MICRON TO MILLIMETER UPSCALING OF SHALE ROCK PROPERTIES BASED ON 3D IMAGING AND MODELING

Shuang Zhang[1], Robert E. Klimentidis[2], and Patrick Barthelemy[1]

[1]VSG – Visualization Sciences Group, Burlington, MA, USA
[2]ExxonMobil Upstream Research Co., Houston, TX, USA

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ABSTRACT

3D tomographic data at various scales is increasingly available through the wide adoption of μCT (Micro Computed Tomography) and FIB-SEM (Focused Ion Beam - Scanning Electron Microscopy) technologies. However, upscaling these observations is very challenging. This paper provides a template of an upscaling protocol between FIB-SEM data on a micron sized sample and μCT data on the same sample region but at millimeter-scale.

We use a Devonian North American shale rock fragment in our study. Due to the large scale variations in the pore structure and drastic petrophysical property heterogeneity, shale rocks are very challenging and costly to study as compared to rock samples from conventional reservoirs. Using μCT with voxel resolution of tens of microns, we are able to identify different rock heterogeneities. A smaller sample from each distinct heterogeneity region is then digitized using FIB-SEM 3D imaging with voxel resolution of a few nanometers. Stokes flow at *pore-scale* is used to model the absolute permeability tensor, an intrinsic rock property associated with each rock heterogeneity. Afterwards, multiphase porous medium flow at *Darcy-scale* is conducted on the μCT data, constrained by the permeability tensor and the porosity calculated from FIB-SEM data that correspond to each heterogeneity identified from the μCT data previously.

This feasibility study provides a framework to model a wide range of petrophysical parameters in a heterogeneous region by combining imaging and modeling protocols at different scales.

INTRODUCTION

Porosity and permeability are petrophysical parameters critical to quantify the mass and recoverabilityof oil and gas in reservoirs. Shale rock is particularly challenging as the size of the voids can vary by a few orders of magnitude from a few millimeters to a few nanometers. The heterogeneity of gas shale comes not only from large scale variation of pores and cracks during rock formation or compaction, but also from porous kerogen material in various stages of maturity. These morphological heterogeneities cause nonuniformity and anisotropy of mechanical and transport properties such as porosity, permeability, wettability and absorption. A number of studies in the literature identify and classify these different porosity types with reported resolution up to 4-5nm [4,5]. Many conventional methods for studying these parameters become inconsistent and unreliable for shale.

Imaging offers great potential in studying shale rocks. While 2D SEM/TEM (Transmitted Electron Microscopy) imaging is of growing importance, its shortcomings in characterizing the pore structure are documented [4]. For example, pores appearing to be isolated in 2D can be connected via the third dimension. Moreover, 2D images provide no insight into connectivity or permeability. This highlights the importance of 3D imaging and the consequent digital rock physics analysis, which is demonstrated in our previous work [8]. Because of the wide adoption of μCT and FIB-SEM technologies, 3D tomography at various scales has become increasingly available. There is a need now to integrate the information such as porosity and permeability extracted from the data at very small scale with the larger scale, i.e., data upscaling.

This paper will focus on setting up a template for an upscaling protocol between FIB-SEM data on a micron size shale rock sample and μCT data on the same sample but at millimeter-scale. This study builds on the work of Zhang et. al. [10] which describes an upscaling approach between μCT and discontinuous borehole images with missing data interpolated with multipoint statistics. In this paper, we use μCT and FIB-SEM as our 3D imaging methods to digitally sample shale fragment and its representative heterogeneities at different scales. We use numerical models at two different scales to link the two digital representations and to estimate the petrophysical properties at the fragment scale.

METHODOLOGY

Porosity can be observed on the microscale (between nanometers to microns) in organic matter, between mineral grains including within pyrite framboids, micro-fossils, clay minerals and in the form of microcracks. While all porosity can be connected as one single pore network, it is associated with different materials (organic or mineral) which cause significant heterogeneity within a single fragment.

In the shale fragment used in this study, we model three kinds of heterogeneities:

- *H1* - The heterogeneity that is caused by voids greater than 10s of microns. These voids relate to large pores or fractures that are either natural or associated with fracturing. This heterogeneity can be imaged with high fidelity using μCT.
- *H2* - The heterogeneity that is dominated by organic matter which is mixed with mineraland nano-scale pores.
- *H3* - The heterogeneity that is dominated by mineral matrix which is mixed with pore space and small volumes of organic matter.

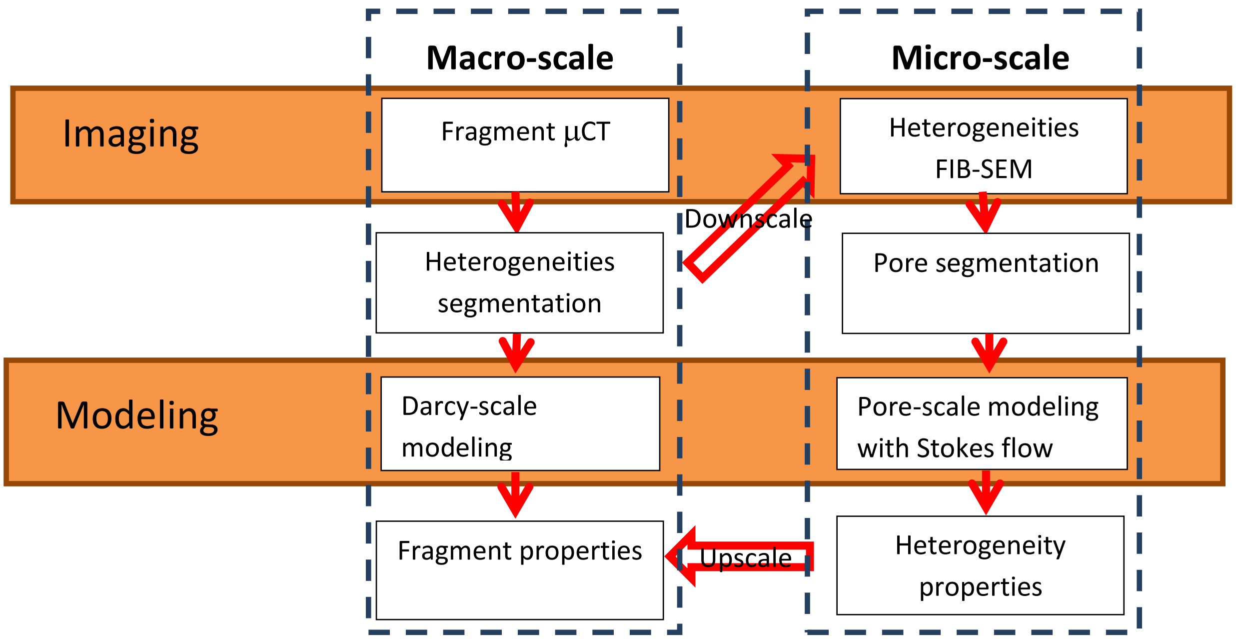

Figure 1. Diagram of the multi-scale imaging and modeling approach

Figure 1 is a diagram showing the basic building blocks and workflow of our up-scaling protocol. Using μCT with voxel resolution of tens of microns (reconstructed at 25μm per pixel), we are able to identify different rock heterogeneities (*H1*, *H2* and *H3*) from the fragment. A smaller sample from individual rock heterogeneities (*H2* and *H3*) is then imaged using FIB-SEM with voxel size of a few nanometers. Upon 3D reconstruction and segmentation, nano-pore networks are extracted from *H2* and *H3* samples. Stokes flow at *pore-scale* (i.e., geometries corresponding to the smallest possible pore in the porous material) is used to model the absolute permeability tensor, an intrinsic rock property which varies for each rock heterogeneity. To simplify the numerical modeling of an extremely complex pore network, this image-based simulation approach uses the binarized FIB-SEM image stack as the input grid without explicitly building the geometrical surface and the unstructured volumetric mesh. This simplification allows us to solve flow equations on systems so large that they would otherwise be computationally intractable, thereby permitting the direct study of fine *pore-scale* details.

Afterwards, multiphase porous medium flow at *Darcy-scale* [2] (i.e., porous material with averaged porosity and permeability as bulk material properties) is modeled on the μCT data with *H1*, *H2* and *H3* heterogeneities, using the permeability tensor and the porosity for *H2* and *H3* calculated in previous step derived from the FIB-SEM data. This modeling approach features *Darcy-scale* continuum mechanics without explicitly encoding the *pore-scale* geometry, thereby drastically reducing the complexity of the simulation mesh, but it retains rich multi-phase multi-physics parameters. Estimates of saturation and capillary pressure curves can be produced at the scale of a shale rock fragment.

DOWNSCALE IMAGING

We use x-ray μCT (Figure 2a) to scan the rock shale fragment sample (Figure 2b). Digitized data are shown in 3D (Figure 2c) and 2D (Figure 2d). Then two small areas from the heterogeneities *H2* and *H3* are identified (as marked in Figure 2d). They are digitized using FIB-SEM (Figure 2g). For *H2*, organic matter dominance is observed (Figure 2h and 2i). For *H3*, we can see mineral dominance with small pores and cracks (Figure 2e and 2f). Following necessary pre-processing, we produced the following three digital rock datasets:

- *Data1*: μCT data for rock fragment, shown in Figures 2b, 2c & 2d.
- *Data2*: FIB-SEM data for *H2* sample, shown in Figures 2h & 2i.
- *Data3*: FIB-SEM data for *H3* sample, shown in Figures 2e & 2f.

Through 3D image processing and segmentation [8], pore space, organic matter (or organic matter dominant heterogeneity *H2* for *Data1*), and mineral matrix (or mineral matrix dominant heterogeneity *H3* for *Data1*) are identified for each dataset. The dimensions of the processed sample and calculated volume fractions are summarized in Table 1. For *Data3*, because the volume fraction of organic matter is very small, we counted it toward pore space without having a significant impact on our simulations.

PORE-SCALE MODELING

Two simulation tools are used in this paper for flow modeling:

- Avizo XLab-Hydro[1] solver for *pore-scale* modeling.
- DUMUx [2] solver for *Darcy-scale* modeling.

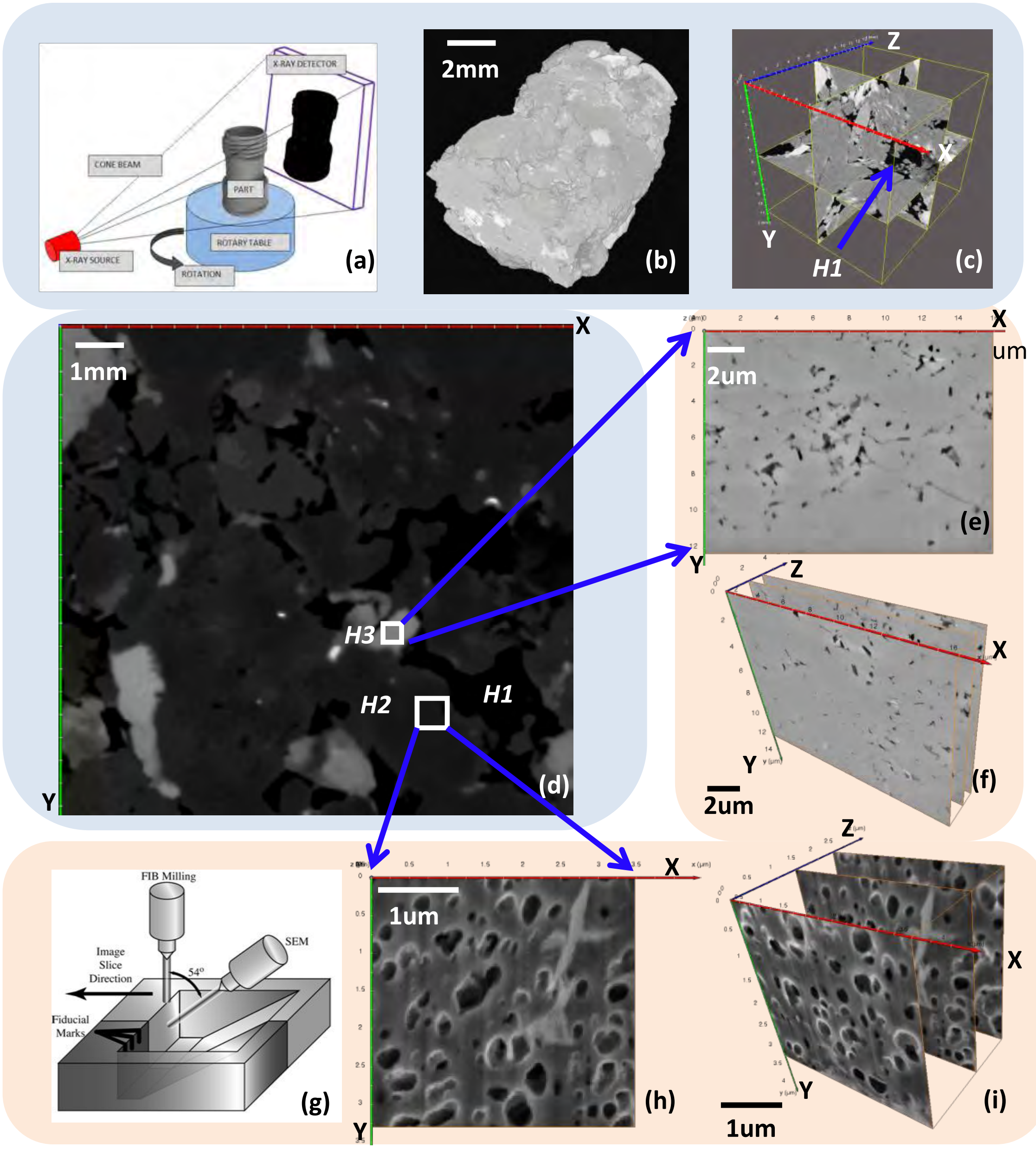

Figure 2. Downscale imaging procedure. (a). Experimental schematic of x-ray computed tomography, which is the imaging methodology to produce results shown in Figures b, c & d. (b). External surface of the irregular shale rock fragment studied in this paper. (c) Digitized fragment using μCT. (d). One XY slice of μCT data on the fragment. (e). One XY slice of FIB-SEM data on a H3 sample. (f). Digitized image stack of a *H3* sample. (g). Experimental schematic of FIB-SEM. (h). One XY slice of FIB-SEM data on a *H2* sample. (i). Digitized image stack of a *H2* sample.

	Data1	**Data2**	**Data3**
Sample	Shale rock fragment	H2 (see Figure 2h & 2i)	H3 (see Figure 2e & 2f)
Acquisition method	μCT	FIB-SEM	FIB-SEM
Dimension	11.25x10.75x12.5 mm	3.5x3.3x2.4 μm	15.9x12.3x3 μm
Voxel Resolution	25 μm	20 nm	20 nm
Pore volume fraction	7.87%	37.7%	4.57%
Organic dominant v. f.	14.61%	58.3%	n/a
Mineral dominant v. f.	77.52%	4%	95.43%

Table 1. Dimension and volume fractions of three datasets.

We first focus on *pore-scale* modeling part. In *pore-scale* modeling, individual pores at various scales need to be explicitly represented with a simulation mesh. Traditionally, this means a surface geometry--equivalent to CAD models in standard engineering simulation practices--needs to be built to represent the interface between the pores and the solid[7,9]. We take a different approach with Avizo XLab-Hydro, by building finite volume mesh directly on the voxels of the segmented 3D imaging data, and solving the Stokes equations as in Equation 1 below.

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0; \boldsymbol{\nabla} p = \mu \boldsymbol{\nabla}^2 \boldsymbol{u} + \boldsymbol{f} \qquad \text{Equation 1}$$

Where $\boldsymbol{u}$ is the fluid velocity vector, p is the pressure, μ is the dynamic viscosity, $\boldsymbol{f}$ is the body force vector which is set to zero. With simplified geometry and flow equations, we can solve for the velocity and pressure fields for complex porous structure that is derived from imaging experiments; this is in contrast to conventional modeling executed on meshes constructed with CAD (Computer Aided Design) tools. Then Darcy's law (Equation 2) is used to evaluate the absolute permeability.

$$k_n = u_n \frac{\mu \boldsymbol{\Delta} x}{\boldsymbol{\Delta} p} \qquad \text{Equation 2}$$

Where n denotes the direction of flow, $\boldsymbol{\Delta} x$ and $\boldsymbol{\Delta} p$ are length and pressure drop across the sample respectively. Using volume averaging, we can derive tensor forms of Equations 1 and 2[5]. The result intrinsic permeability tensor **K** does not depend on the flow conditions and describes the anisotropy of the system. We have validated this solver against theoretical models and standard glass bead packaging models [8]. Interested readers are referred to [7,8,9] and Avizo' s User's Guide which can be downloaded from [1] for more information.

The key simulation results at *pore-scale* are reported in Table 2. For each of the simulations, water (viscosity 0.001 Pa*S) is virtually pushed through the sample with a pressure difference of 30,000 Pa along one direction at a time, while all other boundaries are treated as impermeable walls.

	Sim1	*Sim2*	*Sim3*
Data	*Data1*	*Data2*	*Data3*
Dimension	11.25x10.75x12.5 mm	3.5x3.3x2.4 μm	15.9x12.3x3 μm
Pore volume fraction	7.87%	37.7%	4.57%
Perm. Tensor **xx xy xz** **yx yy yz** **zx zy zz**	(Unit: D) 3.20 0.38 0.26 0.38 1.50 -0.30 0.26 -0.30 1.00	(Unit: μD) 43.0 -5.4 -2.2 -5.4 53.0 -5.7 -2.2 -5.7 44	(Unit: nD) 67.0 -0.91 -12 -0.91 100.0 -24 -12 -24 210
Principal Permeability Axes: Magnitude (same units as permeability tensor above), Declination (degrees), Inclination (degrees)	Mag Dec Inc 3.29 11.1 4.9 1.61 278.4 28.8 0.79 289.9 -60.7	Mag Dec Inc 57.0 108.1 -20.1 45.7 175.7 46.1 37.3 34.1 37	Mag Dec Inc 215.9 249 77.5 95.4 276.6 -11.1 65.7 5.5 5.6

Table 2. Summaries of Stokes simulations at pore-scale. The results for the principal permeability axes are courtesy of Professor David K. Potter during revision.

These simulations provide important information about the connectivity of porous network and its single phase, anisotropic absolute permeability at their respective scales. Specifically, the last row shows three magnitudes (which are identical to eigenvalues, ordered from the largest to smallest) and orientations (declination and inclination with respect to the x, y and z axes) of the three principal permeability anisotropy axes calculated from the permeability tensor. However, the following limitations are recognized. For *Sim1*, with the digitized rock fragment, the measured porosity significantly underestimates the total porosity as the porosity in *H2* and *H3* heterogeneities cannot be directly observed when imaged at this resolution. In other words, the pores that are not resolved with the μCT scan resolution are not modeled. For *Sim2* and *Sim3*, our FIB-SEM imaging method does have sufficient resolution to capture the majority of the pores, but the volume of the sample being studied is very small. Even though they may be representative for its respective porous network, they can definitely be considered unrepresentative at millimeter scale, as other families of heterogeneities exist. Digitizing the whole fragment using FIB-SEM with nano-scale resolution is not practical. These limitations highlight the need for an upscaling solution. In our work, upscaling is achieved by performing Darcy-scale simulations using,

- Heterogeneities meshed from μCT 3D imaging segmentation at mm-scale.
- Simulated intrinsic material properties (porosity and permeability tensor) derived from the FIB-SEM 3D imaging at um-scale resolution for each heterogeneity.

DARCY-SCALE MODELLING AND UPSCALING

DUMUx [2] is a generic simulation framework for multiphase fluid flow and transport in porous media. Object-oriented programming with template paradigm is used to achieve performance, flexibility, and scalability. Maas et al. [3] introduce one dimensional DUMUx simulations into core analysis to study the uncertainties in SCAL measurements and to better interpret them. In this paper, we use the segmentation results from 3D imaging as the mesh input of DUMUx solver. This Cartesian grid features a cell-by-cell definition of heterogeneous material properties such as porosity and permeability. Multiphase flow solutions can be obtained on macro-scale sample with unlimited number of heterogeneities. All *Darcy-scale* simulations are conducted along X direction, with Neumann mass fluxes specified corresponding to a pressure difference of 30,000Pa. Other boundaries are specified as Dirichlet no flux boundaries. Table 3 summarizes the key simulations conducted at *Darcy-scale*. Note the model size of these simulations is limited by the hardware resources used in this study.

	Sim4	***Sim5***	***Sim6***	***Sim7***
Grid	100x100	100x100	100x100x100	100x100x100
Hetero-geneity	Single material with porosity and permeability from *Sim1*	Five layer sample with porosity and permeability tensors computed from sub-regions *Sim1*	Segmentation results of *Data1*, with H2 & H3 porosity and permeability tensors computed from *Sim2* and *Sim3*.	Same as *Sim6*
Models	Single phase, Steady State	Single phase, Steady State	Single phase, Steady State	Two phase, Transient

Table 3. Summary of simulations at Darcy scale

Before the upscaling study, we need to first validate our approach. The pore space segmented from the μCT *Data1* can be treated as a *pore-scale* model where pore sizes are 10 microns or more. A 2D cross section of *Data1* after segmentation is shown in the black polygon in Figure 3. *Sim1* from Table 2 is conducted in 3D on *Data1* after segmentation. In addition to permeability tensors as reported in Table 1, pressure and velocity fields are also solved for all voxels in *Data1*. We integrate the pressure on all YZ planes (note the flow is along X axis), and plot the average pressure, shown as the solid red curve in Figure 3. Five zones with near linear pressure drop are identified and labeled with red numbers.

This *pore-scale* model is translated to a *Darcy-scale* model by specifying porosity and permeability tensor as two constants of the homogenized single phase transport equation, Equation 3,

$$\boldsymbol{\phi}\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{u} = \mathbf{0} \; ; \; \boldsymbol{u} = -\frac{\mathbf{K}}{\mu}(\nabla p + \rho g H) \qquad \text{Equation 3}$$

Where ϕ is porosity, g is gravity, and H is the height. Both ϕ and **K** are spatial variables. They are associated with each heterogeneity later on. In our study, gravity is assumed to be zero. If the flow is incompressible as in our case, simulation of this equation produces a linear pressure drop along the flow direction, which is shown as the dashed curve in Figure 3. With inhomogeneity and anisotropy averaged out, the results from *Sim4* match *Sim1* very well.

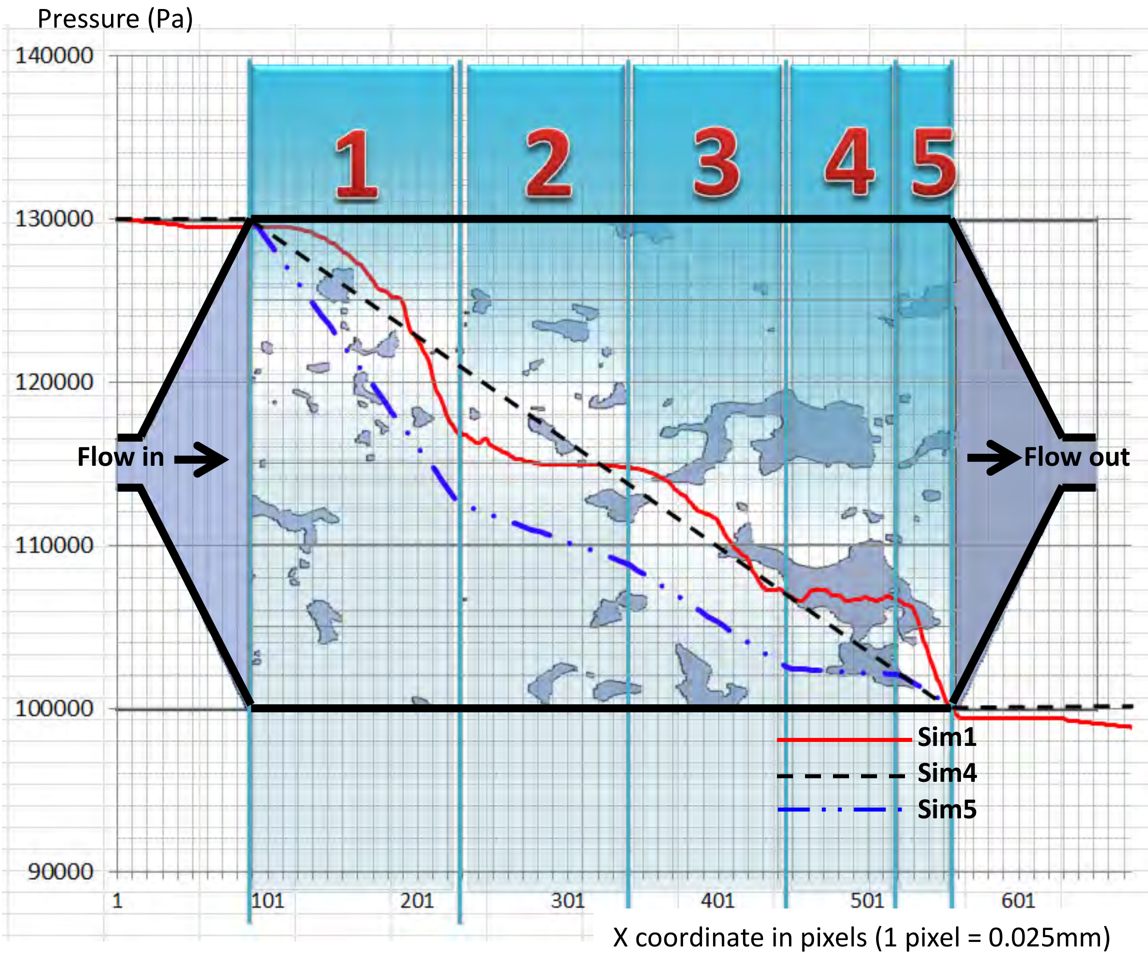

Figure 3. Comparing Darcy scale simulations with pore scale simulations.

A series of *pore-scale* simulations are conducted on each of the linear pressure zones. Porosities and permeability tensors for each zone are computed. These parameters are used as inputs of a *Darcy-scale* model simulation, *Sim5*, with these five zones homogenized. Pressure integral is plotted as blue dash-dot curve in Figure 3. The general trend of pressure drops in the five zones are well captured. However, it does not match exactly the pressure drop integral curve from *Sim1*. The accuracy in zone subdivision and the ignored three dimensional complexity in this one dimensional homogenization (note the simulation is done in 3D, but the five zones is set along x-axis only) can be possible causes. We note that this deviation warrants further investigation.

Figure 4 shows the set-up and key results of *Sim6*. With porous heterogeneities (H2 and H3) taken into account, the pressure drop integral curve displays behavior very different from *Sim1 and Sim4* (Figure 3) where only the pore space is present. We observe pressure extremes outside the range of the specified pressure difference at inlet and outlet.

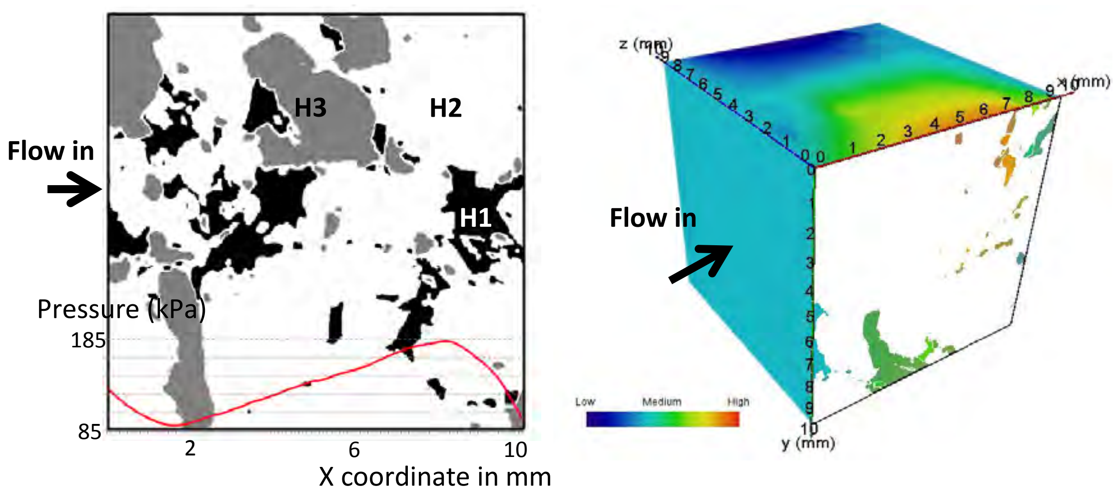

Figure 4. Single phase up-scaled model, *Sim6* results. (a). One 2D slice of 3D segmentation of μCT *data1*; integrated pressure curve is plotted at the bottom. (b). Volume rendering of pressure field.

This framework allows us to conduct more sophisticated simulations with multiphase and multiple chemical component on the *Darcy-scale*. These simulations will produce more important petrophysical parameters such as relative permeability, capillary pressure and non-wetting phase saturation. As a feasibility study, we conducted a two-phase simulation, equation 4,

$$\phi\frac{\partial \rho_\alpha S_\alpha}{\partial t} + \nabla \cdot \rho_\alpha \boldsymbol{u}_\alpha = \boldsymbol{0}\ ; \quad \boldsymbol{u}_\alpha = -\frac{k_\alpha \mathbf{K}}{\mu}(\nabla p_\alpha + \rho_\alpha g H) \qquad \text{Equation 4}$$

Where α denotes different phases. In our two phase study, there is a wetting phase (water, denoted *w* hereafter) and a non-wetting phase (oil, denoted *nw* hereafter).

Figure 5 shows the *Sim7* result. We inject water along the X direction. The sample is originally oil saturated. As the simulation evolves, the oil is gradually displaced by the water influx. Figure 5a shows the oil saturation curve over time. At 1250 seconds, water started to penetrate the sample. We also see the average pressure of water, the wetting phase, as penetrating through (Figure 5b). The evolution of water front is shown in Figure

5c as a series of surfaces. Water saturation, pressure of non-wetting phase (oil), and capillary pressure are also computed but deferred to a follow-up study.

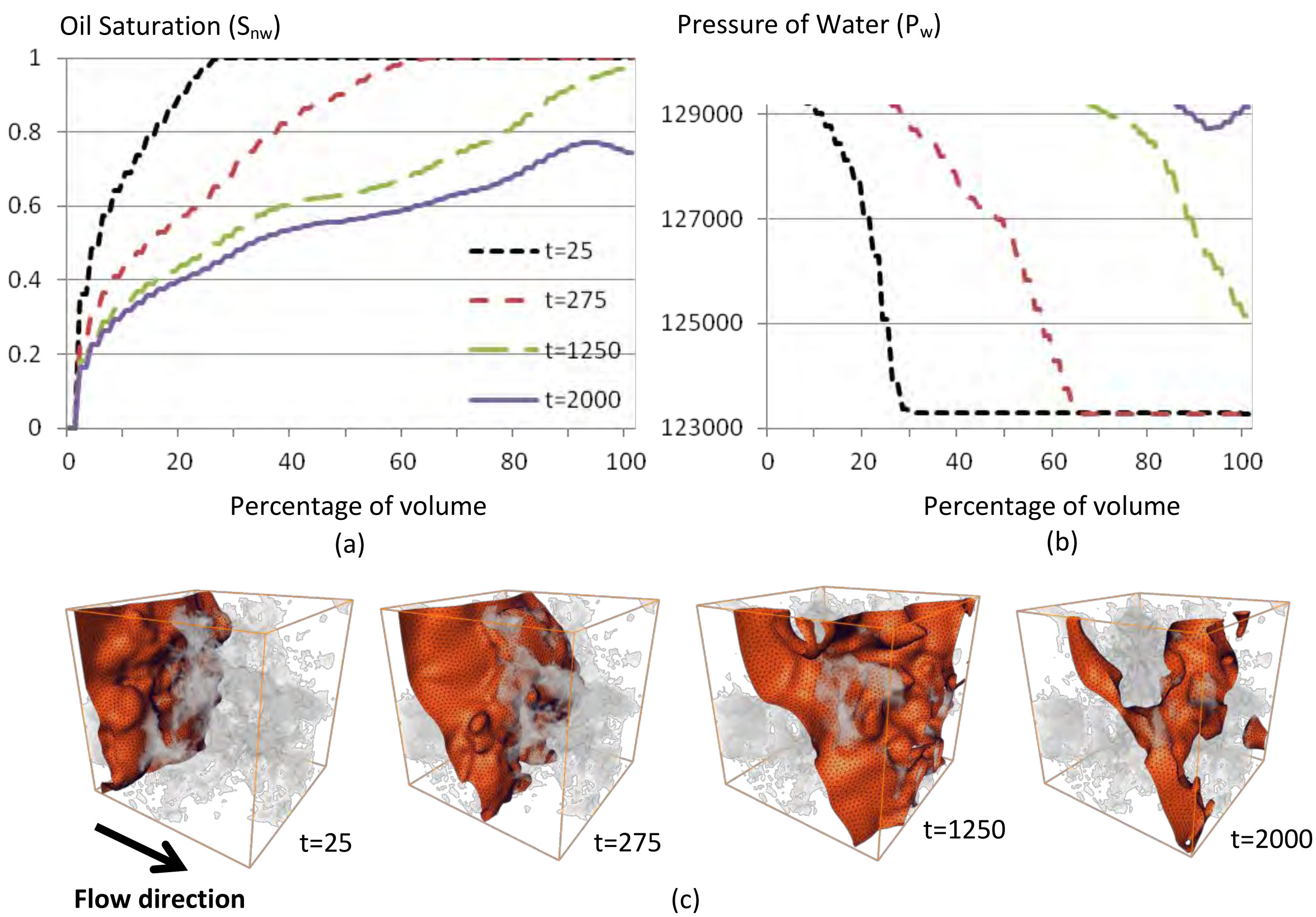

Figure 5. Two phase up-scaled model, *Sim7* results, the time unit is second in all plots. (a). Integrated oil saturation (non-wetting phase) curve at four time steps; (b). Integrated water pressure (wetting phase) curve; (c). Time evolution of water front (surface) through the fragment; pore space is rendered as grey cloud.

DISCUSSION & FUTURE WORK

This work develops a framework to capture the shale-gas reservoir heterogeneity by combining imaging and modeling approaches at different scales. This paper focuses on the conceptual aspects of the framework to prove its feasibility. It touched a very small fraction of possible modeling scenarios and quantitative information that can be extracted. Great potential exists. This framework can be extended to inter-well scale or field scale where digital data for different rock litho-facies may come from different means other than imaging. Moreover, the question from geophysics communities in relationship with "dirty pores" (pores that retain organic matter) can be addressed with this framework. In addition to porosity, permeability, saturation, and pressure, many other petrophysical properties can be upscaled in a similar manner, such as mechanical, electrical, and chemical parameters.

As both the imaging and software technologies continue to evolve, the framework proposed in this paper has significant potential in a vast range of applications. To realize this potential, a number of aspects need to be further addressed. First, the petrophysical parameters at all scales have to be validated against physical experiments. Numerical aspects such as convergence with grid resolution and representative volume determination must be investigated, before numerically modeling complex systems with different phase compositions, different number of phases, and impact of the transport of species.

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