Shale structure reconstruction by X-ray computerized tomography based on total variation regularization

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Abstract. The microstructure knowledge of shale is the basis of shale gas exploration and production. In this paper, we applied parallel X-ray computerized tomography technology rather than conventional surface-based observation methods to recover the shale structure non-destructively. In order to avoid the X-ray hardening, we used the synchrotron radiation source to acquire the projection data. Total variation regularization method was applied to suppress the noise effect and improve the image contrast, and primary-dual algorithm was used to solve it. Experimental tests show that the proposed approach is a feasible and efficient method to reconstruct the shale microstructure precisely and accurately.

1. Introduction
Shale gas is trapped within the non-connected small shale fractures and is difficult to extract. With the advent of energy crisis and development of hydraulic fracturing technology, it attracted more and more attentions in the past decade. Shale gas is considered as one of the unconventional sources of natural gas. The exploration of shale gas becomes one of the most hot research fields gradually.

In order to successfully recover distribution of shale gas, we should get the microstructure of shale, which plays an important role in the gas exploration and production [1]. Traditional surface observations methods, such as optical and scanning electron microscopy, are inadequate to obtain three-dimensional information of the shale sample, and the shale samples are destructed [2]. Therefore, these methods are not ideal because the shale samples are hard to exploit and precious [3].

X-ray computerized tomography (XCT) technique is a well-known noninvasive method to visualize the interior structure, which has been applied in medicine, biology, industry and science successfully from its invention in the 1970’s [4, 5]. Therefore, we attempt to use XCT to reconstruct the shale microstructure nondestructively.

In this paper, the parallel X-ray beams generated by synchrotron radiation (SR) source are used to acquire the projection data. The synchrotron radiation source, which can provide
energy-tunable, monochromatized and naturally collimated X-ray beams, was generated at
beamline BL14W1 XAFS of the Shanghai Synchrotron Radiation Facility (SSRF), by using
NI (National Instrument) LabVIEW’s Data logging and Supervisory Control (DSC) module
communication with experimental physics and industrial control system (see [6] for details).
One of the important reasons for using monochromatized beams is that it can avoid the X-ray
hardening caused by polychromatic beams.

Because the 3-dimensional (3D) information can be obtained slice by slice, we only consider
the 2-dimensional (2D) XCT image reconstruction problem. From the analytical point of view,
the 2D XCT problem is to invert the Radon transform of the X-ray attenuation map $f(x)$ of
the detected material [5, 7]

$$Rf(s, \theta(\alpha)) = \int_{s} f(s\theta(\alpha) + t\theta^\perp(\alpha))dt,$$

(1)

where $\theta(\alpha) = (\cos \alpha, \sin \alpha)^t, \theta^\perp(\alpha) = (-\sin \alpha, \cos \alpha)^t \in S^1$ and $s \in \mathbb{R}$. The $f$ can be
reconstructed by filtered back-projection (FBP) formula from 180$^\circ$ projection data

$$f(x) = \frac{1}{2\pi^2} \int_{0}^{\pi} \int_{\mathbb{R}} \frac{Rf'(s, \theta(\alpha))}{x \cdot \theta(\alpha) - s}dsd\alpha,$$

(2)

where the derivative of $Rf(s, \theta(\alpha))$ is about the first variable $s$.

Another reconstruction technique is algebraic method. Directly approximating the unknown
attenuation map $f$ as an $m \times n$ digital image (also denoted by $f$ for simplicity), and vectorizing
$f$ by lexicographical order, we can formulate the XCT image reconstruction problem as linear
system [5, 7, 8]

$$b = Af + \eta,$$

(3)

where $A \in \mathbb{R}^{M \times N}$ is called imaging matrix, $f \in \mathbb{R}^{N}$ ($N = mn$) and $b \in \mathbb{R}^{M}$ polluted by noise
$\eta$ are the unknown image and the observed projection data [5, 8]. For the unknown image $f$,
the vector form $f \in \mathbb{R}^{N}$ and matrix form $f \in \mathbb{R}^{m \times n}$ are not distinguished hereafter, and its
meaning is determined in the context.

However, neither FBP nor algebraic method could reconstruct ideal images from polluted or
partial data since the XCT reconstruction problem is ill-posed [8, 10]. Regularization methods
are commonly used technique for handling ill-posed problems, and have gradually become
the research hotspot in the field of XCT [9, 10, 11, 12]. The regularization methods are usually
modeled as the following minimization problem

$$\arg \min_{f \in C} \{ \lambda \phi(f) + D(Af, b) \},$$

(4)

where $\phi$ is a convex function (called regularization term) and $C$ is a convex set, representing the
prior knowledge of $f$, and $D(\cdot, \cdot)$ is a distance function(called fidelity term), measuring how $Af$
is fit to the projection data $b$. Here $\lambda > 0$ is called the regularization parameter.

The regularization term and fidelity term are at the core of regularization methods and
studied extensively. There are a lot of choices for regularization term, such as total variation
(TV)- based [10, 13, 14], sparse representations methods based on wavelet, tight-frame and
dictionary basis for XCT image reconstruction [15, 16, 17]. In this paper, we use the total
variation (TV) function as the regularization term. On one hand, shales are typically consisted
of incompatible components, such as clay mineral and quartz grain. Therefore, we can assume
the attenuation map $f$ is a piecewise constant function. On the other hand, it is well known that
total variation minimization method [18] forces the image (or function) to be a piecewise constant
approximation [19, 20]. Therefore, we use the total variation function as the regularization term for the reconstruction of shale information. As for the fidelity term, we use $l^2$ norm as the distance function $D$, i.e. $D(Ax, b) = \frac{1}{2} ||Ax - b||^2_2$, because the noise in the XCT projection data obeys Gaussian distribution. Furthermore, we impose a nonnegativity constraint on the solution, i.e. $C = \{ f \in \mathbb{R}^N | f_i \geq 0 \}$, because the attenuation coefficients are always nonnegative physically. As for the selection of regularization parameter, we determined it by experiments on the simulated projection data with the same noise level as the real projection data.

Efficient algorithm is another key problem for the regularization XCT image reconstruction problem (4). Although several algorithms were developed for total variation minimization problem in the past decade [21, 22, 23, 24], we use the primary-dual algorithm [23] to solve the proposed model in this paper.

We test the proposed method on stimulated data of Shepp-Logan phantom [26] and the experimental data (see [6] for details). The results show that the TV regularization method can suppress the noise effect and preserve the weak edges, which help us to distinguish different components in the shale sample. Therefore, the XCT technology is an efficient method to obtain the interior information of shale, and the TV-based regularization method is more suitable to the reconstruction of shale microstructure than filtered back-projection method.

The contributions of this paper are as follows: (1) We investigated a XCT-based technique to obtain the structure of shale nondestructively. (2) In the implementation, monochromatic X-ray are used to avoid the hardening effecting caused by polymathic X-ray. (3) TV minimization is adopted as the regularization term, because the attenuation map shale can be approximated by piecewise constant function accurately. And we used a strategy to select the proper regularization parameter.

The rest of this paper is organized as follow. In section 2, we illustrate the TV model for XCT image reconstruction and the primal-dual algorithm. Experiments on simulated and practical projection data are presented in section 3. In the last section, some conclusions and discussions are demonstrated.

2. Model and Algorithm

The TV-based model used in this paper is of the form

$$\min_{f \geq 0} \left\{ \lambda TV(f) + \frac{1}{2} ||Af - b||^2_2 \right\}, \quad (5)$$

where the user-defined regularization parameter $\lambda > 0$ is related to the noise level of data $b$. The total variation of a 2D image $f \in \mathbb{R}^{m \times n}$ is computed by

$$TV(f) = \| (\nabla f) \|_1 = \sum_{i,j=1}^{m,n} \sqrt{ (\nabla_1 f)_{ij}^2 + (\nabla_2 f)_{ij}^2 }, \quad (6)$$

where the gradient $\nabla f$ of $f$ is defined as $(\nabla f)_{i,j} = ( (\nabla_1 f)_{i,j}, (\nabla_2 f)_{i,j} )$ with $\nabla_1 f = \left\{ f_{i+1,j} - f_{i,j} \right\}_{i \leq m}$, $\nabla_2 f = \left\{ f_{i,j+1} - f_{i,j} \right\}_{j \leq n}$.

The selection of regularization parameter is very important for the performance of regularization methods. It is well known that the proper regularization parameter is related to the noise level of projection. We firstly estimate the noise level in the projection data in the domain in which the X-ray does not go through the shale (The ideal value should be zero). Then we determined a proper parameter by experiments of simulated data of Shepp-Logan phantom with the noise level.
Let \( G(f) = \begin{cases} 0 & \text{if } f \geq 0 \\ +\infty & \text{otherwise} \end{cases} \), \( F_1(v) = \lambda \sum_{i=1}^{m} |v_{ij}| = \lambda \sqrt{(v^2_{ij})^2 + (v^2_{ij})^2} \) for \( v \in Z = \mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n} \) and \( F_2(w) = \frac{1}{2} \|w - b\|_2^2 \) for \( w \in \mathbb{R}^M \). Then the minimization problem (5) can be rewritten as an unconstrained minimization problem

\[
\min_f F_1(\nabla u) + F_2(Af) + G(f).
\] (7)

The problem (7) is equivalent to the following saddle point problem [9, 23]

\[
\min \max_{v,w} \{ \langle \nabla f, v \rangle - F_1^*(v) + \langle Af, w \rangle - F_2^*(w) + G(f) \}.
\] (8)

Here the conjugate functions \( F_1^* \) and \( F_2^* \) are defined as

\[
F_1^*(v) = \max_{p \in Z} \{ \langle v, p \rangle - F_1(p) \},
\]

\[
F_2^*(w) = \max_{q \in \mathbb{R}^M} \{ \langle w, q \rangle - F_2(q) \},
\]

where the inner products \( \langle p, q \rangle_Z = \sum_{i=1,j=1}^{m,n} (p_{ij}q_{ij}^1 + p_{ij}^2q_{ij}^2) \) for all \( p, q \in Z \), and \( \langle x, y \rangle_{\mathbb{R}^M} = \sum_{i=1}^{M} x_iy_i \) for all \( x, y \in \mathbb{R}^M \).

The general frame of the primal-dual iteration procedure for the saddle point problem (8) can be formulated as Algorithm 1 (see [9, 23] for details). In Algorithm 1, \( A^t \) is the conjugate transpose operator of \( A \) and \( \nabla^t \) is the conjugate operator of \( \nabla \) defined by

\[
\langle v, \nabla x \rangle_Z = \langle \nabla^t v, x \rangle_{\mathbb{R}^N}.
\] (11)

The proximal mapping \( \text{prox}_\sigma[H] \) of a given convex function \( H \) is defined as

\[
\text{prox}_\sigma[H](v) = \min_p \{ H(p) + \frac{1}{2\sigma} \|p - v\|_2^2 \}.
\] (12)

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**Algorithm 1** Primal-dual algorithm for (8)

Initialization: \( k = 0 \), \( \theta = 1 \), \( f^k = f^0 = 0 \in \mathbb{R}^N \), \( v^k = 0 \in Z \), \( y^k = 0 \in \mathbb{R}^M \), \( \tau, \sigma > 0 \) and \( \tau \sigma \left\| \left( \frac{A}{\nabla} \right) \right\|_2^2 \leq 1 \). For \( k = 0, 1, \ldots \), do

\[
v^{k+1} = \text{prox}_\sigma[F_1^*(v^k + \sigma \nabla f^k)];
\]

\[
y^{k+1} = \text{prox}_\sigma[F_2^*(y^k + \sigma Af^k)];
\]

\[
f^{k+1} = \text{prox}_\tau[G] \left( f^k - \tau \langle \nabla v^{k+1}, f^k \rangle + A^t y^{k+1} \right);
\]

\[
f^{k+1} = f^k + \theta (f^{k+1} - f^k);
\]

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In order to use the primal-dual algorithm, one only needs to compute the conjugate functions \( F_1^* \), \( F_2^* \) and the proximal mappings \( \text{prox}_\sigma[F_1^*], \text{prox}_\sigma[F_2^*] \) and \( \text{prox}_\tau[G] \). It has been proved that [9, 23]

\[
F_1^*(z) = \begin{cases} 0, & |z_j| \leq \lambda, \quad \forall j \\ +\infty, & \text{otherwise} \end{cases}
\]

(13)

\[
F_2^*(y) = \frac{1}{2} \|y\|^2 + \langle y, b \rangle_{\mathbb{R}^M}.
\]

(14)
The proximity operators of $F^*_1$, $F^*_2$ and $G$ are

$$\text{prox}_\sigma[F^*_1](z) = \frac{\lambda z}{\max\{\lambda, |z|\}},$$  \hspace{1cm} (15)

$$\text{prox}_\sigma[F^*_2](y) = \frac{y - \sigma b}{1 + \sigma},$$  \hspace{1cm} (16)

$$\text{prox}_\tau[G](f) = \max\{f, 0\}.$$  \hspace{1cm} (17)

Here the divisions in (15) and (16) are componentwise. Therefore, the primal-dual algorithm for the original problem (5) can be illustrated as Algorithm 2.

**Algorithm 2** Primary dual algorithm for TV model

**Step 1 Initialization:** $k = 0$, $\theta = 1$, $f_k = \bar{f}_k = 0 \in \mathbb{R}^N$, and $v_k = 0 \in \mathbb{Z}$, $y_k = 0 \in \mathbb{R}^M$, $\tau, \sigma > 0$ and $\tau \sigma \left\| \left( A \nabla \right) \right\|^2_2 < 1$.

**Step 2 Perform the following iterations until convergence:**

$$y_{k+1} = \frac{y_k + \sigma (A \bar{f}_k - b)}{1 + \sigma},$$  \hspace{1cm} (18)

$$v_{k+1} = \frac{\lambda (v_k + \sigma \nabla \bar{f}_k)}{\max\{\lambda, |v_k + \sigma \nabla \bar{f}_k|\}},$$  \hspace{1cm} (19)

$$f^{k+1} = \max\{0, f_k - \tau (\nabla^t v^{k+1} + A^t y^{k+1})\}.$$  \hspace{1cm} (20)

**Step 3 Update:** $\bar{f}^{k+1} = f^{k+1} + \theta (f^{k+1} - f^k)$, $k = k + 1$, and go to Step 2.

By the definition (11), one can derive the computing formula of $\nabla^t$ as follows \cite{25}

$$(\nabla^t v)_{i, j} = \begin{cases} v_{i+1, j}^1 - v_{i, j}^1 & 1 < i < m \\ v_{i, j}^1 & i = 1 \\ -v_{i-1, j}^1 & i = m \end{cases} - \begin{cases} v_{i, j+1}^1 - v_{i, j}^1 & 1 < j < n \\ v_{i, j}^1 & j = 1 \\ -v_{i, j-1}^1 & j = n \end{cases}.$$  \hspace{1cm} (21)

### 3. Experimental results

In this section, we applied our mathematical model and algorithm on simulated and practical data, and compared the results with that of the traditional FBP method. Beside the visual comparison of the reconstructed image, we also compared the mean square errors (MSEs) for the simulated data. The MSE is defined by

$$\text{MSE}(f) = \sqrt{\frac{1}{m \times n} \sum_{i=1, j=1}^{m, n} (f_{i, j} - f^0_{i, j})^2},$$  \hspace{1cm} (22)

where $f^0$ and $f$ are the original and estimated images, respectively. In our experiments, for Algorithm 2, we choose the two parameters $\sigma = \tau = 0.5$.

#### 3.1. Experiments on simulated data

The simulated data were generated on the Shepp-Logan phantom \cite{26} at 180 directions with 201 equal distance lines. In order to illustrate the noise suppressing effect, we compared the FBP method and the proposed TV method for contaminated projections, which were obtained
Original FBP (MSE=0.2418) TV (MSE=0.0796)

Figure 1. Reconstructed images with simulated data of Shepp-Logan phantom using different methods.

by adding zero mean Gaussian noise (with standard variance 0.005) to the noiseless projection data. The regularization parameter is chose as $\lambda = 0.0005$.

The results by FBP method (2) and the TV method are shown in Figure 1. By visual comparison, we can observe that the TV method is superior to FBP with respect to fine structure reconstruction and noise suppression. The MSE comparison also shows that the TV method is much better than the traditional FBP method.

3.2. Experiments on real data
The experiment was carried out at BL13W1 beamline at Shanghai Synchrotron Radiation (SR) Facility (see reference [6] for details on the setup and shale sample information). The estimated noise level is about 0.005. The regularization parameter $\lambda = 0.0005$. In Figure 2, we present the reconstructed images of one slice of the tested shale sample, and the parts in the rectangle were enlarged for comparison.

From Figure 2, we can observe that TV method is superior to the FBP method visually. Firstly, the image contrast by FBP method is much lower than that by the TV method. Secondly, the TV method suppresses the noise effect and preserves the edge between different components successfully. Therefore, we may conclude that the combination of the SR sources X-ray and TV regularization is a feasible and efficient tool to recover the shale interior information non-destructively.

4. Conclusions and Future works
In this paper, we applied the X-ray computerized tomography technique to obtain the shale interior structure. In order to suppress the noise in the projection data, the total variation regularization method was used to reconstruct shale structures from XCT projection data. The experiments on stimulated and real data showed that the TV method was superior to the filtered back projection method in noise suppression and edge preservation. Based on the observation of the shale, in the future, we will study the segmentation-based method to reconstruct a piecewise constant attenuation function directly, not by the aid of total variation minimization.

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Figure 2. Reconstructed images from experimental data. First row: reconstructed images from projection data; Second row: zoom-in images in the rectangle of the corresponding images in the first row.

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