Unearthing the hidden structure of rocks — that’s what Shuang Zhang and his colleagues achieved by using the combination of VSG’s Avizo 3D Analysis software and COMSOL’s Multiphysics modeling and simulation software.

Since American oil and gas reserves are becoming increasingly more difficult to access, the industry has been turning to the technique of injecting fluid under pressure into rock deposits in order to harvest oil and gas that is trapped in-situ. This process requires knowledge of the structure of the shale formations in an oil field site. The process relies on being able to predict the ability of fluids to penetrate the rock. “There are two important physical parameters in order to determine this,” said Dr. Zhang, “these are porosity and permeability.” Porosity is a measure of how much void space exists in the rock and permeability characterizes how well the fluid will flow through it. “Of course, these two parameters are strongly correlated,” he continued. “The work of discovering these parameters has generally been done by obtaining a rock sample and examining it in a physical laboratory,” said Dr. Zhang.

Dr. Zhang, along with his VSG colleagues and customers demonstrated an innovative method for doing this analysis without using physical laboratory techniques. They took a brick-shaped shale sample (Figure 1a) and deconstructed it by using a focused ion beam-scanning electron microscopy (FIB-SEM) system (Figure 1b) to obtain data at a nanoscale level from the sample (Figure 1c). The Avizo software uses this data to construct a digitized three-dimensional model representing the pore distribution within the sample. “The value of the COMSOL software for our project is its ability to use the geometry representing the pore network of the rock to perform a flow simulation. This flow simulation is very important for determining how permeable the rock,” said Dr. Zhang.

**FIB-SEM**

The FIB-SEM technique uses an ion beam to mill away a layer of the rock sample. Detailed digital data of the structure of the exposed layer is obtained by the scanning electron beam microscope at a resolution down to a few nanometers. By repeating this process over and over, a 3D volume is assembled from the stack of fine-scale images of each layer. After preprocessing to eliminate effects such as misalignment between layers and random noise, the Avizo software is used in an interactive fashion to create a digitized mathematical model of the shale sample. This process is actually quite similar to the way images of the human body are constructed by using tomography techniques as in CAT scans, PET scans and MRIs.

The shale is composed of three types of material: mineral matter, organic matter and void-spaces. These are termed phases and their significance is that the rock is made up of a complex nanoscale arrangement of these phases, which is what ultimately determines the flow characteristics. If the voids are of microscopic size and distribution, FIB-SEM scanning can generate data that would be impossible to find in a physical lab.

**Three-Dimensional Model Reconstruction**

Once the data for the 3D model has been assembled and stored, the Avizo software creates the geometry model and the corresponding volumetric mesh structure. This model can create a display of the three phases rendered with different shadings. A critical feature is the ability to extract a small region of interest (ROI), which will reduce the amount of computation data storage resources needed to a manageable level.

In performing the analysis, data regarding the three phases is separated out (segmented) and quantified, so that the percentages of the total volume for each phase can be calculated. This separation step is called image space segmentation. A further step, called pore...
space segmentation, separates the pores into “dead pores,” “connected pores,” and “pore throats.” These steps enable detailed statistical analysis of the nature and distribution of the pores throughout the volume. It is this pore network that enables the COMSOL software to perform a simulated flow experiment.

“A significant benefit of being able to represent the sample in digitized form is that physics phenomena governed by mathematical models such as partial differential equations can be calculated, using data representing real-world geometry, through the PDE solvers such as COMSOL,” said Dr. Zhang. Properties such as permeability, molecular diffusivity, heat conductivity and electrical resistivity can be determined in this way.

**Flow Simulation**

The two important parameters for determining flow are porosity and permeability. Porosity is calculated with the Avizo software by using the 3D image it has created from the FIB-SEM data. Once the image-based digitized model has been constructed, the COMSOL Multi-physics software can be used to conduct a virtual physical experiment. In order to calculate the absolute permeability, it is necessary to obtain the average fluid velocity and the applied pressure.

“These values are obtained from the flow simulation, which is conducted by the COMSOL software,” said Dr. Zhang.

The COMSOL flow simulation sets up a velocity inlet on one side of the digital sample and a pressure outlet on the opposite face. The four other sides, as well as the pore boundaries are set up as non-slip walls. “Traditionally this type of analysis has to be done in a physical laboratory, where the process is expensive, inaccurate, incomplete, and time consuming,” said Dr. Zhang. COMSOL further outputs the results of this virtual physics experiment in a format that can be used by the Avizo software to create visualizations of the pressure distribution within the pore space, velocity vector plots, and a display of streamlines representing pressure.

**Advantages**

Using FIB-SEM and VSG’s “Virtual Material Studio” enables a detailed and accurate analysis to be performed on a sample of shale from an oil field. Once the digitized data is input using the FIB-SEM technique, a tomographic analysis is used to create a mesh image of the sample. The computer does the rest of the work.

As Dr. Zhang put it, “COMSOL takes the geometry generated by Avizo and performs the flow simulation and Avizo takes the data generated by the simulation and uses it to create powerful visualizations.”

“When our simulation-based method is validated, we will be able to solve things that cannot be measured in a physical lab... We can do things in the digital world a lot cheaper and faster compared to a physical lab,” said Dr. Zhang. He went on to say: “Industry is just becoming aware of this image-to-simulation workflow (Figure 3). An extraordinary amount of information can be extracted from this workflow — much more than we have ever seen before.”

**Reference**