector using the spectrum, \( \varepsilon \), contains two variable factors: 1) detected number of photons; and 2) acquisition time.
These effects are inspected in section 7.5.2. Within this and the next chapter, I apply this correlation to extract quantum information which supports material characterisation (section 7.3) and BH correction (section 8.3 and 8.4).

### 7.3 Transmitted Intensity and Variance (TIV) model for material characterisation

Assuming a monochromatic radiation, the registered X-ray intensity, $I$, can be represented as follows:

$$I(E) = N(E) \cdot E \cdot P(E)$$

where $N(E) = N_0(E) \cdot Q(E)$ is the number of X-ray photons at energy $E$, $N_0(E)$ is the number of photons incident on a detector and $Q(E)$ is the quantum efficiency of the detector. Quantum efficiency $Q(E)$ describes the detector’s stopping probability of the original quanta. $P(E)$ is the proportional contribution of each quantum’s energy to the detected intensity, $P(E) = C(E) \cdot A(E) \cdot T(E)$, that consists of functions that characterise the physical losses including non-detected quanta converted to heat within a certain detector setup, $C(E)$, its amplification of opams, $A(E)$, and inherent digital conversion errors, $T(E)$. For our simulations given the energy range of 0 to 120 keV, the quantum efficiency $Q(E)$ is assumed to be 1.00 and $P(E) = \frac{1}{\text{avg}(E)}$, where avg$(E)$ is the average energy.

Expanding the measured intensity Eqn. 7.3 by considering the polychromatic nature of X-rays (see the full Beer-Lambert law in Eqn. 1.3), results in:

$$I_\varepsilon(E) = -\int_0^{E_{\text{max}}} N(E) \cdot E \cdot P(E) \cdot \exp\left[-\int L \cdot \mu(s,E) \, ds\right] \, dE,$$

where $N(E) = S_\varepsilon(E)$ is the transmitted intensity with the label, $\varepsilon$, related to the X-ray radiation with maximum energy, $E_{\text{max}}$. $I_\varepsilon(E)$ is the registered X-ray intensity on the detector over all photon energies $[0, E_{\text{max}}]$.

From measurement of the Poissonian variation of the measured intensity, $\sigma = \sqrt{N\cdot\text{EP}(E)}$, the statistical variance assuming a polychromatic radiation can be presented as:

$$\sigma^2_\varepsilon(E) = -\int_0^{E_{\text{max}}} N(E) \cdot E^2 \cdot P^2(E) \cdot \exp\left[-\int L \cdot \mu(s,E) \, ds\right] \, dE,$$

where $N(E) \cdot E^2 \cdot P^2(E) = S_\varepsilon(E)$ is the incident X-ray intensity spectrum modulated...
by detector quantum efficiency and spectral transmission of non-sample attenuating materials between source and detector. For further information about the modelling and measurement of $S_\varepsilon(E)$ refer to section 5.3. Considering the photon counts, $N(E)$, and the detector observation of the quanta’s energy, $P(E)$, the X-ray spectrum of Eqn. 5.6 can be represented as follows:

$$\begin{cases} S_{\varepsilon_1}(E) = N(E).E.P(E), \\ S_{\varepsilon_2}(E) = N(E).E^2.P^2(E) = S_{\varepsilon_1}(E).E.P. \end{cases}$$

(7.6)

$S_\varepsilon$ for $\varepsilon \in \{\varepsilon_1, \varepsilon_2\}$ are the X-ray spectra of $I_\varepsilon(E)$ (see Eqn. 7.4) and $\sigma_\varepsilon^2(E)$ (see Eqn. 7.5), that corresponds to dual-energy imaging (see section 5.3.3). $S_{\varepsilon_1}$ and $S_{\varepsilon_2}$ are respectively dominant at photoelectric absorption (PE) and Compton scattering (CS) energy regions. For further information regarding the interactions of X-ray with matter (PE and CS), refer to section 1.2.5. Figure 7.1 shows the dual-energy spectra, $S_{\varepsilon_1}$ and $S_{\varepsilon_2}$.

![Figure 7.1: Simulated energy spectra at 100 keV maximum energy with 0.5 mm aluminium filter (red line) and the spectrum including higher mean energy (blue line); modified to match that seen for our experimental protocol.](image)

From Eqns. 7.3 and 7.5 the Fano factor over the energy range $[0, E^\text{max}_\varepsilon]$, considering no sample ($\mu = 0$), is equal to:

$$\frac{\sigma_\varepsilon^2(E)}{I_\varepsilon(E)} = \frac{\int_0^{E^\text{max}_\varepsilon} N(E) \cdot E^2 \cdot P^2(E)}{\int_0^{E^\text{max}_\varepsilon} N(E) \cdot E \cdot P(E)} = \frac{< S_\varepsilon(E) \cdot E \cdot P^2(E) >}{< S_\varepsilon(E) \cdot P(E) >}.$$  

(7.7)
Eqn 7.7 shows that $\sigma^2_\varepsilon$, on average, is proportional to energy. This proportionality is the reason that $\sigma^2_\varepsilon$ is probing at higher energy than $I_\varepsilon$, as shown in Fig. 7.1.

From section 5.2, I know that dual-energy imaging is able to estimate material properties because the attenuation coefficient can be represented in the form of a two-basis function that describes the contribution of PE at lower energies and CS at higher energies to the total attenuation coefficients, in a typical $\mu$CT imaging energy range [1, 120] keV. PE and CS are, subsequently, proportional to the $Z^{3.2}$ and $\rho$ of sample materials. However, Fig 7.1 and Eqn. 7.7 show that $\sigma^2_\varepsilon(E)$ can be used as an alternative to present the information of higher energy. Consequently, I modified Eqns. 7.8 and 7.10 to be able to apply them for $\rho$ and $Z$ estimations of the sample materials, as such:

\[
I_\varepsilon = - \int_0^{E_{\text{max}}} N(E) E P(E) \exp \left[ \int_L \frac{p(s, E) \, ds}{E^m} + \int_L c(s, E) \, ds f_{Kn}(E) \right] \, dE,
\]

\[
\sigma^2_\varepsilon = - \int_0^{E_{\text{max}}} N(E) E^2 P^2(E) \exp \left[ \int_L \frac{p(s, E) \, ds}{E^m} + \int_L c(s, E) \, ds f_{Kn}(E) \right] \, dE
\]

(7.8)

where projections of $\int_L p(s, E)$ and $\int_L c(s, E)$ represent the contribution of PE and CS to X-ray mean transmitted intensity and statistical variance images. These projections are defined to be $K_1^Z \frac{\rho}{A} Z^{n-1}$ and $K_2^Z \frac{\rho}{A}$ (see Eqn. 5.3), where $K_1$ and $K_2$ are constants, $A$ is atomic weight of material, $Z = Z(s)$ is the atomic number and $\rho = \rho(s)$ is the density of materials (see section 5.2). Section 7.4 and 7.5 demonstrate how I used Eqn. 7.8, henceforth referred to as the TIV method, to estimate $\rho$ and $Z$ of samples.
7.4 Testing the TIV model using simulated intensity and variance images

To be able to compare the results of this section with the results of the full AMTI model, I have chosen the seven reference materials of section 5.4. These materials are: aluminium (Al), carbon (C), acrylic (C₅O₂H₈), marble (CaCO₃), teflon (C₂F₄), glass (SiO₂) and titanium (Ti)) with 10.00, 6.08, 10.00, 9.90, 19.56, 10.00, 6.09 mm diameter, respectively. The source to sample distances (SD) are 33.8, 17.3, 33.8, 34.5, 71, 35.2, 17.8 mm, respectively and camera length (CL) is 1,000,000 mm for all cases. The samples were imaged using the cone beam X-ray radiation in a circle trajectory (shown in Fig. 1.5) at 100 keV maximum energy with 0.5 mm Al filter (S₁₁), as shown in Fig. 7.1. I obtained the attenuation coefficient data \[ \mu ρ(E) \] of the materials, from the NIST database. Having the attenuation coefficients and the information about the setup of the ANU µCT system, I simulated radiographs \[ I_ω(\text{sim}) \] of cylinders of reference materials, \( ω \). Next, I used Eqn. 7.4 to simulate the statistical variance image, \( σ^2_ω \).

The TIV model requires calibration of \( K_1 \) and \( K_2 \) constants before using those to estimate density and atomic number of materials. For these, I simulated \( ρ \) and \( Z_{\text{eff}} \) (see Eqn. 5.4) projections of reference materials to build \( \int_L p(s, E) \, ds \) and \( \int_L c(s, E) \, ds \) projections (see Eqn. 5.3). I used the estimated exponent of energy, \( m = 3.00 \), and atomic number, \( n = 3.20 \) of section 5.4.1.

To calibrate the model, I applied the projections of \( \int_L p(s, E) \) and \( \int_L c(s, E) \) to the TIV model (7.4) to compare with that predicted data (projections of \( I_ω \) and \( σ^2_ω \)) in a least square manner using the relative error, as follows:

\[
\begin{align*}
\text{minimise } & \{ K_1, K_2 \} & \\
\sum_{\ell,ω,i} \| I_ω(\text{sim}) & - \int_0^{E_{\text{max}}} N(E) \, E \, P(E) \, \exp \left[ \frac{\int_L p(s, E) \, ds}{E^m} + \int_L c(s, E) \, ds \, f_{\text{KN}}(E) \right] \, dE \|^2, \\
\sum_{\ell,ω} \| σ^2_ω(\text{sim}) & - \int_0^{E_{\text{max}}} N(E) \, E^2 \, P^2(E) \, \exp \left[ \frac{\int_L p(s, E) \, ds}{E^m} + \int_L c(s, E) \, ds \, f_{\text{KN}}(E) \right] \, dE \|^2. \\
\end{align*}
\]
Figure 7.2: A line through a simulated projection cylinder and the TIV model fit: at 100 keV (red line and dashed cyan line) and 120 keV (blue and dashed green line) maximum energies for a) glass and b) aluminium.

I used the input spectra $S_{\varepsilon_1}(E)$ and $S_{\varepsilon_1}(E)$ of Fig. 7.6. Figure 7.2(a) and (b) show a horizontal line through the simulated projection image of glass and marble cylinders and the TIV model fit on them.

In order to use the calibrated TIV model to estimate the density and atomic number of materials, I applied the Newton-Raphson method to minimise the absolute error of Eqn. 7.9 over all pixels, $i$, to estimate projections of $\rho_{\text{Z}_A}$ and $\rho_{\text{Z}_A}$. The projections are then reconstructed using filtered back-projection algorithm (see section 1.2.7.3) to generate $\rho$ and $Z$ images of the samples. Table 5.2 shows average $\rho$ and $Z$ estimation using the TIV model and theoretical values. The density and atomic number error intervals are [0.45%, 6.16%] and [0.01%, 2.62%] respectively with an average relative error of 3.63% and 1.29%. The $Z$ estimations using the TIV model and simulated data, compared to the results of the simulations of dual-energy material characterisation in sections 5.4.2, shows an average of 0.41% higher error and the $\rho$ estimations have an average 1.17% higher error. This is because the spectra of intensity-variance is not as distinct as the dual-energy spectra of section 5.3.3. However, the TIV method requires image acquisition only at a single-energy spectrum. The flowchart of Fig. 7.5 illustrates the above mentioned processes for calibration of the TIV model and the $\rho$ and $Z$ estimations using the model.
§7.4 Testing the TIV model using simulated intensity and variance images

Data Acquisition; from NIST for \([1, E_{E_1}^{\text{max}}]\), of dual-energy spectra \(*\) from Fig. 5.1

Attenuation coefficient \([\mu(E)]\) of 7 reference material \((\omega)\) in \([1, E_{E_1}^{\text{max}}]\)

Simulate \(I\) projections of materials \(\omega\) for \([1, E_{E_2}^{\text{max}}]\); Eqn. [7.4] for the methods of section 7.3

Simulate \(\sigma^2\) projections of materials \(\omega\) for \([1, E_{E_1}^{\text{max}}]\); Eqn. [7.4] for the methods of section 7.3

Fit \(I\) and \(\sigma^2\) projections on TIV model; Eqn. 7.9

Theoretical \(\rho\) and \(Z\) values of material \(\omega\)

\((m, n); \diamond\) from Fig. 5.8

Parameter estimation; \((K_1, K_2)\)

Calibrate the TIV model

Calibrated TIV model

Parameter estimation; \(P\) and \(C\) intensity images

Estimated \(\rho\) intensity images

Estimated \(Z\) intensity images

CT image reconstruction of \(\rho\)

CT image reconstruction of \(Z\)

Dual-energy spectra; \(S_{E_1} \& S_{E_2}\) from Fig. 7.6

Figure 7.3: Flowchart of the TIV model calibration and \(\rho\) and \(Z\) estimation, using simulated projections of cylinders of 7 reference materials (Section 7.4), with \(\epsilon\) being the energy label. \(P = \int p(s, E)\) and \(C = \int c(s, E)\) from Eq. 5.3
Table 7.1: Estimated effective atomic number and bulk density of reference materials using TIV model (Section 7.4).

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$ using sim data</th>
<th>Relative error of estimated $\rho$</th>
<th>Estimated $Z$ using sim data</th>
<th>Relative error of estimated $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>2.53</td>
<td>6.16 %</td>
<td>13.34</td>
<td>2.62 %</td>
</tr>
<tr>
<td>C</td>
<td>1.43</td>
<td>1.82 %</td>
<td>5.94</td>
<td>1.01 %</td>
</tr>
<tr>
<td>Marble</td>
<td>2.79</td>
<td>0.45%</td>
<td>15.57</td>
<td>1.53 %</td>
</tr>
<tr>
<td>Acr</td>
<td>1.25</td>
<td>5.80 %</td>
<td>6.51</td>
<td>0.01 %</td>
</tr>
<tr>
<td>Teflon</td>
<td>2.03</td>
<td>5.73 %</td>
<td>8.53</td>
<td>0.98 %</td>
</tr>
<tr>
<td>Glass</td>
<td>2.17</td>
<td>2.47 %</td>
<td>11.92</td>
<td>2.37 %</td>
</tr>
<tr>
<td>Ti</td>
<td>4.40</td>
<td>2.99 %</td>
<td>21.89</td>
<td>0.50 %</td>
</tr>
</tbody>
</table>

7.5 Testing the TIV model using simulated images including noise

In this section, the aim is to simulate the mean transmitted intensity and statistical variance images, as would be seen in experimental protocol. Having a priori information of the attenuation coefficient of the seven reference materials in $[1, \varepsilon_{e}^{\text{max}}]$ from the NIST database, along with the geometry of the sample and $\mu$CT setup, explained in section 7.4, I simulated the projections of the reference materials. For each of the reference materials, I then generated a random number of samples, $r$, of the projections from a “normal” distribution. In Eqn. 7.2 for sufficiently large values of $\lambda$, the normal distribution with mean $\lambda$ and standard deviation $\sqrt{\lambda}$, i.e., mean intensity $I = N.E.P(E)$ and standard deviation $\sigma = \sqrt{N.E.P(E)}$ for monochromatic assumption, is an excellent approximation to the Poisson distribution. The average of the generated projection samples works as the mean transmitted intensity, $I_{E,\text{PG}}$. The variance, $\sigma^2$, indicates the deviation of the random samples, $I'_e$, from their mean, and is defined as the square of the standard deviation, $\sigma$, where $\sigma = \sqrt{\frac{1}{r} \sum_{i=0}^{r} (I'_e - I_{E,\text{PG}})^2}$.

In this section, I used the mean absolute deviation because it corresponds better to real life [Gorard, 2005] since it’s more tolerant in extreme values and more accurate in sample measurements than standard deviation as it is a natural weight, whereas in standard deviation, the act of squaring makes each unit of distance of the random samples from the mean exponentially greater and the act of square-rooting the sum of squares does not completely eliminate this bias [Gorard, 2005]. The mean absolute deviation is the mean of the random samples’ absolute deviations around the random samples’ mean. For the normal distribution, the ratio of mean absolute...
Testing the TIV model using simulated images including noise

deviation, $\frac{1}{F} \sum_{i=0}^{F} \| I_{\varepsilon} - I_{\varepsilon}^{\text{avg}} \|$, to standard deviation is $\sqrt{\frac{2}{\pi}}$ [Geary, 1935]. Therefore, I calculated the statistical variance, $\sigma_{\varepsilon}^2$, as follows:

$$\sigma_{\varepsilon}^2 = \left[ \sqrt{\frac{2}{\pi}} \frac{1}{r} \sum_{i=0}^{r} \| I_{\varepsilon} - I_{\varepsilon}^{\text{avg}} \| \right]^2$$  (7.10)

I fitted the TIV model (7.4) on the estimated mean intensity image, $I_{\varepsilon}^{\text{avg}}$, and the statistical variance, $\sigma_{\varepsilon}^2$, in a least square manner using the minimisation of Eqn. 7.9 to estimate $K_1$ and $K_2$ constants.

Next, I used the calibrated TIV model along with the calculated $I_{\varepsilon}^{\text{avg}}$ and $\sigma_{\varepsilon}^2$ to estimate the projections of $\int p(s,E)$ and $\int c(s,E)$. The mean intensity and variance images are 200×200 pixel images in dimension. I assumed the number of acquisitions are 1000 and the number of detected photons are 10,000 on the normalised spectra of Fig. 7.1. Figure 7.4 shows a horizontal line through the simulated projection image of glass and carbon cylinders, along with the calibrated TIV model fit to them.

Section 7.5.1 applies several X-ray energy spectra and filters to examine the accuracy of the density and atomic number estimation using the TIV model. Section 7.5.2 examines the effect of higher acquisition time (number of measured radiographs) and number of detected photons on the TIV model and assess the accuracy of the density and atomic number estimations.

Figure 7.4: A line through a simulated projection and the TIV model fit of the cylinders of a) glass and b) carbon imaged at 100 keV.
Data Acquisition; from NIST for \([1, E_{\varepsilon_1}^{\text{max}}]\), of dual-energy spectra \(\star\) from Fig. 5.1

Attenuation coefficient \([\mu(E)]\) of 7 reference material (\(\omega\)) in \([1, E_{\varepsilon_1}^{\text{max}}]\)

Simulate \(I\) projections of materials \(\omega\) for \([1, E_{\varepsilon_1}^{\text{max}}]\); Eqn. 7.5 including noise for the method of section 7.5

Simulate \(\sigma^2\) projections of materials \(\omega\) for \([1, E_{\varepsilon_1}^{\text{max}}]\); Eqn. 7.5 including noise for the method of section 7.5

Theoretical \(\rho\) and \(Z\) values of material \(\omega\)

Parameter estimation; \((K_1, K_2)\)

Calibrate the TIV model

Calibrated TIV model

Parameter estimation; \(\mathcal{P}\) and \(\mathcal{C}\) intensity images

Estimated \(\rho\) intensity images

Estimated \(Z\) intensity images

CT image reconstruction of \(\rho\)

CT image reconstruction of \(Z\)

Figure 7.5: Flowchart of the TIV model calibration and \(\rho\) and \(Z\) estimation, using simulated projections of cylinders of 7 reference materials (Section 7.5), with \(\varepsilon\) being the energy label. \(\mathcal{P} = \int_{L} p(s, E)\) and \(\mathcal{C} = \int_{L} c(s, E)\) from Eq. 5.3.
7.5.1 Accuracy assessment of TIV model for different X-ray energy spectra

In this section, I examined the effect of the energy and filtering of the spectrum on the $\rho$ and $Z$ estimations using the TIV method by applying several spectra, e.g., with maximum energy of [60, 80, 100] keV for, respectively, no filter, 0.5 mm and 2 mm aluminium filter. I fitted the TIV model on the simulated $I_{\epsilon}$ and $\sigma_{\epsilon}^2$ of section 7.5 and minimised the absolute error of Eqn. 7.9 using the Newton-Raphson method over all pixels, $i$, to estimate $\int p(s, E) \, ds$ and $\int c(s, E) \, ds$. I used the filtered back-projection (see section 1.2.7.3) to reconstruct the projections. Next, I used Eqn 5.3 to estimate $\rho$ and $Z$ images. Table 7.2 and 7.3 show $\text{avg}(\frac{\delta \rho}{\rho})$ and $\text{avg}(\frac{\delta Z}{Z})$ estimations for all reference materials.

<table>
<thead>
<tr>
<th></th>
<th>60 keV spectrum</th>
<th>80 keV spectrum</th>
<th>100 keV spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>No filter</td>
<td>18.34 %</td>
<td>17.15 %</td>
<td>11.02 %</td>
</tr>
<tr>
<td>0.5 mm Al filter C</td>
<td>18.56 %</td>
<td>18.26 %</td>
<td>10.80 %</td>
</tr>
<tr>
<td>2 mm Al filter</td>
<td>28.87 %</td>
<td>21.08 %</td>
<td>13.99 %</td>
</tr>
</tbody>
</table>

Table 7.2: Estimated relative error of effective atomic number of reference materials using TIV model for different X-ray spectra (Section 7.5.1).

<table>
<thead>
<tr>
<th></th>
<th>60 keV spectrum</th>
<th>80 keV spectrum</th>
<th>100 keV spectrum</th>
</tr>
</thead>
<tbody>
<tr>
<td>No filter</td>
<td>5.46 %</td>
<td>7.00 %</td>
<td>9.53 %</td>
</tr>
<tr>
<td>0.5 mm Al filter</td>
<td>5.80 %</td>
<td>7.46 %</td>
<td>9.60 %</td>
</tr>
<tr>
<td>2 mm Al filter</td>
<td>9.66 %</td>
<td>12.8 %</td>
<td>13.70 %</td>
</tr>
</tbody>
</table>

Table 7.3: Estimated relative error of the bulk density of reference materials using TIV model for several X-ray spectra (Section 7.5.1).
7.5.2 Accuracy assessment of TIV model for detected X-ray photons

In this section, I examined the effect of the number of image acquisitions and the photon counts on the accuracy of the $\rho$ and $Z$ estimations. I applied the simulated $I_{\text{avg}}^\varepsilon$ and $\sigma^2_{\varepsilon}$ of section 7.5 to fit on the TIV model (7.4) using the 100 keV energy spectra with 0.5 mm aluminium filter (see Fig. 7.1) and estimated $\rho$ and $Z$ images of reference materials as explained in section 7.5.1. Table 7.4(a) shows the estimations of $\text{avg}(\frac{\delta \rho}{\rho})$ and $\text{avg}(\frac{\delta Z}{Z})$ for the number of image acquisition of [1000, 10,000, 100,000] times per sample with 1000 detected photons, and table 7.4(b) shows the estimated $\text{avg}(\frac{\delta \rho}{\rho})$ and $\text{avg}(\frac{\delta Z}{Z})$ for the number of the detected photons of [1000, 10,000, 100,000] with 10,000 times image acquisitions of the sample. This table shows slight differences of 0.26% and 0.31% between 10,000 and 100,000 image acquisitions, thus I chose to estimate the $\rho$ and $Z$ of table 7.5 with the number of acquisition of 10,000 and photon counts of 100,000. Table 7.5 shows the estimated atomic numbers and densities using the TIV model for the mentioned X-ray spectra, number of image acquisitions and detected photon for the ANU $\mu$CT setup. The density and atomic number error intervals are [1.89%, 17.58%] and [0.12%, 17.24%] respectively with an average relative error of 4.96% and 3.66%. Comparing to the results of the AMTI model using experimental images of these seven materials in section 5.4.3, the TIV model in this section shows an average of 2.09% and 2.40% higher error for $\rho$ and $Z$ estimations.

<table>
<thead>
<tr>
<th># of photons</th>
<th>avg($\frac{\delta \rho}{\rho}$)</th>
<th>avg($\frac{\delta Z}{Z}$)</th>
<th># of acquisition</th>
<th>avg($\frac{\delta \rho}{\rho}$)</th>
<th>avg($\frac{\delta Z}{Z}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>16.56%</td>
<td>15.20%</td>
<td>1000</td>
<td>5.80%</td>
<td>6.50%</td>
</tr>
<tr>
<td>10,000</td>
<td>10.80%</td>
<td>9.60%</td>
<td>10,000</td>
<td>4.96%</td>
<td>3.66%</td>
</tr>
<tr>
<td>100,000</td>
<td>5.80%</td>
<td>6.50%</td>
<td>100,000</td>
<td>4.65%</td>
<td>3.40%</td>
</tr>
</tbody>
</table>

Table 7.4: Average estimated relative error of the $\rho$ and $Z$ of the seven samples for a) detected photon with 1000 image acquisition, and b) acquisition number with 100,000 detected photon.
### Table 7.5: Estimated effective atomic number and bulk density of reference materials using TIV model for chosen acquisition time and photon counts (Section 7.5.2).

<table>
<thead>
<tr>
<th>Material names</th>
<th>Estimated $\rho$ using sim data</th>
<th>Relative error of estimated $\rho$</th>
<th>Estimated $Z$ using sim data</th>
<th>Relative error of estimated $Z$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>2.60</td>
<td>3.57 %</td>
<td>13.22</td>
<td>1.72 %</td>
</tr>
<tr>
<td>C</td>
<td>1.43</td>
<td>1.89 %</td>
<td>7.03</td>
<td>17.24 %</td>
</tr>
<tr>
<td>Marble</td>
<td>2.84</td>
<td>5.50 %</td>
<td>15.22</td>
<td>0.76 %</td>
</tr>
<tr>
<td>Acr</td>
<td>1.38</td>
<td>17.58 %</td>
<td>6.22</td>
<td>4.47 %</td>
</tr>
<tr>
<td>Teflon</td>
<td>2.07</td>
<td>3.42 %</td>
<td>8.46</td>
<td>0.13 %</td>
</tr>
<tr>
<td>Glass</td>
<td>2.29</td>
<td>2.74 %</td>
<td>11.66</td>
<td>0.12 %</td>
</tr>
<tr>
<td>Ti</td>
<td>4.50</td>
<td>3.68 %</td>
<td>21.73</td>
<td>1.21 %</td>
</tr>
</tbody>
</table>

### 7.6 Conclusion

The available methods to estimate the $\rho$ and $Z$ of materials in $\mu$CT used a simplified form of the Alvarez and Macovski model (see section 5.2). I calibrated and used the full form of the AMTI model in chapter 5. The AMTI model and its simplified forms (see section 6) require dual-energy imaging. In this chapter, I presented the transmitted intensity and statistical variance (TIV) model. This model requires only single-energy imaging because the statistical variance image works as the required information of the higher energy. The average intensity and variance image obtained from repeated observation of the same sample. The registered X-ray intensity on the detector and the Poisson noise in repeated measurements, are proportional to the quanta of the X-ray spectrum. From that, the Fano factor $\sigma^2 / \mu$ is proportional to the average energy. This proportionality is the reason that $\sigma^2$ images can substitute the higher energy information of the dual-energy imaging. This method considers the X-ray spectrum in its full form. It also assumes the energy dependency of attenuation coefficients of materials. The choice of dual-spectra, the acquisition time and number of photons affect the accuracy of the estimated results (see section 7.5.2 and 7.5.1).

Since only one energy is used, the energy is selected according to the right contribution of photoelectric absorption and scattering.

For the simulated projections of section 7.4 the relative error of the $\rho$ and $Z$ estimation have intervals of [0.45%, 6.16%] and [0.01%, 2.62%], respectively, with an average relative error of 3.63% and 1.29%. This, compared with the AMTI results using the simulated images (see section 5.4.2), show higher errors of 0.41% and 1.17% for $\rho$ and $Z$ estimations respectively.

Section 7.5 simulates the projections as would be seen in experimental protocol. In
this section, the average error of the $\rho$ and $Z$ estimations have intervals of [1.89%, 17.58%] and [0.12%, 17.24%], respectively, with an average relative error of 4.96% and 3.66%. Here, I compared these results with that of the AMTI, AMP and SK methods using the real images of the seven sample materials, respectively, in section 5.4.3, 6.2.1 and 6.3.1. The accuracy benchmark of the TIV (table 7.5), AMTI (table 5.2), AMP (table 6.2) and SK (table 6.5) models show the average error, avg\(\overline{\delta Z}\), of the estimated atomic number for all reference materials using these models, respectively, are 1.26%, 3.66%, 5.36% and 7.44%. The average error of the estimated density values, avg\(\overline{\delta \rho}\), for all reference materials, respectively, are 2.87%, 4.96%, 4.00% and 6.63%. This shows that the results of the TIV model in section 7.4 have higher average errors of 2.09% and 2.40% for $\rho$ and $Z$ estimations, in comparison with the AMTI model in section 5.4.3. However, the atomic number estimations using the TIV model are on average 3.78% and 1.7% more accurate than the AMP and SK models respectively. The density estimations using the TIV model have 1.69% higher error than the AMP model. The AMTI model and its simplified forms require dual-energy imaging (see Fig. 5.6). In this thesis, the dual-energy imaging was performed at 60 and 120 keV. These energies are considered as the dominant energies for the PE absorption and CS effects in section 1.2.5. However, the TIV method requires image acquisition only at a single-energy spectrum. The spectra of intensity-variance is not as distinct as dual-energy spectra (see Fig. 7.1).

The presented TIV model has some benefits such as: 1) the model only requires imaging at single-energy; 2) the model inherently accounts for BH and the reconstructed $\rho$ and $Z$ lacks BH artefacts; and 3) it can yield a good estimation of the $\rho$ and $Z$ of sample materials. Based on the above assessment, the TIV model in the setup of section 7.4 and 7.5 on average, shows 1.25% and 1.78% higher relative errors for $\rho$ and $Z$ estimations than the results of AMTI model, which is an acceptable range compared to the requirement of dual-energy imaging for the AMTI model. For future work, the experimental data can be used within the same procedure of this chapter to investigate the practicality and accuracy of the TIV model for the real data.

As shown in table 6.2, the main focus of this study is to to establish an accuracy benchmark to investigate the the trend of relative errors of the $\rho$ and $Z$ estimation using the TIV model. We compared the material characterisation results of this study with that of Alvarez and Macovski dual-energy model (AMTI), AMP and SK models in this section. I also note that the feasible number of acquisition is expected to be much less than that presented in table 7.4(a). The results of table 7.4(a) and (b) shows that increasing the number of photons and number of acquisitions decreases the the average estimated error of the $\rho$ and $Z$. An accuracy assessment also performed for the applied energy spectrum and filters in section 7.5.1 table 7.2 and 7.3. The fact that the photon counts of images should be over 1,000,000 counts support the idea of the TIV model. At the time of performing the study of this chapter there was no clear idea about the number of photon counts of the images.
Beam hardening correction using single-energy imaging and statistical variance

8.1 Introduction

In chapter 7, the transmitted intensity and statistical variance (TIV) model was presented and applied to estimate the density ($\rho$) and atomic number ($Z$) of the sample materials. Unlike the AMTI model (see chapter 5) and its simplified forms (see chapter 6) that require dual-energy imaging (see section 5.3.3), the TIV model requires measurements of intensity only at a single-energy spectra because the statistical variance images yield the same information as the higher energy information required at dual-energy imaging. For further information, please refer to section 7.3.

Although the objective of the TIV and AMTI models are to estimate $\rho$ and $Z$ of the sample materials, i.e., material characterisation, the beam hardening (BH) artefacts (see section 2.2) were also noticeably corrected in the reconstruction of the estimated $\rho$ and $Z$ images. The BH correction occurs because the TIV and AMTI models inherently account for BH by considering the polychromatic nature of the X-ray spectra and the energy dependency of the X-ray attenuation. However, the conventional reconstruction algorithms assume monochromatic radiation, which causes inconsistent values in the reconstructed images that is evident in the form of cupping and streaking artefacts. This happens because the lower energy radiation is being attenuated as it passes through the material which leaves harder X-rays, i.e., BH. For further information about BH, please refer to section 2.2.

This chapter modified the TIV model to be directly applied for BH correction. The structure of this chapter is as follows. Section 7.3 describes the theory of BH correction using single-energy imaging and statistical variance. I simulated projections of the cylinders of the sample using the attenuation coefficient data obtained from the National Institute of Science and Technology (NIST). I generated a number of projections randomly in a Gaussian distribution manner, from which the mean and
statistical variance images were calculated to form the input data as would be seen in experimental protocol (see section 7.5). Next, the TIV model is applied to estimate the two sets of the projections corresponding to the contribution of photoelectric absorption (PE) and Compton scattering (CS) images (see section 1.2.5). These images are functions of the $\rho$ and $Z$ of the sample material and are not energy dependent. Finally, the reconstruction of these images were directly substituted in the Alvarez and Macovski attenuation coefficient (AMAC) model (Eqn. 5.1) to estimate the tomogram of the sample material at a single-energy, $E_{\text{avg}}$. The BH artefacts are corrected in the resultant tomograms. Section 8.4 presents a simplified form of the TIV model (STIV) for BH correction. This model firstly estimates the average energy as mentioned above and then normalises the reconstruction of the beam hardened data using the proportionality of Eqn. 7.7.

The modified TIV and STIV models for BH correction eliminates the requirements of the measurement of BH curves and finding an appropriate model to linearise the projection data by fitting the model on the BH curve and remapping the inverse of the model on the data, as shown in section 3. They also don’t require the iterative computations of the post-correction iterative BH correction methods mentioned in section 2.2.3 by comparing the original projections with the corrected re-projections.

This research was carried out in the “Computed Tomography” group of Applied Mathematics Department at the Australian National University (ANU). I modified the TIV model of section 7.3 to allow it to be used for BH correction. I simulated the projections of reference materials using the polychromatic spectrum. The resultant images include BH artefacts. I then calibrated the modified TIV model and applied it on the projections to reduce the BH artefacts. The research here in chapter 8 is an extension of that described in chapter 7, which included my discussions with Dr Andrew Kingston about using the proportionality of Eqn. 7.7. In section 8.4 I proposed the STIV model for BH correction. For the presented research within this chapter, I am preparing a manuscript with the title and author list as follows:

8.2 The performance of energy in beam hardening correction (BH) methods

As mentioned in section 2.2, BH is seen with polychromatic X-ray sources. As the X-ray passes through the sample, low energy X-ray photons are attenuated more easily, and the remaining high energy photons are not attenuated as easily, thus, the BH does not follow the exponential decay seen with monochromatic X-rays (see section 1.2.6; Beer-Lambert law). This is a particular problem with high atomic number materials such as metals. Compared to low atomic number materials, these high atomic number materials have dramatically increased attenuation at lower energies.

Chapter 2.2 reviews two forms of BH software correction methods, including linearisation methods (see section 2.2.2) and post-reconstruction iterative methods (see section 2.2.3). I implemented five different BH linearisation correction models that are fitted on a BH curve, i.e., the linearised projections versus the thickness of sample material, to remap the data by applying the inverse of the model on the projection data (see chapter 3). One of these models, the Bimodal model (see section 3.3.2), presents a model by assuming dual-monochromatic radiation. As shown in section 1.2.5, X-rays interact with matter differently in different energies, i.e., PE and CS (see section 1.2.6). The Bimodal model demonstrated that the BH curve behaves differently, thus, should be modelled in different manners in the dominant energy regions of PE and CS.

The AMAC model in Eqn. 5.1 presented the attenuation coefficient, $\mu$, in the form of a two-basis function, where for low energy X-rays, attenuation is primarily due to PE and is proportional to the $Z$ of materials, i.e., $\frac{\rho Z^{m-1}}{E}$, and at high energies attenuation is primarily due to CS and is proportional to $K_2 \frac{Z^2}{\rho f_{\text{KN}}} f_{\text{KN}}$. $f_{\text{KN}}$ is defined in Eqn. 5.2 [Klein and Nishina, 1928], $E$ is the energy, and $m = 3.00$ and $n = 3.20$ for ANU \textmu CT facility (see section 5.4.1). The energy dependency of attenuation coefficients and the polychromatic nature of X-rays are considered in the AMAC and AMTI models, thus, these models inherently account for BH. The estimated $\rho$ and $Z$ cross-section of 3D images of the Berea sandstone (see Fig. 5.14) using the AMTI model shows that the model indeed corrects the BH artefacts. Similarly, the TIV model used for estimation of the $\rho$ and $Z$ of the sample materials in section 7.3 accounts for BH inherently. The TIV model requires imaging at a single-energy spectra and estimates the statistical variance image to perform as the required information in the CS energy region. This is because the statistical variance is proportional to the mean intensity image with a factor of average energy. For further information, please refer to section 7.2. Although the main objective of the TIV model is material characterisation (see chapter 7), the above mentioned reason motivates using the TIV model directly for BH correction. This is carried out in the following sections.
8.3 Transmitted intensity and statistical variance (TIV) model for BH correction

In this chapter, I present a method for BH correction from the measurements of the mean transmitted intensity and statistical variance images, by modifying the TIV model to be directly applied for BH correction of the mean transmitted intensity images. I used 40 keV spectrum to be able to simulate the BH effect on the tomograms. Figure 8.1 shows the dual-energy spectra correspond to the spectrum of $I_{\text{avg}}^\varepsilon$ and $\sigma^2$.

Figure 8.1: Simulated energy spectra at 40 keV maximum energy with no filter (red line) and the spectrum including higher mean energy (blue line); modified to match that seen for our experimental protocol.

Within this procedure, firstly I simulated the projections of sample materials using NIST attenuation coefficients by generating a random number of samples, $r$, from a “normal” distribution. The average of the simulated samples are estimated to be the mean transmitted intensity, $I_{\text{avg}}^\varepsilon$. The variance, $\sigma^2$, is then simulated as in Eqn. 7.5. These simulations include noise as expected in an experimental protocol. Next, I fitted the TIV model (7.4) on the simulated $I_{\text{avg}}^\varepsilon$ and $\sigma^2$ in a least square manner using the minimisation of Eqn. 7.9 to estimate $K_1$ and $K_2$ constants. I used the minimisation of Eqn. 7.9 using the calibrated TIV model along with the estimated $I_{\text{avg}}^\varepsilon$ and $\sigma^2$ to estimate the projections of $P = \int p(s, E)$ and $C = \int c(s, E)$. The mean intensity and variance images are 200×200 pixel images in dimension. I assumed the number of acquisitions to be $N = 1000$ and the number of detected photons on the normalised
s spectra of Fig. 7.1 to be 1000. For more information, please see section 7.5.2.

This process does not follow to estimate $\rho$ and $Z$ values as in section 7.4 and 7.5 instead, I used the filtered back-projection algorithm (see section 1.2.7.3) to reconstruct $p(s, E)$ and $c(s, E)$ (see Eqn. 5.3). $p(s, E)$ and $c(s, E)$ are subsequently functions $Z$ and $\rho$, and obviously are not energy dependent. Therefore, substituting the $p(s, E)$ and $c(s, E)$ reconstructions into the AMAC model (Eqn. 5.1) at the average effective energy, $E_{avg}$ yield a BH corrected tomogram. Considering the proportionality of Eqn. 7.7, the $E_{avg}$ within this process are estimated as:

$$E_{avg} = \frac{C}{P}$$ (8.1)

Flowchart of Fig. 8.3 charted the BH correction method by modifying the TIV. Figure 8.2 shows the uncorrected and corrected average intensity and statistical deviation of glass and marble. Here, glass is borosilicate with the chemical structure of 80.60% silica ($\text{SiO}_2$), 12.60% boric oxide ($\text{B}_2\text{O}_3$), 4.20% sodium oxide ($\text{Na}_2\text{O}$) and 2.20% aluminium oxide ($\text{Al}_2\text{O}_3$), and 3.00% mixed of ($\text{Fe}_2\text{O}_3$, $\text{CaO}$, $\text{MgO}$, $\text{Cl}$) according to the NIST database. The RMS error of the applied power law BH correction method compared to a smooth disc in this section is estimated to be 0.82%.

Figure 8.2: A line through reconstruction of glass imaged at 40.0 keV tube voltage showing the average intensity captured at 40 keV (blue line), statistical variance (green line) and the applied TIV BH correction in section 8.3 (red line). The reconstruction of this study are from a single radiograph. Since the same noise copied to the all projection angles, the line profile of the reconstructed image also include ring artefacts.
Data Acquisition; from NIST for \([1, E_{\epsilon_1}^{max}]\), of dual-energy spectra from Fig. 7.6

Attenuation coefficient \([\mu(E)]\) of 7 reference material \((\omega)\) in \([1, E_{\epsilon_1}^{max}]\)

Simulate \(I\) projections of materials \(\omega\) for \([1, E_{\epsilon_1}^{max}]\); Eqn. 7.5 including noise

Simulate \(\sigma^2\) projections of materials \(\omega\) for \([1, E_{\epsilon_1}^{max}]\); Eqn. 7.5 including noise

Dual-energy spectra; \(S_{\epsilon_1}\) & \(S_{\epsilon_2}\) from Fig. 7.6

Theoretical \(\rho\) and \(Z\) values of material \(\omega\)

Parameter estimation; \((K_1, K_2)\)

Calibration of the TIV model

Calibrated TIV model

Parameter estimation; \(P\) and \(C\) intensity images

CT image reconstruction of \(p(s, E)\)

\(E_{\text{avg}}\) from Eqn. 8.1

Calculate \(\mu\) using AMAC model; Eqn. 5.1

BH corrected reconstructed images

\(\diamond\) from Fig. 5.8

\((m, n)\)

Fit \(I\) and \(\sigma^2\) projections on TIV model; Eqn. 7.9

Draft Copy – 21 November 2016

Figure 8.3: Flowchart of the modified TIV model for beam hardening correction, using simulated projections of cylinders of 7 reference materials (Section 8.3), with \(\epsilon\) being the energy label. \(P = \int_L p(s, E)\) and \(C = \int_L c(s, E)\) from Eq. 5.3.
8.4 Simplified Transmitted Intensity and Variance (STIV) model for BH correction

In this section, a simplified form of the section 8.4 is used for BH correction. Similarly, I obtained the attenuation coefficient data \( \mu(E) \) of the sample materials, from the NIST database. I chose the spectrum with maximum energy of 40 keV with no filter to produce the BH artefacts in the images. Having the attenuation coefficients and the information about the setup of the ANU \( \mu \)CT system, I simulated radiographs \( I_\omega \{ \text{sim} \} \) of cylinders of the sample materials, as explained in section 7.5 to be as seen in experimental protocol. These images include severe cupping artefacts. Next, I used Eqn. 7.4 to simulate the statistical variance image, \( \sigma^2 \). These images along with the TIV model are used to estimate \( P \) and \( C \) using the minimisation of Eqn. 7.9. Next, I estimated \( E_{\text{avg}} \) from Eqn. 8.1. For every intensity bin, normalising \( I_\epsilon \) by the quantity of Eqn. 8.2, I anticipate BH corrected projections.

\[
I_{\text{corrected}} = I_{\text{BH}} \times \frac{E_{\text{BH}}}{E_{\text{avg}}} = \frac{\sigma^2}{E_{\text{avg}}}
\]  

where \( I_{\text{corrected}}, I_{\text{BH}} \) and \( \sigma^2 \) are the corrected, beam-hardened and the statistical variance images. These images are reconstructed using filtered back-projection. Figure 8.4 shows a line through reconstruction of the average intensity image captured at 40 keV (blue line), statistical variance image (green line) and the corrected image using the STIV method (red line). The RMS error of the applied power law BH correction method compared to a smooth disc in this section is estimated to be 0.44%. 

Draft Copy – 21 November 2016
Beam hardening correction using single-energy imaging and statistical variance

Figure 8.4: A line through reconstruction of marble, showing the average intensity captured at 40 keV (blue line), statistical variance (green line) and the applied TIV BH correction in section 8.4 (red line).

8.5 Conclusion

The TIV model was used in chapter 7 to estimate the $\rho$ and $Z$ of materials. I noticed that BH artefacts are corrected in the reconstructed images of $\rho$ and $Z$. This is because this model accounts for energy and thus also for the BH effect. In this chapter, I modified the TIV model to be used directly for BH correction. I estimated the projections of $P$ and $C$ (see section 5.3) using the TIV model and reconstructed them using filtered back-projection. The reconstruction of $p(s, E)$ and $c(s, E)$ were directly substituted in the AMAC model (Eqn. 5.1) with an average energy to estimate the $\mu$ of sample material. The resultant tomogram does not contain observable beam hardening artefacts. Section 8.4 is a simplified form of the TIV BH correction that normalises every bin in the average intensity having the statistical variance and average energy. These methods indeed correct the BH as shown in Fig. 8.2 and 8.4.
Conclusion and Future Work

Through the presented thesis, I discussed two main issues that micro computed tomography ($\mu$CT) suffers from: 1) the beam hardening (BH) artefacts that are evident on the tomograms in the form of cupping and streaking artefacts, which happens due to ignoring the polychromatic nature of X-rays in the standard tomographic reconstruction algorithms. The BH artefacts make the quantitative analysis and segmentation of the tomograms difficult; and 2) $\mu$CT produce micro resolution structural images of a sample but not the compositional information. In geology and the petroleum industry, understanding the compositional information of the samples, i.e., material characterisation, provides valuable input towards geological classification of sedimentary rock texture and subsequent alterations by diagenetic processes during burial. One of the main applications is the extraction of oil and gas from reservoir rocks, since the minerals and their distribution strongly affect properties such as wettability, which is highly relevant to recovery from conventional reservoirs by waterflooding, or brittleness, which dictates whether an unconventional reservoir is amenable to hydraulic fracturing. $\mu$CT material characterisation can aid in distinguishing the minerals such as quartz from feldspars or calcite from dolomite. This improves understanding of the geomechanical and transport properties [Golab et al., 2010] of rocks.

Within this thesis, I contributed by addressing these fundamental issues, i.e., BH correction and material characterisation in $\mu$CT, by presenting and applying the “energy selective techniques” that consider the energy dependency of $\mu$CT. In this sense, chapter 1 reviews the the basics of tomography with special emphasis on the physics of the X-ray spectrum, interaction of X-rays with matter and full energy dependent form of X-ray attenuation and chapter 2 is a review of the definition of the BH and material characterisation problems in $\mu$CT and the description of many available energy selective solution methods.

In chapter 3 I investigated five different the BH linearisation techniques including polynomial, bimodal, power law, cubic spline and linear spline models. Every value on the models is corrected towards the linear trend line, which is expected in the monochromatic case. Several samples have been imaged at the ANU $\mu$CT facility separately. I measured the BH curves directly from projections and fitted them with
these five models and remapped the inverse of the model to data to linearise the data and finally determine the model which has average lowest error for all the sample materials. Bimodal modelled the BH curve differently where it lies in the dominant energies of photoelectric absorption (PE) and Compton scattering (CS) effects (see section 1.2.5), assuming dual-monochromatic radiation. Linear spline is the approximation and extension of the bimodal model. These models found to be noise sensitive. Even though Spline, power law, and polynomial models don’t have a defined physical background, they found to have lowest RMS errors of, respectively, $6.36 \times 10^{-1}\%$, $6.24 \times 10^{-1}\%$, and $6.41 \times 10^{-1}\%$ for all samples. Considering that only two parameters needs to be estimated in the power law model and the slight difference in the errors when compared with the polynomial and spline models, it is reasonable to conclude that the power law model is a good, simple model for the ANU µCT system.

Chapter 4 is based on a published conference proceeding paper in the “International Conference of Tomography of Materials and Structures (ICTMS2013)” [Paziresh et al., 2013]. In this chapter, I applied the chosen model from the assessment of chapter 3, i.e., the power law model, for multiple nested-cylinder specimens. The amount of BH varies depending on the material composition of the specimen and the incident X-ray spectrum. The inversion of the power law is performed per-cylinder with the corrected projection calculated as the sum of per-material corrected projections. Several single and nested-cylinders samples such examples have been included to demonstrate that the method reduces the cupping and streaking artefacts. For this chapter, the future work could include developing an automatic method to determine the execution of cylindrical and non-cylindrical beam hardening correction code.

The research presented in chapter 5 is based on a published paper in the “Journal of Applied Physics” [Paziresh et al., 2016]. In this chapter, I applied the Alvarez and Macovski model in its full form. The model has been used broadly in simplified forms [Alvarez and Macovski, 1976; Siddiqui et al., 2004; Derzhi, 2012; Heismann et al., 2003; Park and Kim, 2011; Abudurexiti et al., 2010; Kaewkhao et al., 2008]. For the full model, I calibrated PE coefficient ($K_1$), CS coefficient ($K_2$), energy exponent ($m$) and atomic number exponent ($n$) by fitting the full AMAC model and the National Institute of Science and Technology (NIST) attenuation coefficient data for a particular setup of reference materials. I showed that given precise knowledge of spectra, the full Alvarez and Macovski transmitted intensity (AMTI) model is able to differentiate and identify materials via the $\rho$ and Z mapping. I also calibrated the AMTI model using the simulated projections of cylinders of the reference materials. I applied the calibrated AMTI model to estimate the $\rho$ and Z projections of materials which are later reconstructed to $\rho$ and Z images. The accuracy benchmark shows the AMTI model has 1.96% and 5.00% average and maximum relative error for $\rho$ estimation and 0.88% and 1.82% average and maximum relative error for Z estimation. I also applied the calibrated AMTI model to estimate $\rho$ and Z projections of three rocks (Bentheimer and Berea sandstones and a carbonate) and reconstructed
3D projections using filtered back-projection. To obtain the $\rho$ and $Z$ maps of the main components of rocks (quartz in sandstones and calcite and dolomite in carbonate), the $\rho$ and $Z$ tomograms were masked to exclude “material-boundary” voxels determined by standard deviation of local grey levels and fitted Gaussians to the histograms of the masked images. The segmented $\rho$ and $Z$ regions includes 2.80% and 1.50% relative average density and atomic number estimation error. In this chapter, I showed that given precise knowledge of spectra (see section 5.3.3), the AMTI model is able to differentiate and identify materials via the $\rho$ and $Z$ mapping even if the constituent materials have similar attenuation coefficients in one energy spectra, provided their $\rho$ and/or $Z$ values vary. The proposed model calculations require precise knowledge of spectra and reference materials including $Z_A$ values for the unknown rock sample, however it has some benefits such as: 1) the model reasonably corrected for BH effects in reconstructed $\rho$ and $Z$ images; 2) it can yield good average estimated $\rho$ and $Z$ material properties with average errors of 2.62% and 1.19% and maximum errors of 7.85% and 2.64% of expected values respectively; and 3) the materials are still identifiable through $Z$ estimation even if the $\rho$ of two constituent materials of a sample have similar values and $Z$ is not dependent on $\frac{\rho}{\mu}$. Also, $Z$ estimations are 1.43% more accurate on average than $\rho$ estimations because the images captured at 120 keV suffer from low SNR due to the heavy filtering at high voltage. For further improvement, we plan to apply an iterative modification of the density and atomic number estimations on material matching with a material dictionary. In the reconstruction algorithm, we include an iterative update on the initial $\rho$ and $Z$ estimations of materials through the full model and a probabilistic classification to manage the materials distributions based on the material library [Recur et al., 2014b].

In chapter 5, I calibrated and applied two simplified forms of the Alvarez and Macovski model: 1) the Alvarez and Macovski Polynomial (AMP) model [Alvarez and Macovski, 1976], and 2) the Siddiqui and Khamees (SK) model [Siddiqui et al., 2004] to compare with the results of the AMTI model of chapter 5. The implementation of the full model requires calibration, exact knowledge of the spectra, expensive computation and consideration of the inadequacy of the model described in section 5.4.1. Alvarez and Macovski presented the AMTI model, however they used a polynomial approximation of the model to estimate the $\rho$ and $Z$ of the sample materials. SK simplified the AMTI model by assuming dual-monochromatic radiation. Similar to the previous chapter, I built an accuracy benchmark for the $\rho$ and $Z$ estimations. The accuracy benchmark for the imaged reference materials shows that the results of the AMTI model are more consistent, and have lower maximum error compared to the results of the AMP and SK models, i.e., 12.60% and 11.36% in atomic number estimation and 1.24% and 6.22% in density estimation, respectively. The AMP model performs the analyses on projections, while the SK model is applied on the reconstructed images. Similarly, the results of the AMTI model for the rocks, when compared to the AMP and SK models, are more accurate by 11.52% and 25.62% in atomic number and 7.2% and 22.24% in density, respectively. The results from the SK method are more stable since analysis is performed directly on the tomogram.
Conclusion and Future Work

However, since BH correction (see chapter 3) must be performed on the low-energy reconstructions, this hinders any accurate estimation of $\rho$ and $Z$. The full AMTI model, by contrast, analyses the projection images directly and inherently accounts for BH. It is therefore more accurate in estimation of material properties but less stable, i.e., more noisy. This can be seen in the results of the carbonate presented in Fig. 5.15. Although applying the full model requires precise knowledge of the spectra, the full model yields, on average, 7.81% and 15.9% for atomic estimation and 4.73% and 13.00% for density estimation more accurate results than AMP and SK respectively. Reference materials are required for calibration for both full and simplified forms of the Alvarez and Macovski model. The full model is able to identify calcite from dolomite even though they have similar attenuation coefficients. Finally, the full model accounts for BH reasonably well.

In chapter 7 I proposed the transmitted intensity and statistical variance (TIV) model to estimate the $\rho$ and $Z$ of the sample materials. This model requires only single-energy imaging because the statistical variance image works as the required information of the higher energy. The registered X-ray intensity on the detector and the Poisson noise in a repeated measurements, are proportional to the quanta of the X-ray spectrum. From that, the Fano factor $\sigma^2 / \epsilon$ is proportional to the average energy. This proportionality is the reason that $\sigma^2 / \epsilon$ images can substitute the higher energy information of the dual-energy imaging. This method considers the X-ray spectrum in its full form. It also assumes the energy dependency of attenuation coefficients of materials. I simulated the X-ray transmitted intensity and statistical variance images for a given setup using the attenuation coefficient data of a set of reference materials obtained from the National Institute of Science and Technology (NIST), then applied the TIV model to estimate the $\rho$ and $Z$ images. The relative error of the $\rho$ and $Z$ estimation have intervals of $[0.45\%, 6.16\%]$ and $[0.01\%, 2.62\%]$, respectively, with an average relative error of 3.63% and 1.29%. This compared with the AMTI results using the simulated images (see section 5.4.2) shows higher errors of 0.41% and 1.17% for $\rho$ and $Z$ estimations respectively. This chapter also simulate the X-ray transmitted intensity images using the simulated projections of the cylinders of materials generated randomly in a gaussian distribution, and their statistical variance. This works as a simulation of noise seen in experimental protocol. Using this data, the TIV model is used to estimate the $\rho$ and $Z$ of the sample materials. I established a benchmark for the model in terms of accuracy in sections 7.5.2 and 7.5.1, respectively, by increasing the detected X-ray photons and by applying several different energy spectra. The accuracy benchmark of the results shows that the average error of the $\rho$ and $Z$ estimations have intervals of $[1.89\%, 17.58\%]$ and $[0.12\%, 17.24\%]$, respectively, with an average relative error of 4.96% and 3.66%. Here, I compared these results with those of the AMTI, AMP and SK methods using the real images of the seven sample materials, subsequently, in section 5.4.3, 6.2.1 and 6.3.1. The accuracy benchmarks of the TIV (table 7.5), AMTI (table 5.2), AMP (table 6.2) and SK (table 6.5) models show the average error, $\text{avg}(\delta \frac{Z}{Z})$, of the estimated atomic number for all reference materials using these models, respectively, are 1.26%, 3.66%, 5.36% and 7.44%. The average er-
ror of the estimated density values, $\text{avg}(\delta \rho)$, for all reference materials, respectively, are 2.87%, 4.96%, 4.00% and 6.63%. This shows that the results of the TIV model in section 7.4 have higher average errors of 2.09% and 2.40% for $\rho$ and $Z$ estimations, in comparison with the AMTI model in section 5.4.3. However, the atomic number estimations using the TIV model are on average 3.78% and 1.7% more accurate than the AMP and SK models respectively. The density estimations using the TIV model have on average 1.69% higher error than the AMP model. The AMTI model and its simplified forms require dual-energy imaging (see Fig. 5.6). In this thesis, the dual-energy imaging was performed at 60 and 120 keV. These energies are considered as the dominant energies for the PE and CS in section 1.2.5. However, the TIV method requires image acquisition only at a single-energy spectrum. The spectra of intensity-variance is not as distinct as dual-energy spectra (see Fig. 7.1). The presented TIV model has some benefits such as: 1) the model only requires imaging at single-energy, 2) the model inherently accounts for BH and the reconstructed $\rho$ and $Z$ lacks BH artefacts, and 3) it can yield a good estimation of the $\rho$ and $Z$ of sample materials. Based on the above assessment, the TIV model in the setup of section 7.4 and 7.5, on average, shows 1.25% and 1.78% higher relative errors for $\rho$ and $Z$ estimations than the results of the AMTI model, but are in an acceptable range comparing to the requirement of dual-energy imaging for the AMTI model. For future work, the experimental data can be used within the same procedure of this chapter to investigate the practicality and accuracy of the TIV model for the real data.

In chapter 8, I proposed a modified form of the TIV model to directly be applied for BH correction, along with a simplified form of it (STIV). Although the objective of the TIV and AMTI models is to estimate $\rho$ and $Z$ of the sample materials, i.e., material characterisation, the BH artefacts (see section 2.2) were also noticeably corrected in the reconstruction of the estimated $\rho$ and $Z$ images. The BH correction occurs because the TIV and AMTI models inherently accounts for BH by considering the polychromatic nature of the X-ray spectra and the energy dependency of the attenuation coefficients of the materials. This chapter uses the simulated projections of the cylinders of the sample and generated number of projections randomly in a gaussian distribution manner, from which the mean and statistical variance images are calculated to form the input data as would be seen in experimental protocol (see section 7.5). Next, the TIV model is applied to estimate the two sets of the projections correspond to the contribution of PE and CS images (see section 1.2.5). These images are functions of the $\rho$ and $Z$ of the sample material and are not energy dependent. Finally, the reconstruction of these images were directly substituted in the AMAC model (Eqn. 5.1) to estimate the tomogram of the sample material at a single-energy, $E_{avg}$. The BH artefacts are corrected in the resultant tomograms. Section 8.4 presents a simplified form of the TIV model (STIV) for BH correction. This model estimates the average energy as mentioned above and then normalises the reconstruction of the beam hardened data using the proportionality of Eqn. 7.7. The modified TIV and STIV models correct the BH artefacts, also eliminate the requirements of the measurement of BH curves and finding an appropriate model to linearise the projection
data by fitting the model on the BH curve and remapping the inverse of the model on the data. They also don’t require the iterative computations of the post-correction iterative BH correction methods mentioned in section 2.2.3 by comparing the original projections with the corrected re-projections.

The two main issues of $\mu$CT that I aimed to investigate and improve, which impact on the ability of this technology in quantitative analysis of the images of the samples such as rocks, are BH artefacts on tomograms and the requirement of more accurate modelling of compositional distribution of the sample materials. These difficulties are significantly reduced by the use of the BH linearisation, AMTI and TIV models investigated in this thesis. Work to extend these findings includes: investigating an automatic method to determine the execution of BH correction codes for cylindrical and non-cylindrical samples (chapter 4); applying an iterative modification of the density and atomic number estimations and probabilistic classification for materials distributions based on the material library (chapter 5); and using the experimental data within the procedure presented in chapter 7 and 8 to investigate the performance of the TIV model for real data.
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