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Mini Review

Data-Constrained Modelling of Material Microstructures and Properties

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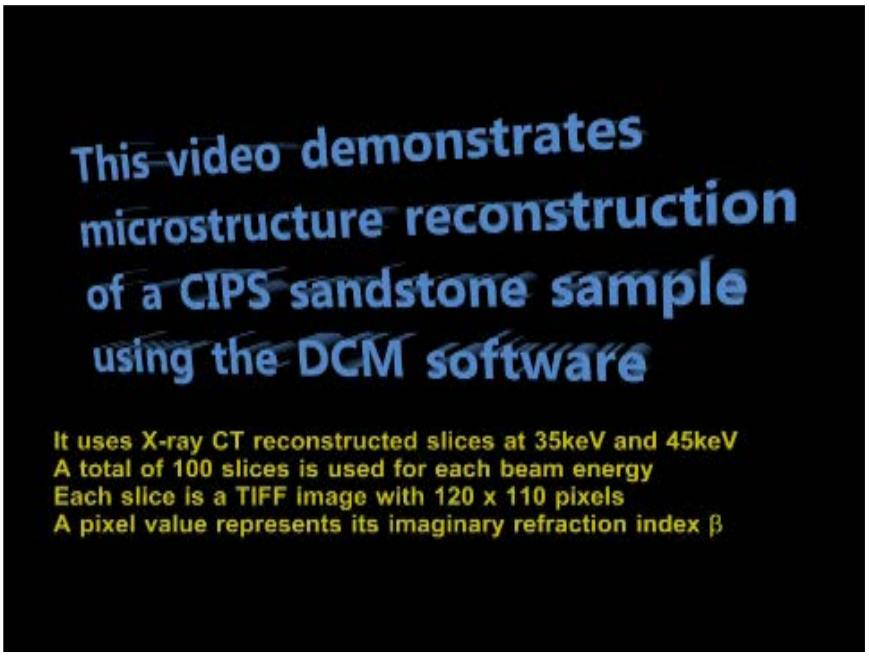
Abstract

This article is a review of our recent development in data-constrained modelling (DCM) methodology for quantitative and sample-non-destructive (SND) characterization of 3D microscopic composition distribution in materials, and microstructure-based predictive modelling of material multi-physics properties. Potential impacts are illustrated with examples in a range of R&D disciplines.

Introduction

Although the X-ray CT and threshold image segmentation approach is widely used in the R&D community for sample-non-destructive (SND) characterization of internal microstructures of various materials [1], it is subjective and imposes an arbitrary length-scale cut-off at the X-ray CT voxel size. It generally assumes that each X-ray imaging voxel has a discrete material composition. That is, there are no finer structures smaller than the X-ray imaging voxels. The smallest X-ray CT voxel size is at the order 1/1000 of the sample size. In other words, the mainstream X-ray CT approach is inadequate to characterize material internal structures smaller than the order of 1/1000 of the sample size. This makes it not suitable for materials with multi-scale internal structures such as tight oil & gas reservoirs including shale, carbonate and tight sandstone; manufactured materials such as 3D-printed metal components, and corrosion inhibitive print primers [2-4]. As image segmentation is based on the X-ray CT slice image grey-scale, it is not sensitive enough to discriminate material compositions with similar X-ray attenuation properties.

The problem is addressed with the recent development in data-constrained modelling (DCM) method using quantitative X-ray CT [5,6]. By integrating statistical physics and multi-energy quantitative X-ray CT, DCM Video 1 explicitly reconstructs 3D microscopic distributions of materials and incorporates fine structures below X-ray CT image resolution as voxel compositional partial volumes. This offers a more accurate 3D representation of a material microstructure and enables more quantitative modelling of its properties. The DCM formulation will be presented in the next section, followed by a selection on case studies and references.



Model Formulation

For DCM, a material sample is represented numerically on a simple cubic grid of $N = N_x \times N_y \times N_z$ cubic vowels. On the nth voxel where n=1,2,...,N, the DCM model minimizes the following objective function:

$$T_n = \sum_{l=1}^{L} \left[\delta\mu_n^{(l)} \right]^2 + E_n \qquad (1)$$

This is equivalent to minimize the discrepancy between the expected and the measured linear absorption coefficients and to maximize Boltzmann distribution probability [7]. In Equation (1), $\delta\mu_n^{(l)}$ is the difference between the expected and CT reconstructed linear absorption coefficients, and E_n is the dimensionless phenomenological interaction energy [5,8]. The optimization is achieved by adjusting the volume fraction variables $v_n^{(m)}$ (m=0,1,... ,M) for each material composition m, where M is the total number of non-void compositions, subject to the following constraints

$$\begin{cases} 0 \le v_n^{(m)} \le 1 \\ \sum_{m=0}^{M} v_n^{(m)} = 1 \end{cases} m = 0,1,\ldots,M \qquad (2)$$

Numerical solution to the above has been implemented as a DCM software [5,6]. Figure 1 is a typical main window of the DCM software. In DCM, sub-voxel structures are incorporated as coexistence of multiple compositions in the same voxels.

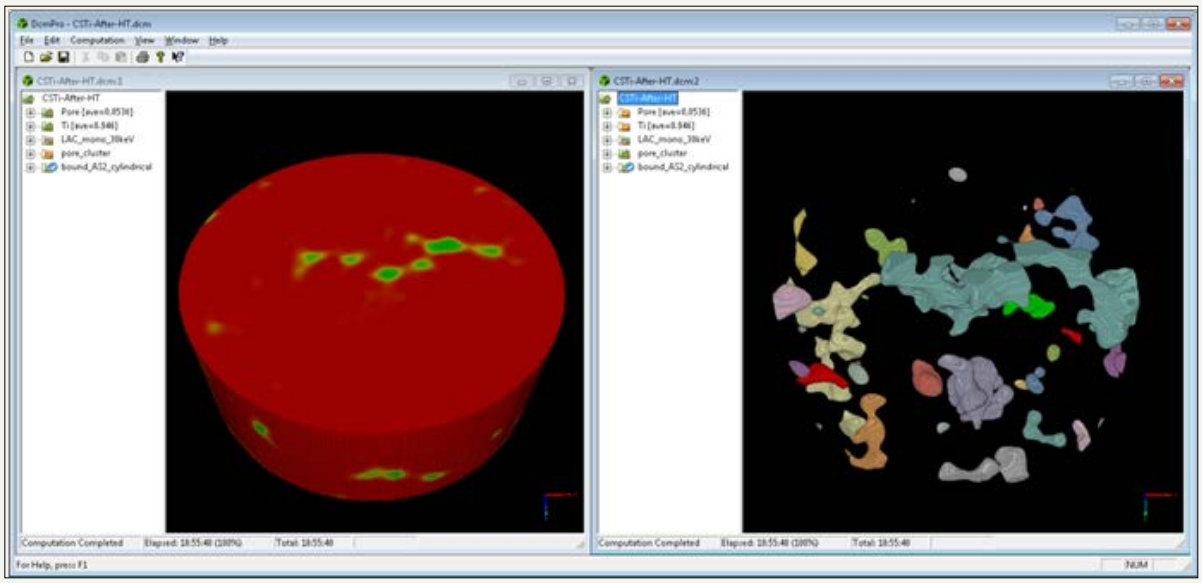
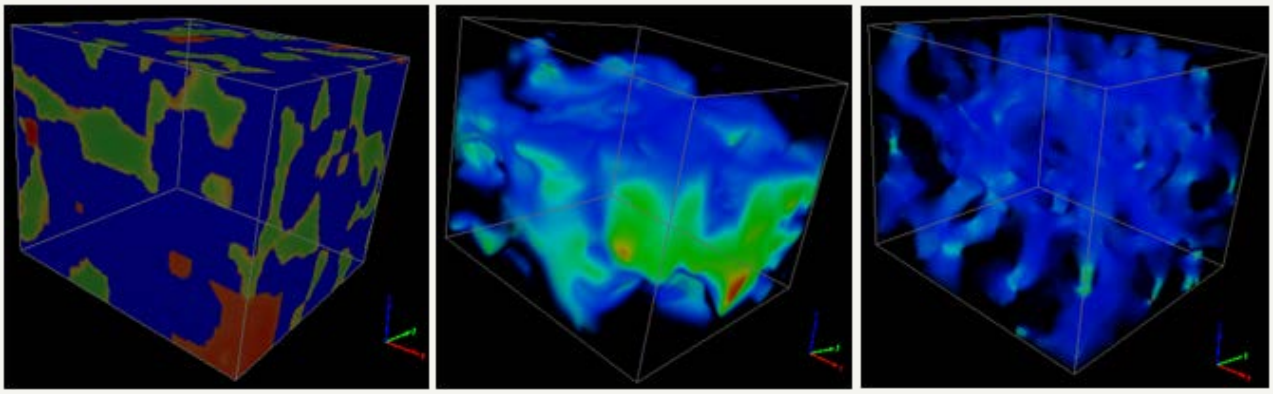


Figure 1: DCM software main display window for a case-study on cold-spayed Ti sample.



(a) **(b)** **(c)**

Figure 2: Microstructure and properties of a CIPS sandstone sample.

2a: Compositional distribution where quartz is displayed as blue, calcite as red and pores as green. Coexistences of multiple compositions in the same voxels are displayed as mixed colours.

2b: Induced electric potential when the pores are filled with the sea water and an external potential difference is applied along the Z-axis.

2c: Fluid speed distribution when a pressure difference is applied along the Z-axis.

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Microstructure Characterization and Properties Modelling

As a demonstration case study for synthetic CIPS (Calcite In-situ Precipitation System) sandstone, which consists of quartz grains cemented by calcite, and pores? It was X-ray imaged at beam energies 35 and 45keV. The multi-energy X-ray datasets were analyzed using the DCM non-linear optimization algorithm [5]. The procedures of the analysis are demonstrated by the accompanying video https://research.csiro.au/static/dcm/DCM-CIPS-sandstone-web-demo.mp4. Each voxel represents a sample volume of microns. Assuming the pores are filled with the sea water, its electrical conductivity and permittivity had been calculated using a finite-difference DCM plugin [9]. Its fluid permeability was calculated using a DCM plugin for partially percolating voxels [10,11]. Its composition distribution, induced voltage and fluid flow speed are illustrated in Figure 2.

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