Journal of Geochemical Exploration 144 (2014) 84–96

Contents lists available at ScienceDirect

Journal of Geochemical Exploration

journal homepage: www.elsevier.com/locate/jgeoexp

From characterisation of pore-structures to simulations of pore-scale fluid flow and the upscaling of permeability using microtomography: A case study of heterogeneous carbonates

Jie Liu [a,*], Gerald G. Pereira [b], Klaus Regenauer-Lieb [a,c]

[a] Laboratory for Multiscale Earth System Dynamics and Geothermal Research, School of Earth and Environment, University of Western Australia, 35 Stirling Hwy, Crawley, WA 6009, Australia
[b] CSIRO Mathematics, Informatics and Statistics, Private Bag 33, Clayton South, VIC 3168, Australia
[c] CSIRO Earth Science and Resource Engineering, 26 Dick Perry Ave., Kensington, WA 6151, Australia

A R T I C L E I N F O

Article history:
Received 26 September 2013
Accepted 26 January 2014
Available online 2 February 2014

Keywords:
Microtomography
Characterisation
Permeability
Upscaling
Percolation theory
Computational modelling

A B S T R A C T

We propose a workflow to provide detailed characterisation of microstructures, simulations of permeability at micro-scale, and to analyse the upscaling of permeability. The workflow is fully tested using two very different microtomographic datasets of carbonate samples with strong heterogeneity. The characterisation of microstructures includes not only routine parameters but also anisotropy of the pore-structure. The critical pore diameter is also obtained through morphological implementations. The method of stochastic analysis of extended local porosity theory is used to determine the sizes of representative volume elements (RVE). We demonstrate criteria for determining the size of the RVE and show a sample that satisfies the criterion. We also discuss a sample that does not suffice the RVE criterion, because of the strong anisotropy. Permeabilities are computed using Lattice-Boltzmann (LB) simulations on the RVE and compared with laboratory measurements. Techniques and procedures are used to extract scaling parameters for both of the samples including: 1) percolation threshold — by using a shrinking/expanding algorithm; 2) crossover length — by analysing the mass density; 3) the critical exponent of correlation length — by using the finite-size scaling scheme; and 4) the critical exponent of permeability — by running LB simulations on a series of derivative models close to the percolation threshold. Our results of critical exponents are different from the previous studies and the mass density distributions are irregular. This pilot study provides new information on the relationships between microstructures and permeability of natural rocks with complex microstructures. The study also reveals the scaling parameters. Our results clearly put into question whether natural rocks can be idealised by classical theoretical solutions. A robust workflow for embracing a computational approach of microstructures may provide a solution.

1. Introduction

Mineral systems involve multiple processes and multiple scales in nature (Gow et al., 2002; Hobbs et al., 2000; Ju et al., 2011; Lin et al., 2006; Liu and Zhao, 2010; Liu et al., 2005, 2008, 2011; Ord et al., 2002; Sorjonen-Ward and Zhang, 2002; Zhang et al., 2003, 2008; Zhao et al., 2008a, 2009). To simulate an ore-forming system numerically, both parameters and different methods are needed for describing different aspects of the system (Zhao et al., 2008a, 2009 and the references therein included). Since pore-fluid flow plays an important role in transporting minerals from one place to another, porosity and permeability become two key parameters to reflect the flow pathways in porous rocks and to affect the mineralisation patterns in ore-forming systems (Zhao et al., 2009). Although computational modelling has been used to solve a broad range of pore-fluid flow problems in both geoscience systems (Awadh et al., 2013; Lin et al., 2003, 2008, 2009; Mugler et al., 2012; Schmidt Mumm et al., 2010; Xing and Makinouchi, 2008; Yan et al., 2003; Zhao, 2009; Zhao et al., 2008a, 2009) and geoenvironmental systems (Charifo et al., 2013; Khalil et al., 2013; Sung et al., 2012; Zhao et al., 2008b, 2010), a numerical model that can be used to reflect the microstructure change of a porous rock due to chemical dissolution and precipitation is still lacking (Zhao et al., 2008b, 2010). Obviously, such a microstructure change can have an important effect on the permeability that is commonly used to reflect the flow pathways in porous rocks.

Microtomography enables quantification of the relationship between the microstructure of rocks and transport properties, which may be used in both geoscience and geo-environmental fields. Fluid transport properties have been studied with considerations of microtomographic characterisation (Arns et al., 2005; Knackstedt et al., 2006; Moreno-Atanasio et al., 2010). Carbonate samples have been proved to be notoriously difficult to analyse owing to their complexity. We provide detailed information of characterisation of carbonate samples with strong heterogeneity and the corresponding permeability in this study. In addition, as the sizes of microtomographic samples are limited to the millimetre scale

* Corresponding author. Tel.: +61 8 6488 4227.
E-mail address: liujieigcea@gmail.com (J. Liu).

0375-6742/$ – see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.gexplo.2014.01.021

to provide high-resolution images, upscaling is the associated problem to derive whether the properties at the micro-scale can be used in large scales. We analyse the upscaling of permeability using percolation theory, focusing on the critical exponent of permeability for heterogeneous rocks. This pilot study provides basic information of natural samples with complex microstructures about the relationship of microstructures and permeability, and the upscaling of permeability.

We understand the characterisation of microstructures as describing the structures in micro-scale using parameters or statistical data (Baker et al., 2012). Porosity is generally the most important and popular parameter for assessment of reservoir rocks. Pore-size or pore-throat distribution is the second. Not all pores but only those connected ones are effective for fluid flow. Thus the connectivity of pores and effective porosity are essential parameters for fluid flow problems. Percolation theory (Stauffer and Aharony, 1994) deals with the connectivity of sites or bonds. We use percolation theory for microtomographic analysis and the connectivity of pores as the first question to be addressed. We conduct specific surface area of pores which denotes the roughness of the surface of pores, and to some extent, tortuosity as well. An orientation tensor (Ketcham, 2005; Liu et al., 2009) is used to describe the anisotropy of the pore structure representing the anisotropy of permeability. In addition, the critical pore diameter (Katz and Thompson, 1987) is the largest throat of the network where most fluid flows through. It is obtained through a morphological technique presented in this study.

We derive the permeability of the samples on a representative volume element (RVE) if it exists from stochastic analysis (Liu et al., 2009). Using RVEs ensures that the simulated permeability is representative for the specific sample. To determine the permeability numerically we can use a variety of numerical techniques but they all depend on obtaining the steady state flow field and then using Darcy's Law to extract the permeability. Numerical methods such as the finite element method (FEM) (Arns et al., 2002), random walk methods, network models (Blunt et al., 2002; Pereira, 1999), smoothed particle hydrodynamics (SPH) (Pereira et al., 2011, 2012) and Lattice-Boltzmann (LB) methods (Ahrenholz et al., 2008; Chai et al., 2010; Lin et al., 2005; Narvaez et al., 2010; Pan et al., 2006) have been used in the past.

In this study, the two main criteria for selecting the numerical method are (i) the capability to easily input the complex, three-dimensional (3-D) digital data into a numerical method to calculate the flow fields and (ii) computational speed and accuracy. Methods such as the FEM and SPH method need to construct suitable solid boundaries from the digital data. However, this can lead to approximations, which degrade the accuracy of the solution. This is especially a problem for real rock data where the boundaries are not smooth. Network models approximate real pores and connecting throats with simplified (ball and stick) models. However, for the LB method no such approximations or simplifications are required. One can simply take the digital data and input it into the LB code. No approximations need to be made regarding this input geometry and the numerical resolution is the same as the resolution of the digital data. Regarding the speed of the method we have previously (Pereira et al., 2012) made an in-depth comparison for sample porous media (consisting of solid spherical or cubical grains) between the LB and SPH methods. We found that the LB method was vastly superior to the SPH method, even for single core simulations. Moreover, one clear advantage of the LB method over other numerical methods is its inherent parallelism. It can be shown that the major computational part of the algorithm is completely localised, so that processors do not need to talk to each other. In this case, LB scales vary almost linearly with number of processors. In this work we have used this scalability to easily (and rapidly) simulate relatively large (real rock) data sets (up to 500^3 voxels).

Upscaling considers how the permeability obtained at micro-scale can be used in large scales. Different methods can be used for upscaling such as effective-medium theory, stochastic homogenisation and others (Farmer, 2002). A new strategy and methodology was proposed (Liu and Regenauer-Lieb, 2011) to determine the percolation threshold, fractal dimension, the critical exponent of correlation length, and other scaling parameters from static natural samples by referring to percolation theory. The theory for upscaling of microtomography was considered the first choice since it is the most direct method based on the observed statistics. Further to our previous study, we focus in this paper on the critical exponent of permeability and try to apply the percolation theory on heterogeneous rocks. The critical exponent of permeability describes the exponential change of permeability when the porosity approaches the percolation threshold, which is scale independent. When porosity and the percolation threshold are known, permeability is predictable through the critical exponent of permeability for all scales. Scaling laws are the relationships of critical exponents and the critical exponent of permeability is one of the exponents. However, the relationships between the critical exponent of permeability and the others are not well established, only the relationships between the critical exponents of permeability and conductivity are given (Feng et al., 1987; Halperin et al., 1985; Sahimi, 1998). Thus more efforts are required for this scientific topic. Our present study provides a contribution from the point of view of heterogeneous rocks characterised by microtomographic data.

2. Workflow and methodology

2.1. Workflow

In this study, we use the workflow shown in Fig. 1. We start our work from segmentation after data acquisition. Segmentation converts greyscale images to binary images and all the following analyses use the binary images. There are the two columns in the major part of the workflow. The left column comprises: 1) geometrical analysis to get characterisation, so that the fractal dimension can be calculated, 2) stochastic analysis to determine the size of an RVE, and 3) pore-scale simulation on the RVE to obtain permeability at the micro-scale. The right column comprises the detection of percolation threshold and the extraction of the critical exponents of correlation length and permeability, by using finite size scaling scheme and simulations of a series of derivative models. Scaling laws are defined while the fractal dimension and critical exponents are known. These constrain whether the permeability obtained at the micro-scale can be extended to a large scale. We present a new version of the workflow published previously (Liu and

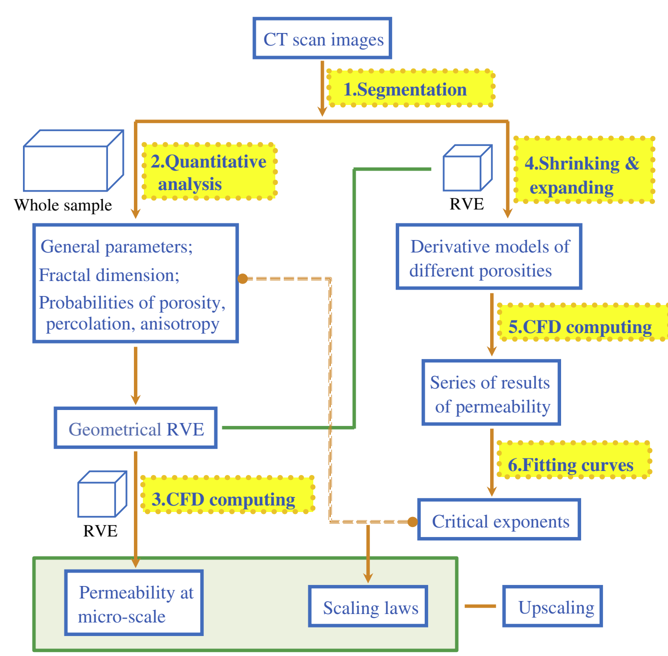

Fig. 1. Workflow for microtomographic analysis and upscaling of permeability.