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Editorial

# Advances in multiscale numerical and experimental approaches for multiphysics problems in porous media

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**Abstract:**
Research on the scientific and engineering problems of porous media has drawn increasing attention in recent years. Digital core analysis technology has been rapidly developed in many fields, such as hydrocarbon exploration and development, hydrology, medicine, materials and subsurface geofluids. In summary, science and engineering research in porous media is a complex problem involving multiple fields. In order to encourage communication and collaboration in porous media research using digital core technology in different industries, the 5th International Conference on Digital Core Analysis & the Workshop on Multiscale Numerical and Experimental Approaches for Multiphysics Problems in Porous Media was held in Qingdao from April 18 to 20, 2021. The workshop was jointly organized by the China InterPore Chapter, the Research Center of Multiphase Flow in Porous Media at the China University of Petroleum (East China) and the University of Aberdeen with financial support from the National Sciences Foundation of China and the British Council. Due to the current pandemic, a hybrid meeting was held (participants in China met in Qingdao, while other participants joined the meeting online), attracting more than 150 participants from around the world, and the latest multi-scale simulation and experimental methods to study multi-field coupling problems in complex porous media were presented.

## 1. Introduction

Porous media are widely found in natural and industrial systems, such as soil, groundwater resources, oil and gas reservoirs, human and animal tissues and organs, plants, composite materials, fuel cells, concrete, ceramics, textiles, and nanochips (Ingham and Pop, 1998; Blunt, 2017). Due to the complex pore structure and a wide range of flow and transport processes (Perkins and Johnston, 1963; Ghanbarian et al., 2013), further experimental and numerical studies are required (Knackstedt et al., 2009; Madonna et al., 2012; Yang et al., 2015). Most recent research has a focus on multiscale and multiphysics problems, especially for upscaling, ranging from the molecular scale to macroscale (Pan et al., 2006; Yang et al., 2020a, 2020b).

In this context, the China InterPore Chapter, the Research Center of Multiphase Flow in Porous Media at the China University of Petroleum (East China) and the University of Aberdeen, provided a platform for global scholars to share ideas and exchange studies of multiscale numerical and experimental approaches for multiphysics problems in porous media. The Research Center of Multiphase Flow in Porous Media focuses on academic exchanges, internationalization, as well as basic and original innovation research. Since 2012, four International Conferences on Digital Core Analysis have

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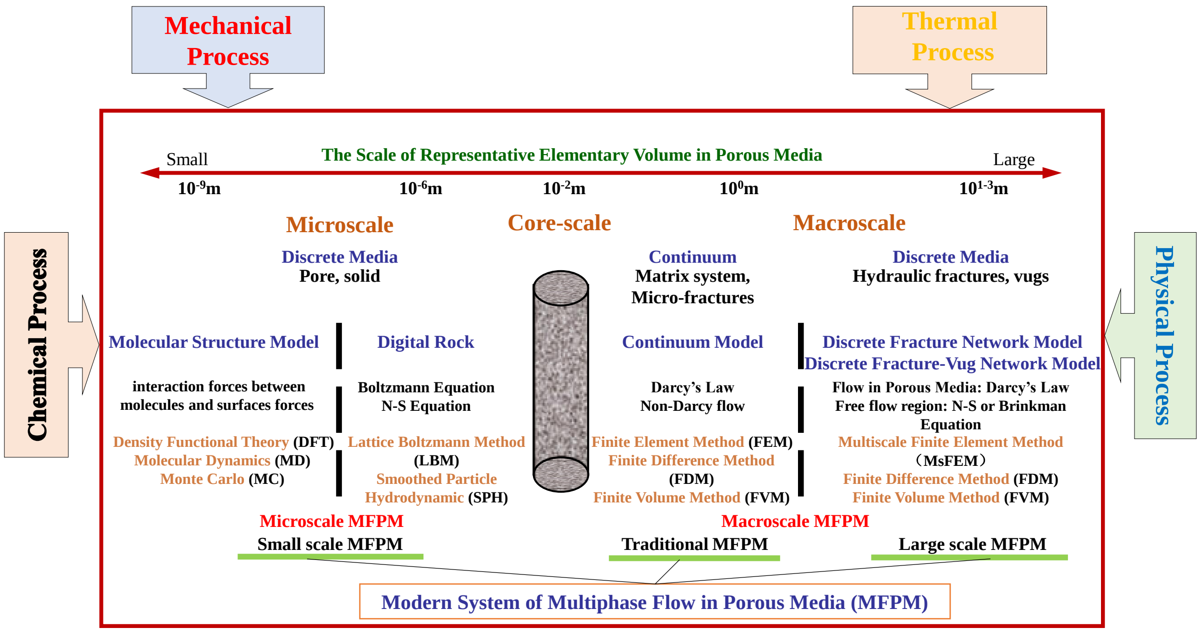


**Fig. 1.** Pedigree chart of the modern system of multiphase flow in porous media over different length scales (Yao et al., 2018).

been successfully held. Their team with PI Prof. Jun Yao also proposed the research frame on modern system of multiphase flow in porous media coupled with multiple fields, see Fig. 1 (Yao et al., 2018).

During April 18-20, 2021, the 5$^{th}$ International Conference on Digital Core Analysis & the Workshop on Multiscale Numerical and Experimental Approaches for Multiphysics Problems in Porous Media was held in Qingdao. Due to the inconvenience of traffic caused by COVID-19, experts from the UK presented their work online and participants in China attended the on-site meeting. The research topics covered in this workshop are summarized as below.

## 2. Experiments on porous media via micro-CT scanning and nanochips

Micro-CT scanning is considered as one of the efficient approaches to obtain the topological structure of porous media. Martin Blunt, from Imperial College London, delivered a lecture entitled "Flow in porous materials: A tale of X-rays, minimal surfaces and wettability". Using dynamic tomography with synchrotron radiation at high time and spatial resolution, he discussed the presence of minimal surfaces and determined thermodynamic based wettability during mutiphase flow in porous materials. Prof. Blunt also introduced trapping mechanisms in the context of $CO_2$ geological storage, and the importance of pore structure and wettability on fluid flow in other porous materials, such as surgical masks and fuel cells. He first shared his experiences on micro-scale fluid phase experiments and the related theory based on minimal surfaces and wettability. Then, he presented the pore scale approach to quantify the flow properties in porous rocks, various wettability measurements, three-phase flow and the flow in various porous materials in nature. He then ended his presentation with discussions on capture efficiency and maximizing flow in porous materials.

Yihuai Zhang, from Imperial College London, presented a talk entitled "Quantification of nonlinear multiphase flow in porous media". He quantified and predicted theoretically the onset of a transition from linear (Darcy) to nonlinear flow. For traditional multiphase flow in porous media, Darcy's law is valid, where the capillary number has a linear relationship with pressure gradient during steady-state multiphase flow; however, studies in recent years showed that there is a regime where the flow rate depends on the pressure drop as a power law with an exponent different than one, called the "intermittent flow" regime. For this phenomenon, the pressure difference during two-phase flow across a sandstone sample for a range of injection rates and fractional flows of water, the wetting phase, during an imbibition experiment was measured. The onset of the transition was quantified to a nonlinear power-law dependence and the exponent in the power-law was a function of fractional flow. Lastly, he used energy balance to accurately predict the onset of intermittency for a range of fractional flows, fluid viscosities, and different rock types.

Yongfei Yang, from China University of Petroleum (East China), gave a presentation on "X-Ray microtomography characterization of dynamic pore structure changes and fluid flow". Based on micro-CT equipments, a set of laboratory micro displacement and in situ scanning system were established. The dynamic changes of pore structure caused by acid rock reaction, fluid injection, stress cycling and thermal shock were characterized, and he also described the distribution of remaining oil in sandstone with different permeability during water and polymer flooding, respectively. Meanwhile, the results of gas-water two phase flow in porous, fractured and vuggy limestones were compared. He also discussed the potential application of micro-CT characterization in the context of $CO_2$ storage and oil/gas recovery in different types of reservoirs.

In a lecture entitled "Investigation on wellbore cement carbonation under geologic carbon storage conditions using micro-CT", Liwei Zhang, from the Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, based on CT scanning experiments, proposed the evaluation basis of cement carbonization degree, carbonization index for the first time, revealed the change of 3D pore structure and the distribution of reaction layer, found that the dense calcium carbonate layer formed by carbonization could prevent the penetration of high concentration $CO_2$ into the cement, and the calcium carbonate precipitation formed in the internal fracture of cement could reduce the fracture opening.

In the talk on "Nanofluidics: From oil/gas recovery to a clean energy future", delivered by Junjie Zhong, from China University of Petroleum (East China), emphasized the significance of exploring fluid behavior at the nanoscale. Nanofluidics is a visualization experiment platform where phase parameters and mass transfer parameters of oil, gas and water such as bubble/dew point, supercritical point, effective viscosity and diffusivity can be directly measured. In addition, micro-effect and mechanism of field development strategies, e.g., recovery of fracturing fluid, geothermal exploitation and gas injection, can be also characterized and evaluated. At last, he presented the combination of nanofluidics and artificial intelligence for the development of intelligent detection.

In the lecture of "Multiscale mechanism study of smart waterflooding", by Yongqiang Chen, from University of Manchester, he described the mechanism to control wettability alteration and the reason for the secondary low salinity waterflooding which recovers more oil than the tertiary low salinity waterflooding. Ion exchange, mineral dissolution and surface complexation reaction are responsible for the pH increase, then the pH increase contributes to the oil recovery. Through the pore scale observations, the secondary low salinity waterflooding could recovery the oil from both big pores and small pores while the tertiary low salinity waterflooding could only recovery the oil from the existing flow path.

Singh Kamaljit, from Heriot-Watt University, presented a talk entitled "3D imaging of flow in porous materials-from rocks to termite nests". Drainage and imbibition process were performed in 3D view based on synchrotron X-ray imaging. A new type of snap-off event was identified. He also discussed the imaging technology of fluid flow process in porous media and the impact of wettability system heterogeneity. The pore space structure and flow field features of termite nests were discussed at last.

## 3. Simulations of fluid transport and rock fractures

Spontaneous imbibition is an important mechanism of water flooding for oil recovery in fractured tight reservoirs. Accurate microstructure characterization of tight media is fundamental to analyze and evaluate reservoirs. Jianchao Cai, from China University of Petroleum (Beijing) and China University of Geosciences (Wuhan), gave the presentation on "Microstructure characterization and pore scale simulation of spontaneous imbibition in tight oil reservoir" to introduce fractal approaches for the characterization of pore structures based on core CT data. The reconstruction of a more accurate multi-scale digital core based on multiple resolution images was presented. Finally, the influence of wettability and pore-throat structure on recovery ratio, imbibition rate and changes of leading edge during spontaneous imbibition was discussed.

Cong Lu, from the Southwest Petroleum University, delivered a presentation on "Experiment and numerical model of conductivity of self-propped fractures in shale". A testing system for the conductivity of self-propped fractures in shale was established, which could get the conductivity accurately and establish the industry standard for conductivity testing. A numerical model for calculating the conductivity of self-proppant fractures in shale was also established, and the accuracy of the model was verified by experiments, with an average relative error of 9.3%. The numerical model of this study is not only applicable to support self-propped fractures, but the other rough fracture diverting capacity calculation.

In the lecture named "Preferential imbibition in a dual-permeability pore network", presented by Haihu Liu, from Xi'an Jiaotong University, he proposed a Lattice Boltzmann Method (LBM) to simulate the process of imbibition in a pore doublet structure. He also discussed the impact of capillary number and mobility ratio on the imbibition process in a pore network with dual permeability.

Coupled multiphase flow and reaction transport processes in porous media are widely used in energy, petrochemical, environment and other fields. Li Chen, from Xi'an Jiaotong University delivered a talk on "Pore-scale numerical simulation of multiphase reactive transport processes in porous media". In his talk, several difficult problems in the pore scale were systematically studied by using LBM. First of all, interphase interface transport and restricted domain mass transfer were developed in the mass transfer model to solve multiphase flow and mass transfer problems. Meanwhile, volumetric reaction and interface reaction model and solid volume evolution model were proposed to research reaction and evolution of solid structure phenomena. These models have also been used in many engineering applications including carbon dioxide geological sequestration, oil, gas and water three-phase miscible displacement (oil recovery), and new energy.

In the talk "Scaled-coupled CFD for next generation digital rock physics", given by Julien Maes, from Heriot-Watt University, he proposed a Darcy-Brinkman-Stokes framework to simulate the process of multi-physical single/multi-phase flow in multi-scale in digital rock, which was capable for modelling the reactive transport in multi-scale digital rock with relatively less expensive calculation. Also, a machine-learning method for the integrated upscaling of digital rock was proposed.

Pore-scale direct numerical simulation is a potentially powerful numerical tool to analyze flow and transport processes in various energy systems. In the lecture on "Numerical simulation of the reactive transport at the pore scale", Vadim Lisitsa, from Novosibirsk State University, presented a state-of-the-art methodology to estimate the evolution of pore space and hydrodynamic parameters of the core samples during the reactive transport at the pore scale using the level set method. Due to the computationally efficient of construction of the persistence diagrams and their classification, the methodology based on persistence homology can be used in 2D and 3D to classify the pore space evolution during chemical fluid–solid interaction.

Hu Jia, from the Southwest Petroleum University, delivered a lecture entitled "Flow model of ionic liquids in porous media under coupled electromagnetic & seepage fields". He introduced the problems existing in the water injection development, and the concept of ionic liquid and the application and theory of enhanced oil recovery by ionic liquid were summarized. He proposed an intelligent displacement technique for ionic liquids using Lorentz force to study the electromagnetic response of ionic liquids in a capillary model, and in further research discovered the effect of electrically induced heat on the flow of ionic fluids in porous media.

Yongcun Feng, from the China University of Petroleum (Beijing), delivered a presentation on "The influence of pore structure on rock mechanical properties". He discussed the problems of macroscopic mechanical properties and rupture characteristics. Combined with theoretical analyses and digital imaging technology, he presented the investigation on the influence of pore structure characteristics, especially on mechanical characteristics of rock damage and crack propagation.

In a presentation on "Multiscale multiphysics geocomputing and its potential applications in unconventional reservoirs", given by Huilin Xing, from Ocean University of China, he presented physics based multiscale multiphase multiphysics geocomputing on supercomputers. PANDAS, a novel finite element and/or Lattice Boltzmann method (FEM/LBM) based software is introduced, it has been successfully applied for simulating highly coupled geomechanical-fluid flow-thermal-chemical reaction systems involving heterogeneously fractured – porous geomaterials to address key scientific and technological challenges across different scales spanning from the pore to the lab and filed scale. Prof. Xing also highlighted further research on cross-scale issues needed to improve and optimize software functions for engineering applications.

Dispersed bubbles in the pore space is important for $CO_2$ sequestration, and whether it is hydrodynamically most stable or not is very important. In "Thermodynamic stability of bubbles in porous media", Ke Xu, from Peking University, focused on the coarsening effect that happens in porous media. He explored this research topic using microfluidics, and mentioned that there are amount of small bubbles in porous media, and they finally evolve to large bubbles and maybe become mobile gas cap at subsurface conditions. As he concluded, thermodynamic stability as bubbles in porous media was shown, and the kinetics for the bubbles to rich to get to the final equilibrium was also shown.

Quan Gan, from the University of Aberdeen, UK, presented a talk entitled "Heat transfer and induced fault reactivation in enhanced geothermal systems (EGS)". Deep geothermal development depends on the heat conduction process between the matrix and the cold water in fractures, and the derived thermal-hydrological-mechanical-chemical coupling process can significantly change the permeability and porosity of the reservoir at different stages. At the same time, faults are widely existed in deep geothermal, and the heat exchange process of rock can easily cause activation slip of faults due to the reduction of fault load. Prof. Gan had embedded 2D and 3D discrete pore and fracture structural models into the coupling model TACK-FLAC3D to improve the fluid flow in fractured reservoirs under stress conditions, and successfully applied them to simulate the production process of reservoirs, shale gas, geothermal, etc. This study enabled accurate descriptions of supercritical gas fracturing, geothermal fracture permeability evolution, and generated earthquakes.

Matteo Icardi, from the University of Nottingham made an interesting presentation on "Peatlands modelling and other porous media research at the GeoEnergy Research Centre" Firstly he introduced some hot topics in their group containing: coupled problems in fluid mechanics mixing and reaction in heterogeneous flow and interdisciplinary fluid mechanics. Then he focused on peatland models and proposed a fully coupled mechanical-ecohydrogical model of Pearland development. As he emphasized, mechanical process had an essential role in the peatland development as it affects physical properties through compression. Meanwhile, mechanical process influenced peatland ecohydrology and carbon stock resilience and they studied the long-term impact of climate change on the global carbon balance.

## 4. Application on unconventional oil and gas development

There are many problems for the development of unconventional reservoir, caused by the abundant nanopores and micropores in reservoir rock. In this section, seven researchers induced current progress for the fluid flow and transport in porous media.

Jun Yao, from China University of Petroleum (East China), delivered a talk entitled "Challenge and development trend on modern system of multiphase flow in porous media". He proposed the mechanics of flow through porous media in extreme condition which presenting as extreme high temperature, pressure and stress. Three scientific problems had been introduced, which were the evolution mechanism of rock mechanical properties, the rule of phase state change and the mechanism of multi-scale thermal fluid-solid coupling flow in porous media. According to these scientific problems, Prof. Yao posed a technical question named "Numerical simulation of thermal fluid-structure coupling in deep and ultra-deep reservoirs".

In "Multiscale simulation of gas transport in porous media", Wei Su, from the University of Edinburgh, presented a general synthetic iterative scheme (GSIS), an efficient and accurate numerical method, to obtain the apparent gas permeability of porous media. The new scheme breaks the limitations of conventional iterative scheme and can be used for multiscale simulation of rarefied gas flows. She applied the method to obtain the apparent gas permeability through 2D porous media represented by the Sierpinski fractal model and a pore body/throat system. The GSIS gave an accurate prediction of apparent permeability, while its computational efficiency could be greatly improved by 700 times compared with the conventional scheme. On the basis of simulation results, she found a universal expression of the Klinkenburg's correction.

Yonghao Zhang, from the University of Edinburgh, delivered a talk on "Non-equilibrium gas transport at the pore scale-slip flow, Knudsen diffusion & confinement". The low variance deviational simulation Monte Carlo method was used to solve the gas kinetic models, proposing two new parameters: pore activity and surface activity, which also provided the way to calculate effective porosity. The results also showed that Darcy's law may be invalid even as Kn and Re approach zero in ultra-tight porous media.

Shu Jiang, from China University of Geosciences (Wuhan), presented a talk entitled "Development mechanism of multi-scale pore-fracture system and occurrence state and flow simulation of fluids in the shale reservoir". He introduced the pore types and pore-throat distribution in shale reservoirs, and discussed the influence of organic matter (OM) abundance, shale compositions, and OM types on the pore development and connectivity. The fracture system in the shale reservoir could be classified into two types: macro-scale tectonic fractures and micro-scale untectonic fractures. He talked about the adsorption characteristics in the shale nano-porous system and analyzed the contributions of OM and clay minerals to the adsorption capacity of shale. He proposed a generalized equation of state equation coupling the confined phase behavior to get phase diagrams for nanopores, and used LBM to obtain oil-water relative permeability based on micro-scale digital rock images. Then, embedded discrete fracture model (EDFM) was coupled with multi-porosity model to build a three-continua shale reservoir model, and multi-physics compositional simulation considering different mechanisms was performed.

In the presentation "Reservoir seepage automatic history matching method for formation and fracture parameter inversion", Kai Zhang, from China University of Petroleum (East China), systematically introduced the different methods of fracture identification and prediction using dynamic monitoring data. This included a prediction method for the geometric distribution of large-scale fractures proposed based on the DFM model, a hierarchical parameterization method for multi-scale fracture network based on the EDFM model, a method for massive multi-scale complex fracture system by compressing the high-dimensional inversion parameters into low dimensional continuous parameters based on deep sparse autoencoder, a method for tight reservoir based on the monitoring inversion of micro-seismic events and fractal DFM, a method for shale reservoir based on MVPSO to predict and reduce the uncertainty of attribute parameters by integrating static and dynamic data.

Yanbin Yao, from China University of Geosciences (Beijing), proposed a talk titled "Prediction model of permeability change induced by hydrate decomposition in silty sandstones". He discussed primary and secondary hydrate synthesis processes, pore water distribution changes during hydrate formation and hydrate saturation changes during depressurization. A new cubic model was proposed to predict permeability changes during depressurization. And the model was validated by the experimental data.

In the presentation on "Pore-scale modeling of elastic properties in hydrate-bearing sediments", given by Yingfang Zhou, from University of Aberdeen, he introduced a work-flow combining the CT scanning and finite-element method (FEM) to estimate the elastic properties of hydrate-bearing. At first, core samples were scanned by a high-resolution synchrotron radiation imaging device. Then, grayscale rock images were segmented into four phases (sand, brine, hydrate, and methane), and the analysis of representation elementary volume was performed. At last, the rock geometry and properties of each phase were read by the FEM to calculate the effective elastic properties. He found that the dominant hydrate morphology changes from pore-filling to pore-bridging and to cementation during the hydrate formation process. Elastic moduli and sonic wave velocities increase with hydrate saturation, and different increase trends can be shown under different saturations.

## 5. Geotechnical engineering

Liping Li, from Shandong University, presented a talk entitled "Fluid-solid coupling simulation method for the catastrophic evolution process of water inrush in deep-buried long tunnels". The mechanism of water inrush in the rock failure based on Peri Dynamics simulation was discussed. By coupling DEM-CFD, water inrush in seepage failure was simulated and performed. Risk assessment and dynamic prediction method of water inrush disaster was finally introduced in detail.

In "The effect of high temperature and high pressure on creep characteristics of salt rock in deep formation", Jianfeng Liu, from Sichuan University, revealed the creep characteristics of salt rock in different temperature and deviator stress conditions, for example, room temperature, and high-temperature condition. Creep at high temperature was more critical that in the former condition which could be ignored. The influence of the temperature and deviator stress on creep characteristics was also discussed. The creep strain was proportional to the square of temperature and deviator stress, whereas in deep formation with high stress, the effect of temperature on the stable-creep rate of salt rocks was more significant.

Hai Pu, from the China University of Mining and Technology, delivered a presentation on "Numerical simulation of water and sand migration in mining fracture". In the study of water and sands bursting, he used LBM-DEM and SPH-DEM methods to realize the coupling between particle and fluid, fluid and solid boundary, particle and solid boundary. He found that the rough structure of the fracture surface hindered the water and sand migration, and the upper constant pressure caused the water and sand migration secondary acceleration after the velocity is reduced, and the varying apertures fracture appeared blocked, and the upper constant pressure caused the blocked structure with small opening section to be dispersed to form secondary acceleration.

Yixin Zhao, from the China University of Mining and Technology (Beijing), presented a talk entitled "Effect of reserved size and anisotropy on mechanical features of coal". He used micro-CT to characterize the pore structure in coal. Through experiments, the influence curves of size and anisotropy on uniaxial compressive strength, peak stress, elastic modulus, internal structure and acoustic emission characteristics of coal were obtained, and the generalized sizing-anisotropy formula of coal strength was given, which could be used to help coal development.

## 6. Others

Wenbo Zhan, from the University of Aberdeen, delivered a talk on "Characterization of transport properties of drugs in brain tissue using computational fluid dynamics". He introduced that the brain tumors respond poorly to drug treatment, which is due to the presence of the blood-brain barrier that reduces the distribution of drugs in the brain. He pointed out that tissue permeability and drug diffusivity in brain tissue coefficient influence drug transport significantly, and these properties were characterized by performing computational fluid dynamics in nerve fibers reconstructed from the microstructure of the brain.

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## Conflict of interest

The authors declare no competing interest.



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