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Data-constrained modelling of an anthracite coal physical structure with multi-spectrum synchrotron X-ray CT

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HIGHLIGHTS

- A DCM model with multi-spectrum synchrotron X-ray CT is used to characterise an anthracite coal physical structure.
- This model enables detection of mixed composition distributions at length scales smaller than X-ray CT resolution.
- The 3D physical structure of the sample is obtained and the partial volume effect is addressed with DCM.
- Voids and some minerals at length scales smaller than X-ray CT resolution have been detected and displayed.

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ABSTRACT

A data-constrained modelling (DCM) approach with multi-spectrum synchrotron X-ray CT has been used to characterise the physical structure of Yangquan coal sample. Three sets of X-ray CT data have been acquired with monochromatic beam energies at 14, 18, and 30 keV respectively. A DCM approach is used to derive compositional volume fractions on each voxel, by minimising the differences between the expected and CT reconstructed absorption coefficients with a nonlinear optimization algorithm. Voxel based 3D compositional maps are generated with colours and intensities representing compositions and volume fractions respectively. The results are relevant in quantitative modelling of coal-bed gas transportation and coal processing.

1. Introduction

Coal is playing an essential role in energy supply system in many places of the world, including China. It will continue to hold its position at some extent in future. The development of clean coal technologies is one of the primary tasks for sustainable development of our society. Quantitative information of microscopic spatial distributions of minerals in coal as well as visualising the physical structure of coal will help understanding the transformation of the minerals during coal processing and the fluid transportation in coal matrix during ECBM (enhanced coal-bed methane) process.

Coal is mainly composed of three physical components: coal matrix (organic components), void (pores and fractures), and mineral (inorganic constituents) [1]. Recently, various techniques have been used to characterise and visualise distributions of these components, such as SEM [2,3], AFM [4,5], CCSEM [6–8], X-ray CT (computed tomography), etc. [9–21]. Among all those techniques, X-ray micro-CT (μCT) has a unique advantage in sample non-destructive 3D characterization.

In the process of using CT techniques, the interpretation of CT absorption images is a very important issue. In 1996, Verhelst et al. [9] studied the correlation of 3D-CT scans and 2D-colour image analysis of coal. In 1997, Simons et al. [10] assumed that the correlation was true only for certain energy ranges. In 2000, a method of dual-energy was used to get the physical density of coal components from the X-ray linear attenuation coefficient [11].

By now, dual-energy microfocus X-ray CT technique has been a main method for quantitative μCT, which is widely used to investigate the distribution of coal components and fluid transportation in coal matrix. In the technical development process, different methods have also been used to minimise the beam hardening artefact [15,21]. Besides dual-energy CT, image threshold

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segmentation is another main method in quantitative analysis of μCT data, which has been well demonstrated by Yao et al. [17].

Despite the efforts that have been made, there still exist some problems related to this technique. Firstly, 3D distributions of minerals are sometimes difficult to be identified by X-ray CT due to that different mineral phases may exhibit similar X-ray absorption property. Secondly, the sizes of some minerals particles or pores in coal are smaller than the resolution of CT equipments. It makes the quantitative detection and identification of these fine compositions much more difficult by dual-energy method or image segmentation method. The reason for this is that a voxel (volumetric pixel – the minimum unit of the CT slice image) in the reconstructed CT image may contain multiple particles with different compositions. The CT value of the voxel represents an average value for their properties. This is the so-called partial-volume effect [22]. Although an increase in image resolution can reduce this effect, the sample size will have to be decreased accordingly. Reducing sample size may worsen the statistical representativeness. In addition to the above, with lab-based X-ray CT imaging, it is difficult to eliminate beam hardening effect, which usually causes pernicious artifact.

In this study, a data-constrained modelling (DCM) with synchrotron-based multi-spectrum X-ray CT approach is applied to investigate the compositional distributions and the physical structure of a coal sample. The DCM approach had been used in characterisation of compositional microstructures for a range of applications in relation to material science and hydrocarbon reservoir characterizations [23–29]. The synchrotron-based high quality X-ray beam has made it possible for quantitative interpretation of CT reconstructed 3D absorption images with a high resolution. The problem such as beam hardening is eliminated due to the excellent monochromaticity of X-ray beam. The light intensity of the X-ray beam effectively shortens the sample exposure time. This can reduce the impact of the uncertainties associated with time. The DCM approach enables detection of mixed composition distributions at length scales smaller than X-ray CT resolution. Consequently, the greyscales variation of "coal matrix" (fine mineral particles or fractures at the sub-voxel scale would lead to this variation) can be resolved more accurately. In other words, the partial volume effect is addressed naturally with DCM.

2. Sample description

2.1. Sample and properties

Coal sample investigated in this study was collected from underground mine in Yangquan, originating from Qinshui basin, which is one of the gas rich coal basins of China. The coal sample for the CT experiment was cut off from a big coal lump at air dry state. It was carefully sanded by hand into a cylindrical shape with a diameter of 5 mm and a length of 10 mm. To avoid sample damage and dust entering the sample, the sanding was gentle and along a single direction. There were no obvious cracks or pores existing in the sample surface. As the volume of the sample used in the CT experiment was small, two coal samples near the one used for the CT experiment were cut off from the coal lump to do the coal property analysis and total porosity testing before the X-ray CT experiment. The results of the standard proximate and ultimate analyses of the coal sample are listed in Table 1. The ions in ash were analysed according to Chinese standard GB/T 1574-2007. The vitrinite reflectance (VRr) and carbon content are 2.3% and 89.0%, respectively. This type of coal is classified as anthracite.

The total porosity of coal sample is obtained by Eq. (2.1) according to the Chinese standard GB/T 23561.4-2009:

$$P_{void} = \left(1 - \frac{\rho_{ARD}}{\rho_{TRD}}\right) \times 100\% \tag{2.1}$$

where P_{void} denote the total porosity of the coal sample, ρ_{ARD} and ρ_{TRD} are the apparent relative and true densities of coal sample respectively. The apparent relative density of coal sample was measured with the sealing wax method according to the Chinese standard GB/T 23561.2-2009. The true relative density was measured using the expansion of helium gas replaced method according to the Chinese standard GB/T 23561.2-2009. With measured values of ρ_{ARD} = 1.51 g/cm^3 and ρ_{TRD} = 1.58 g/cm^3, the total porosity of the coal sample was estimated as 4.43%.

2.2. Pre-analysis

Accuracy of DCM analysis is related to X-ray CT experimental parameters, including sample size, image resolution, and X-ray beam energies. A pre-analysis is required to optimise the sample-specific experimental parameters.

The overall compositions and their volume fractions of the coal samples are estimated from the metal ion data listed in Table 1. The estimation is based on the following assumptions:

(a) The original minerals of the coal sample exist as the common forms of coal minerals as listed in Table 2 (reproduced from Guo et al. [30]).
(b) Metal ions in each ash composition were originated from the common minerals in the coal sample. That is, the percentage of metallic element of the coal sample is equal to the ion percentage in ash compositions multiplied by the ash percentage in coal.
(c) The volatilisation of metal ions during the ash analysis process is negligible.
(d) The volume of the coal sample is equal to the sum of individual component volumes: minerals, coal matrix, and void.
(e) The organic component formula is given directly by the elemental proportion analysis.

Based the assumptions (a) and (b), the percentage of each metallic elements in the coal is obtained. Comparing the common mineral forms in coal (Table 2) and the formulations of minerals, the mineral forms in the coal and the percentage of each mineral have been derived. Using the above assumptions and the data listed in Table 1, Table 3 is the derived list of compositions and their overall volume percentages.

When X-ray passes through the sample, the X-ray attenuation by each composition depends on both its volume fraction and X-ray absorption coefficient. The average attenuation by each compositions vs X-ray beam energies was calculated using an in-built function in the DCM software, which is based on the best known elemental absorption properties [31].

Figs. 1 and 2 show the X-ray absorption ratio of each mineral composition compared to the coal matrix under different X-ray beam energies, which is calculated as.

$$y = \frac{\mu_i(x) \times v_i}{\mu_m(x) \times v_m} \tag{2.2}$$

where i denotes for different minerals, x represents X-ray energy; $\mu_i(x)$ and $\mu_m(x)$ are the X-ray linear absorption coefficients of mineral composition (i) and coal matrix at the X-ray energies at x keV respectively; v_i and v_m are the volume fractions of mineral composition (i) and coal matrix respectively as quoted in Table 3. From Fig. 2, the X-ray absorptions of Pyrite, Dolomite, Plagioclase, and Manganese dioxide are small as compared with coal matrix. Given that the noise level of X-ray CT is typically at 1%, in the context of pre-analysis, they have been ignored. However, if any such minor