重庆大学 CHONGQING UNIVERSITY

第二届全国多孔介质渗吸理论与应用学术会议
暨第三届全国青年渗流力学学术会议，2025年4月25-27，北京

自发渗吸微观动力学与升尺度研究

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研究学术 造就人才 佑启乡邦 振导社会

Outline

Journal of Petroleum Science and Engineering 110 (2013) 268–293

Contents lists available at ScienceDirect

Journal of Petroleum Science and Engineering

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

Developments in spontaneous imbibition and possibilities for future work

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ARTICLE INFO

Article history:
Received 14 January 2013
Accepted 2 August 2013
Available online 24 August 2013

Keywords:
spontaneous imbibition

ABSTRACT

Spontaneous imbibition controls many processes of practical importance. The subject is undergoing rapid growth in terms of the number of publications. This paper is a selective review of the literature which concentrates on the last ten years or so but also highlights, as necessary, earlier work. Insight into the mechanism of spontaneous imbibition is provided through consideration of the behavior of strongly wetted uniform tubes of any cross-section. The significance of cross-flow on the mechanism of advance of interfaces in tubes is related to imbibition in much more complex pore spaces. Details of the mechanism of

Spontaneous imbibition is the process by which a wetting fluid is drawn into a porous medium by **capillary action** (Morrow and Mason, 2001).

1. 研究背景与目的
2. （正向）自发渗吸动态孔隙网络模型
3. 自发渗吸的毛管力与相渗曲线
4. 自发渗吸达西尺度数值模拟
5. 结论与展望

研究背景与目的（Background & Motivation）

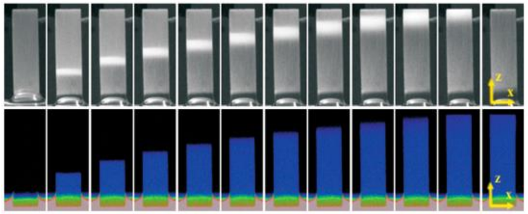
自发渗吸的定义：

- ❑ 典型的两相流动
- ❑ 毛管力是驱动力
- ❑ 正向与逆向自发渗吸
- ❑ 很多地下工程与工业应用的重要物理过程

研究问题与挑战：

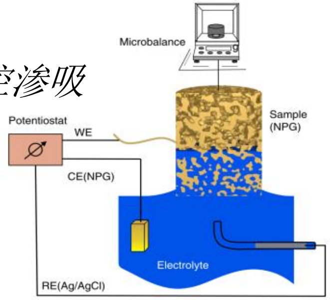
- ❑ 正向、逆向和准静态自发渗吸在孔隙尺度的流动机制有什么区别？
- ❑ 孔隙结构、粘度比、润湿性是如何影响与控制渗吸速率、润湿性圈闭和渗吸前缘演化的？
- ❑ 是否可以在达西尺度准确预测自发渗吸？

渗吸前缘演化



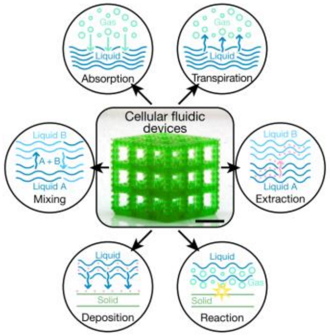
(Gruener, et al., 2012, PNAS)

可控渗吸

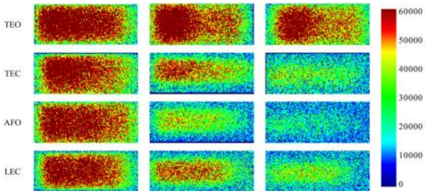


Xue, et al., 2014, Nature Commu.

Dudukovic et al.,Nature,2021



油气提采

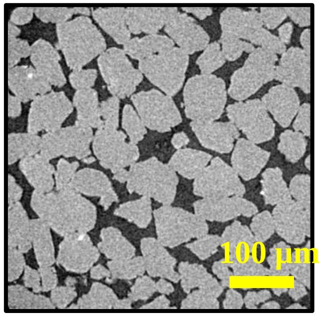


Cheng, et al., 2018, Energy & Fuels

数字岩心渗流模拟技术

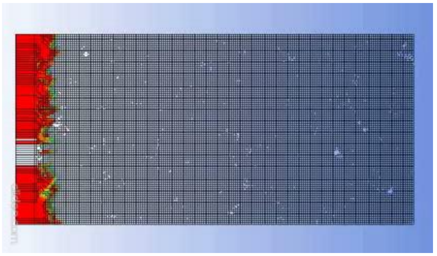
本次报告聚焦复杂的渗吸模型

Nubian砂岩



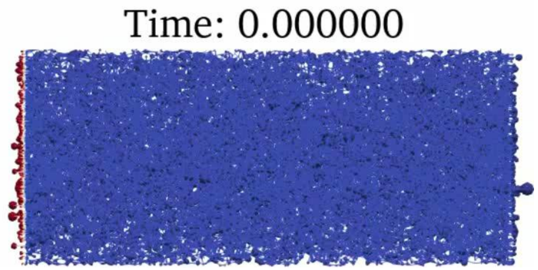
数字岩心

模型复杂



自发渗吸数值模拟,
100×100×200 图像

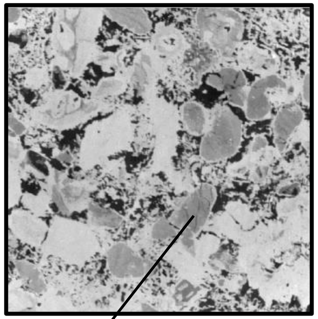
(*Qin et al.*, *AWR*, *2021*)



900×900
×2000
image

自发渗吸动态
孔隙网络模拟

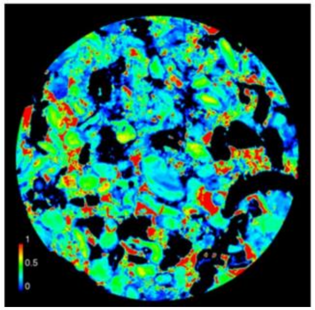
Estaillades碳酸盐岩



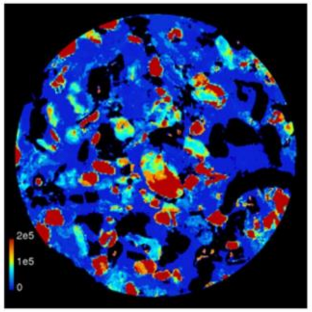
亚分辨率微孔区

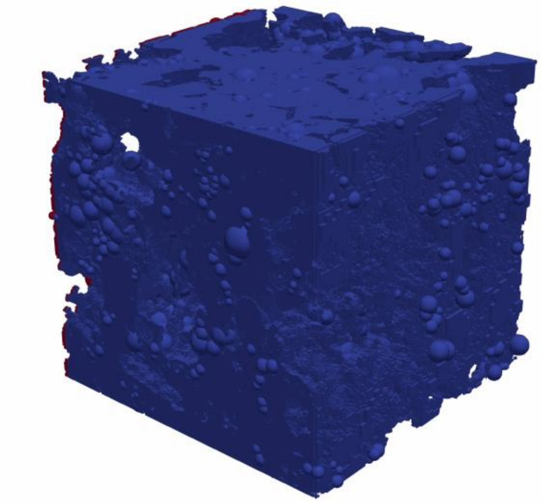
孔隙结构复杂

孔隙度分布



孔径分布





孔隙网络-连续介质混合模型

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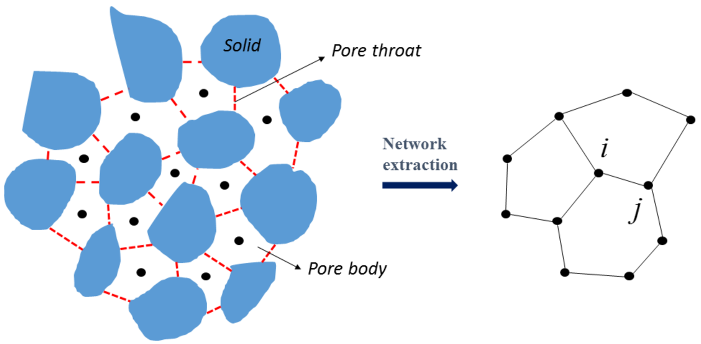
自发渗吸动态孔隙网络模型：控制方程

控制方程:

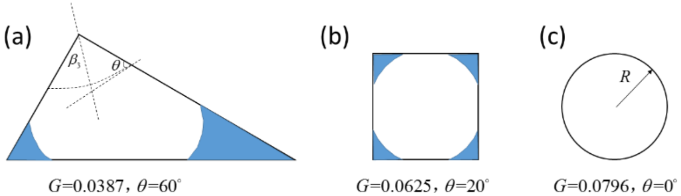
$$V_i \frac{ds_i^\alpha}{dt} = -\sum_{j=1}^{N_i} K_{ij}^\alpha \left(p_i^\alpha - p_j^\alpha\right), \qquad \alpha = \{n, w\}$$

$$p_i^n - p_i^w = p_i^c\left(s_i^w\right) \qquad s_i^n + s_i^w = 1$$



多样化理想孔隙单元:

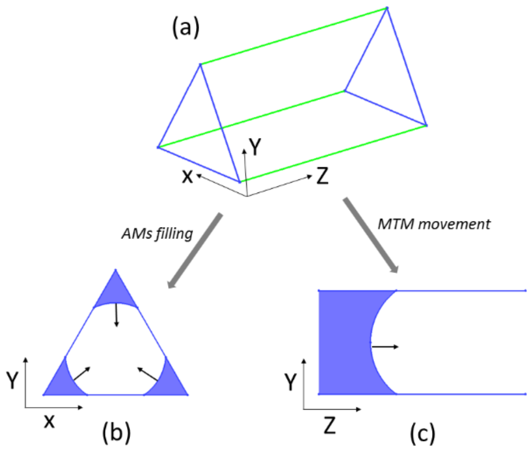
- ❑ As simple as possible;
- ❑ To be image-based;
- ❑ Tackle mixed-wettability.



(Qin and van Brummelen, AWR, 2019)

Key local rule of the competition between AMs and MTM filling (*Ma et al., 1996; Mason and Morrow, 1991***):**

- ❑ Flag a pore of MTM or AMs;
- ❑ Consider snap-off and topological entrapment;
- ❑ Switch from AMs to MTM;
- ❑ Set a pre-wetting film in a dry pore.

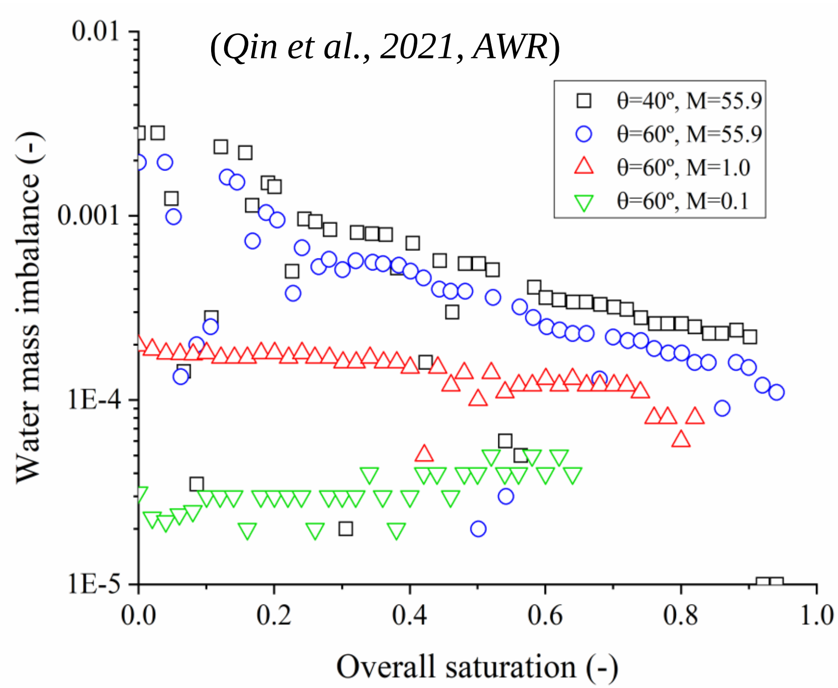


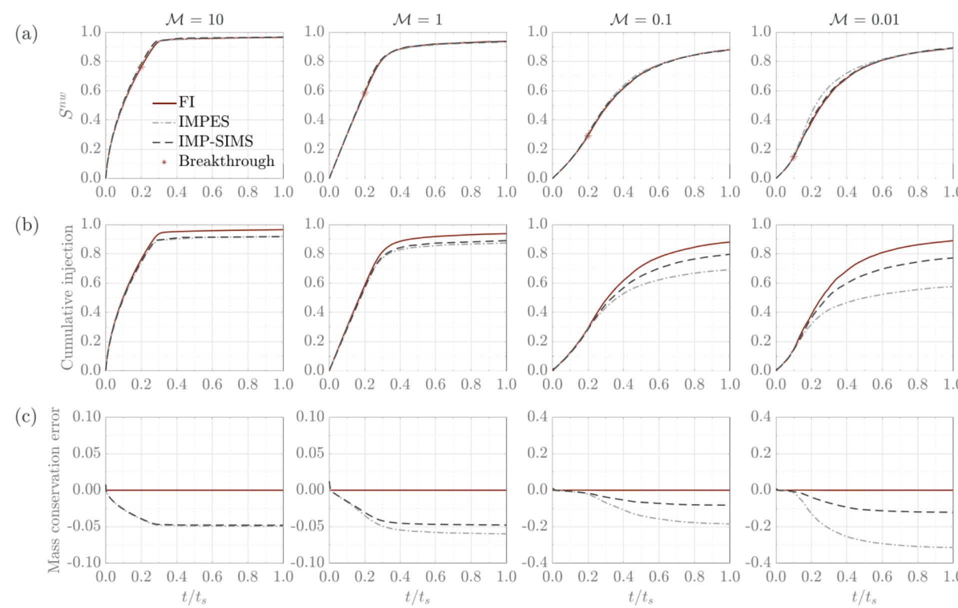
显式格式的质量守恒问题

IMPES:

$$\sum_{j=1}^{N_i}\left(K_{ij}^n + K_{ij}^w\right)\left(\bar{p}_i - \bar{p}_j\right) = -\sum_{j=1}^{N_i}\left\{\left[K_{ij}^n s_i^w - K_{ij}^w\left(1 - s_i^w\right)\right]p_i^c + \left[K_{ij}^w\left(1 - s_j^w\right) - K_{ij}^n s_j^w\right]p_j^c\right\}$$

$$V_i\frac{ds_i^w}{dt} = -\sum_{j=1}^{N_i}K_{ij}^w\left(p_i^w - p_j^w\right) \qquad \bar{p}_i = p_i^w s_i^w + p_i^n\left(1 - s_i^w\right)$$

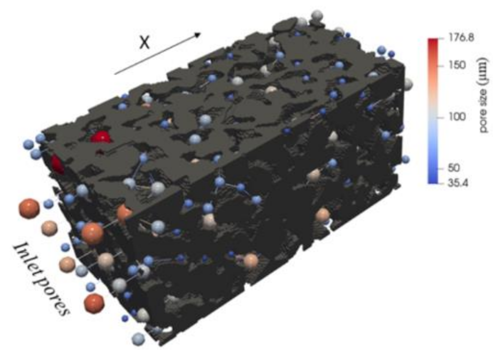




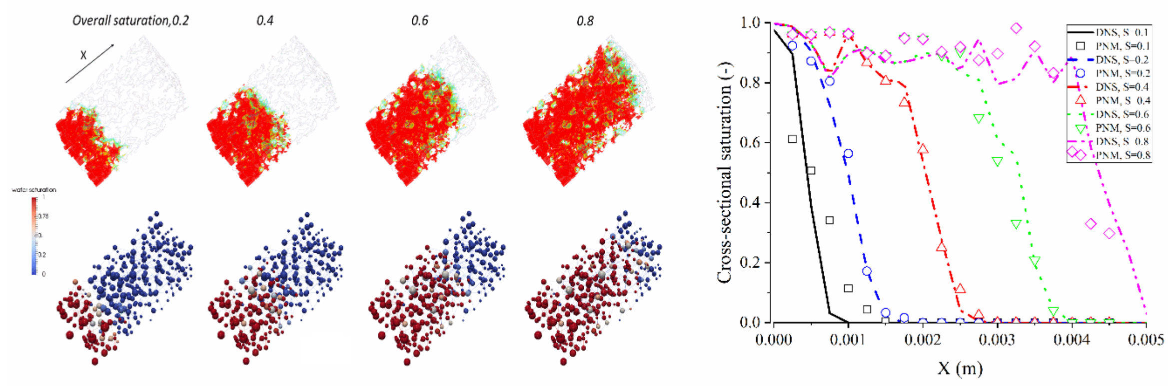
(Chen, Qin and Guo, WRR, 2020)

与直接数值模拟对比的数值验证

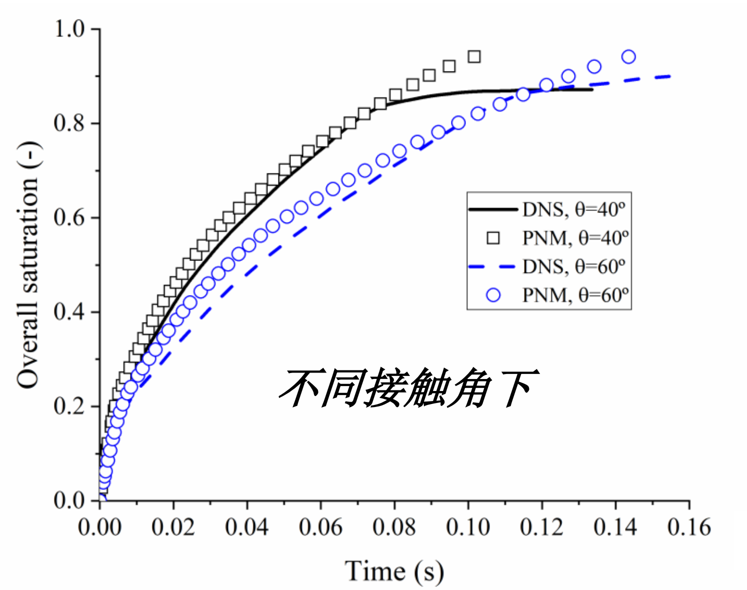
100×100×200 image

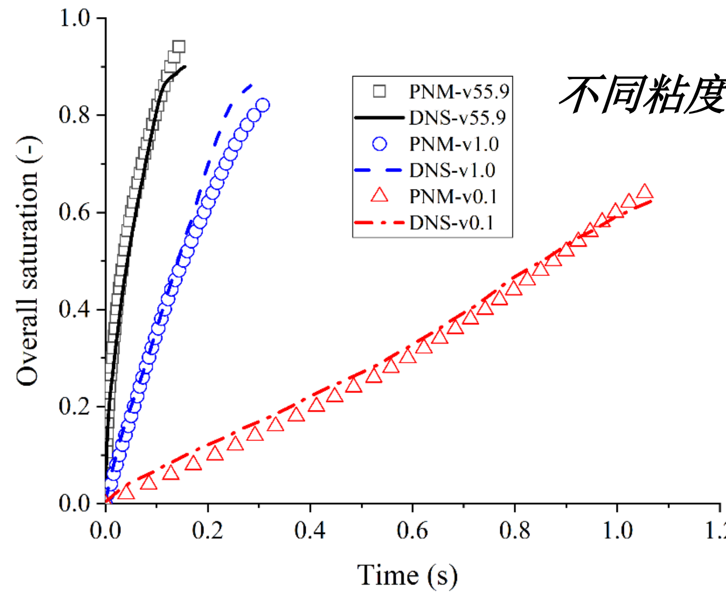


(Qin et al., AWR, 2021) *Air-water system, saturation profiles*



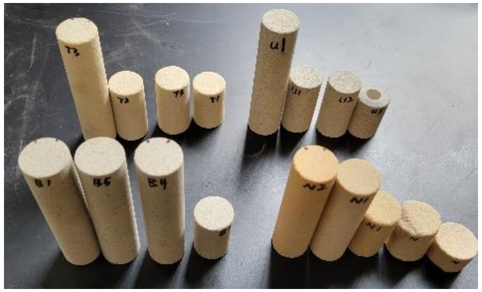
A B

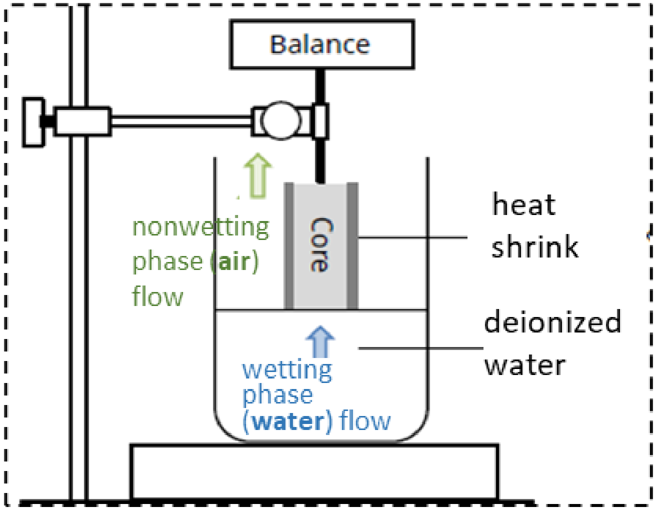


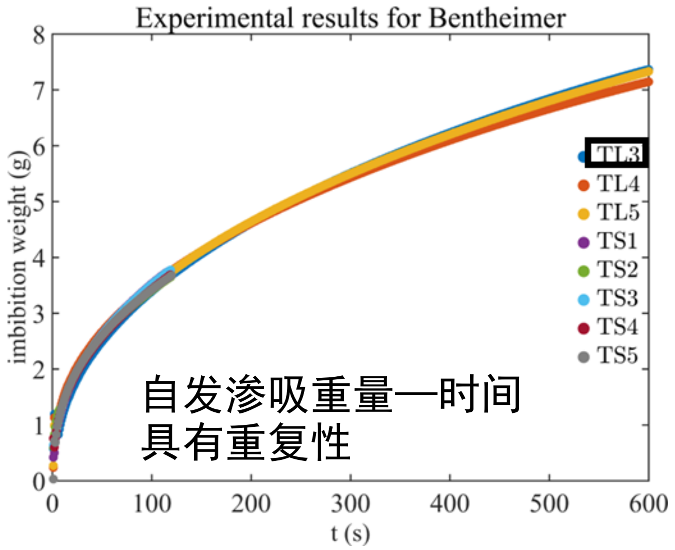


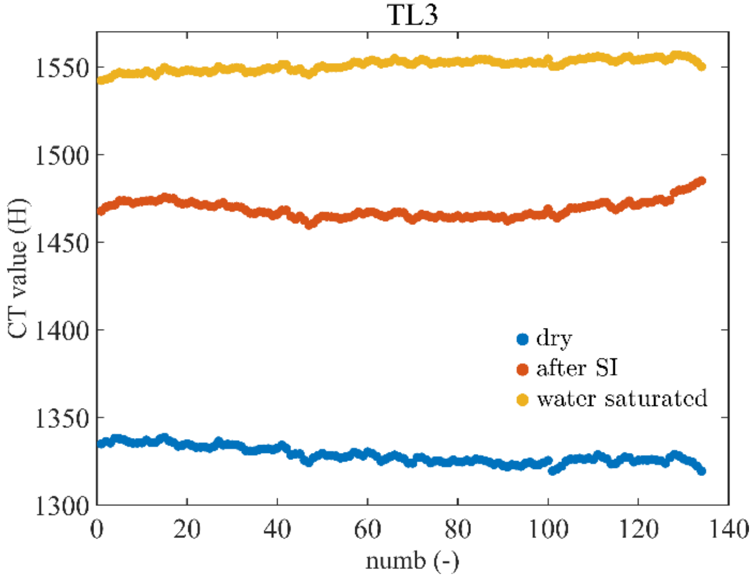
砂岩岩心自发渗吸实验验证研究：岩心渗吸实验

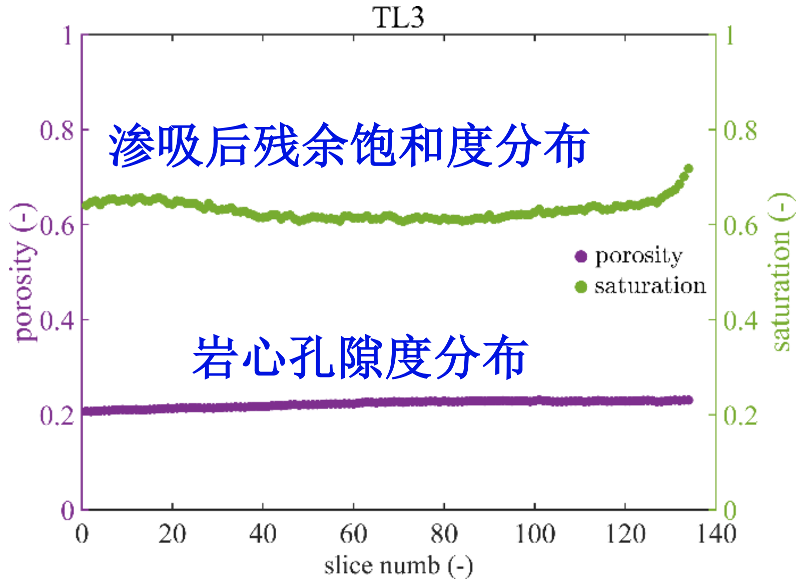
(Wang et al, AWR, 2025)







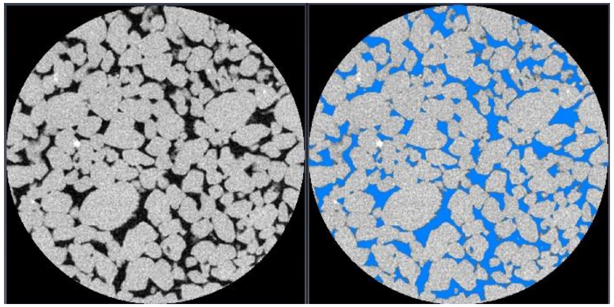




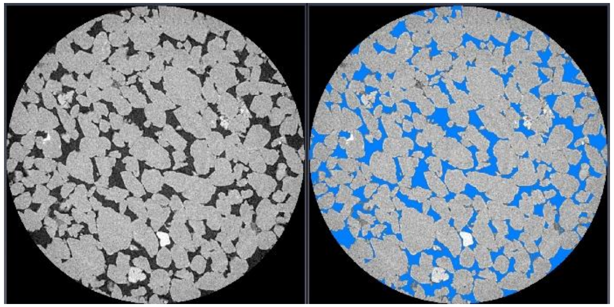
医学CT扫描，确保实验岩心的均质性

砂岩岩心自发渗吸实验验证研究：孔隙结构提取

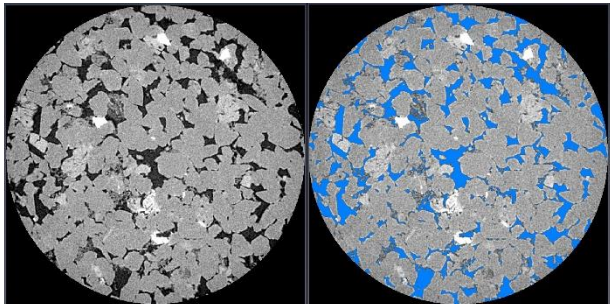
微米CT扫描获取样品的数字岩心



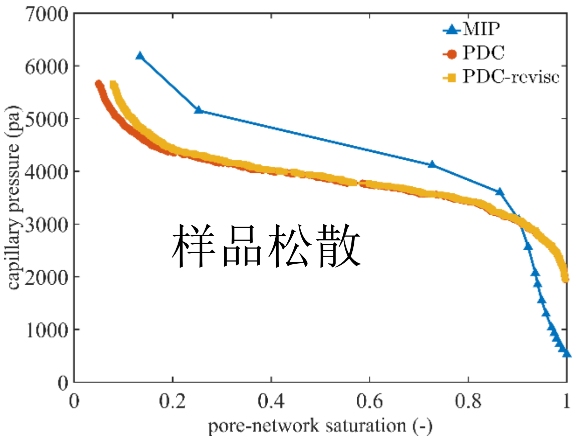
Nubian (voxel size: 4 μm)

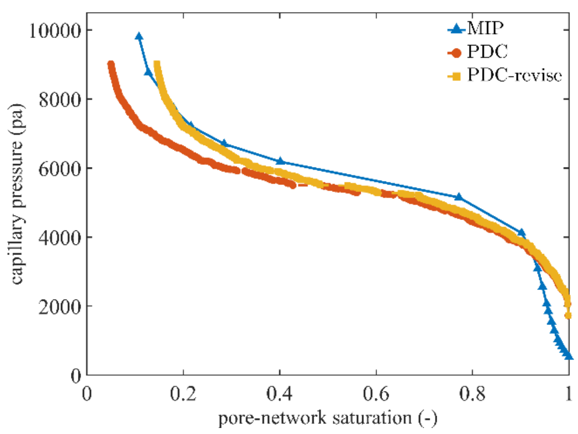


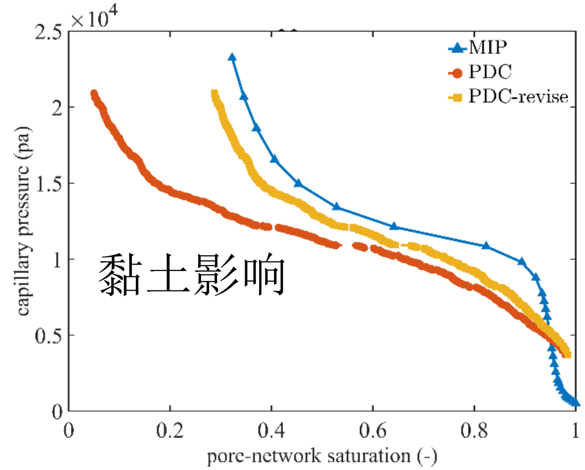
Bentheimer (voxel size: 3 μm)



Upper Berea (voxel size: 2 μm)

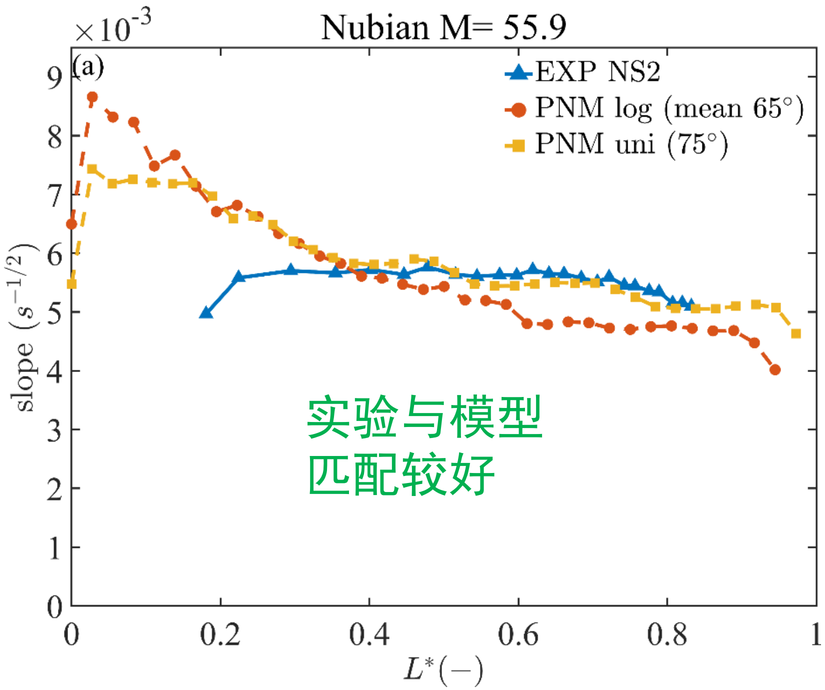


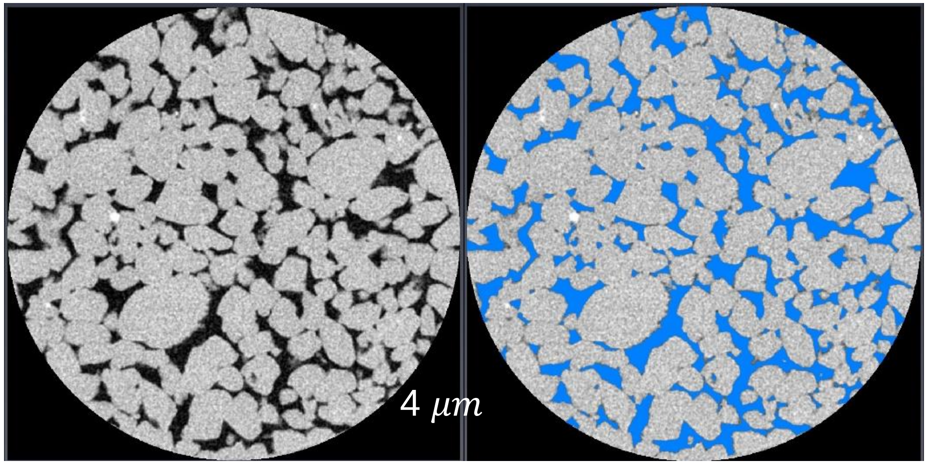




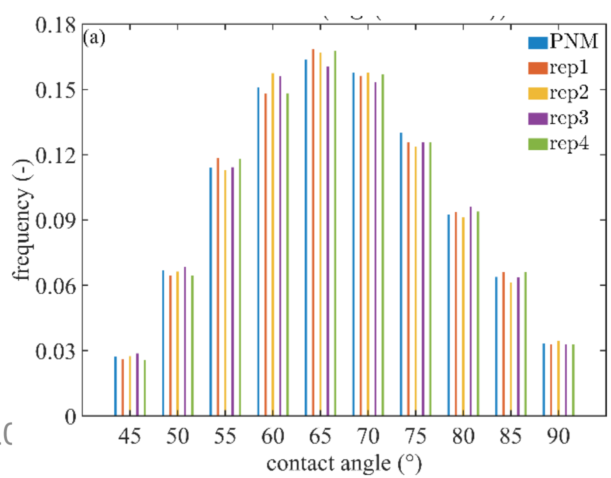
孔隙结构复杂程度的判断为: Nubian < Bentheimer < Upper Berea.

实验验证结果与分析：渗吸速率[1]





Voxel size: 900 × 900 × 900

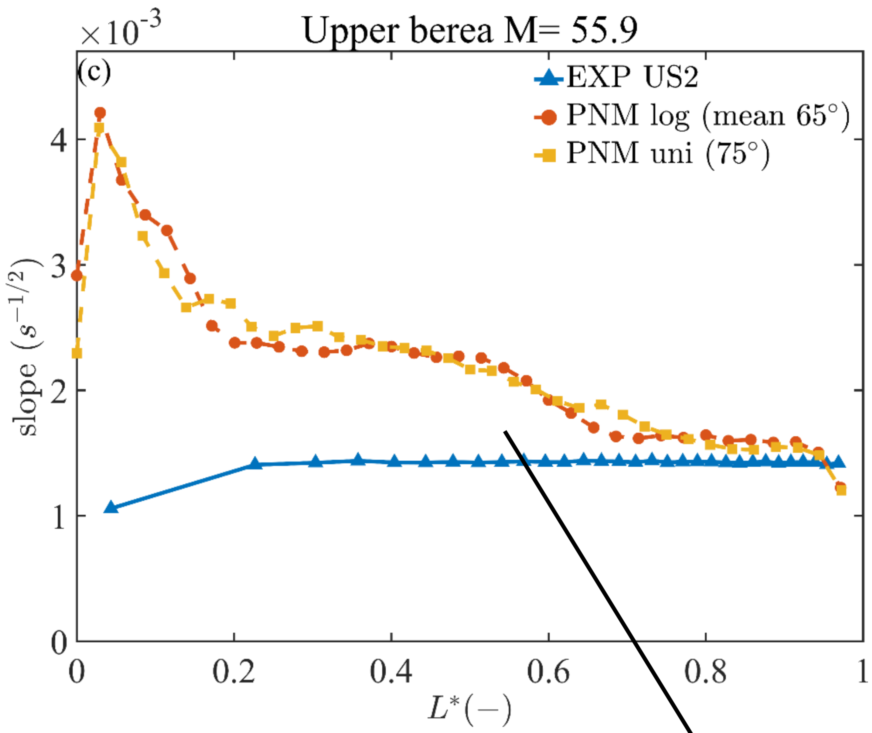


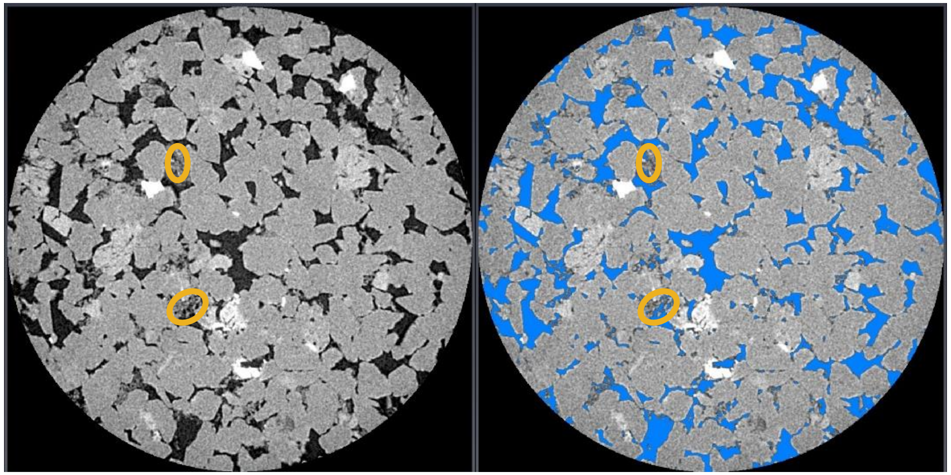
两种有效接触角：

- 对于**Bentheimer和Nubian**孔隙结构较为简单的砂岩，匹配效果很好。
- 模型输入所需**有效接触角远大于静态接触角**。

实验验证结果与分析：渗吸速率[2]

(*Wang et al., AWR, 2025*)





- 实验中微孔优先自发渗吸，延缓大孔的自发渗吸。
- 模型需要更高的有效接触角：由于更复杂的岩石表面粗糙度和非均质性、孔隙结构的收缩和扩张。

分布接触角需要模拟更大的REV！

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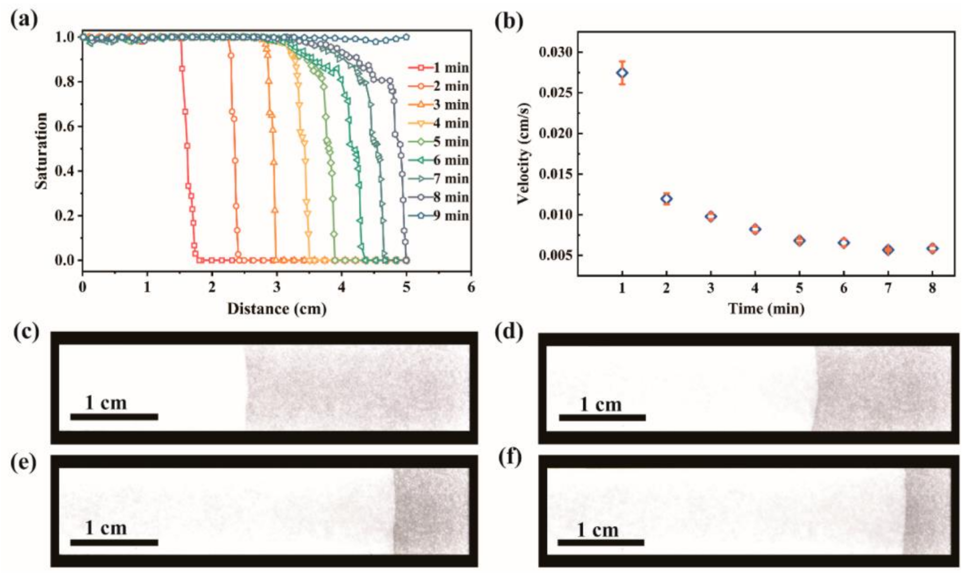
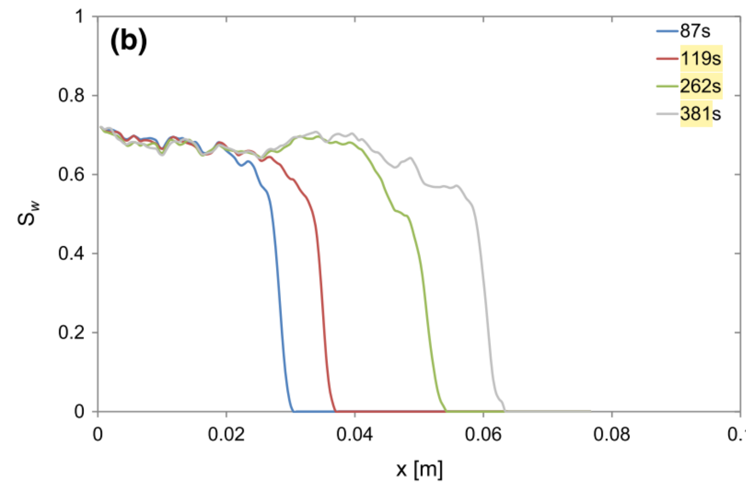
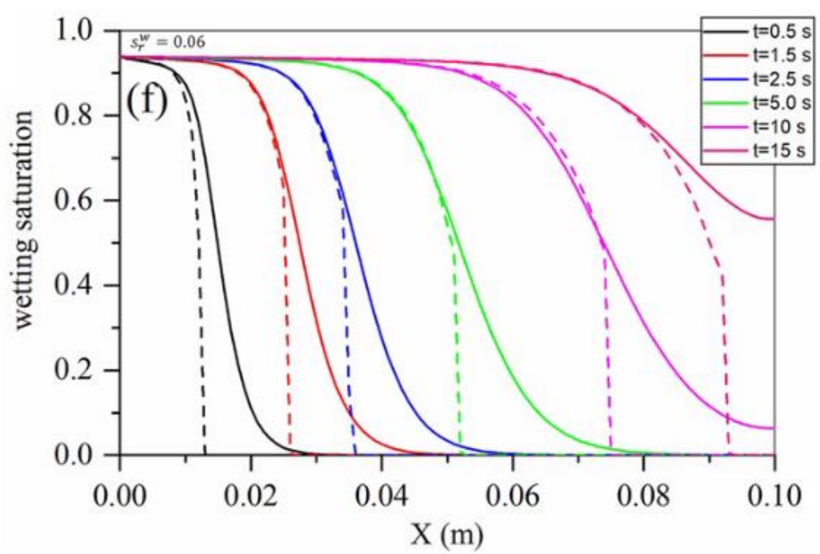
自发渗吸的毛管力与相渗曲线：偏离准静态/稳态曲线



(Wang, et al., Langmuir, 2022)

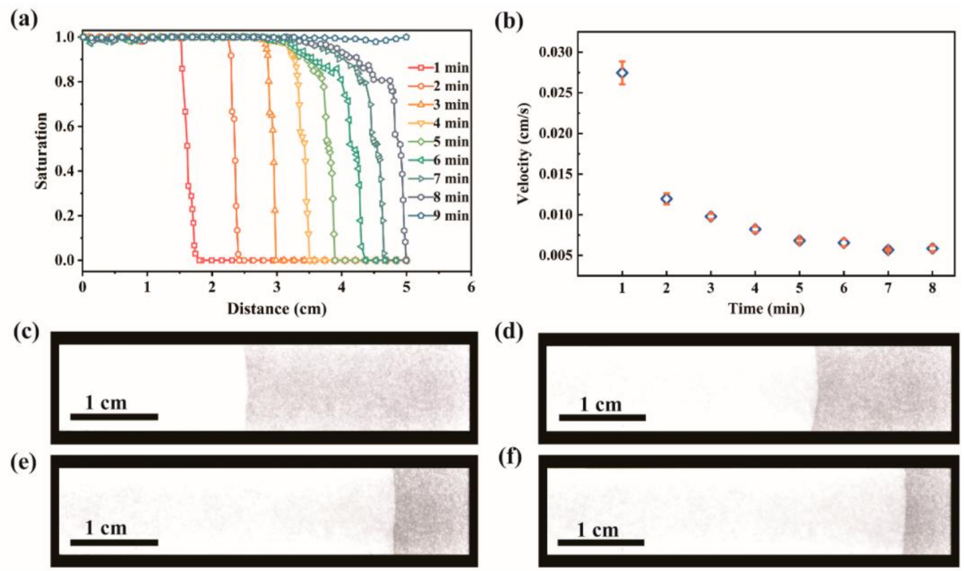


(Alyafei, et al., TiPM, 2016)

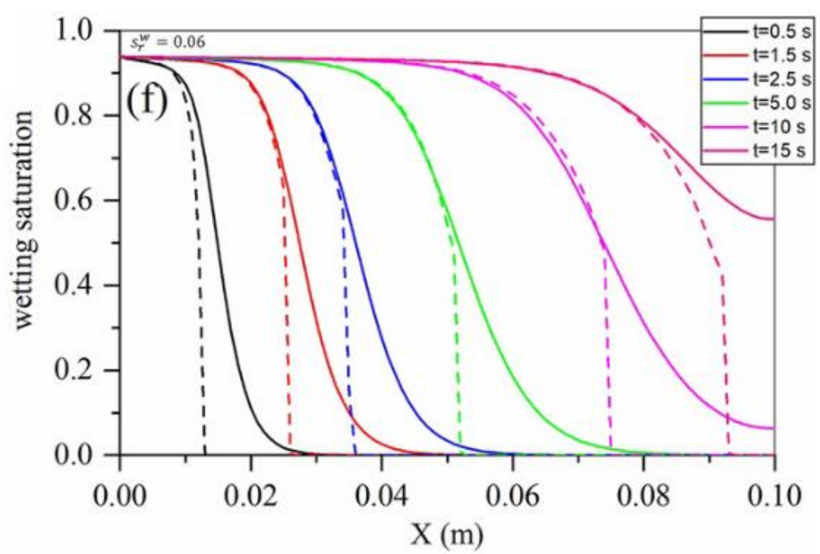


Input parameter	Estaillades	Ketton	Portland
S_{wi}	0	0	0
S_{gr}	0.28	0.28	0.29
n	10	10	8
$k_{rw,max}$	0.05	0.05	0.21
m	1.5	1.5	1.5
$k_{rg,max}$	0.8	0.8	0.8
$P_{c,entry}$ (Pa)	1,10,000	35,000	1,50,000
α	−1.5	−1.3	−1.3

自发渗吸的毛管力与相渗曲线：偏离准静态/稳态曲线



(Wang, et al., Langmuir, 2022)

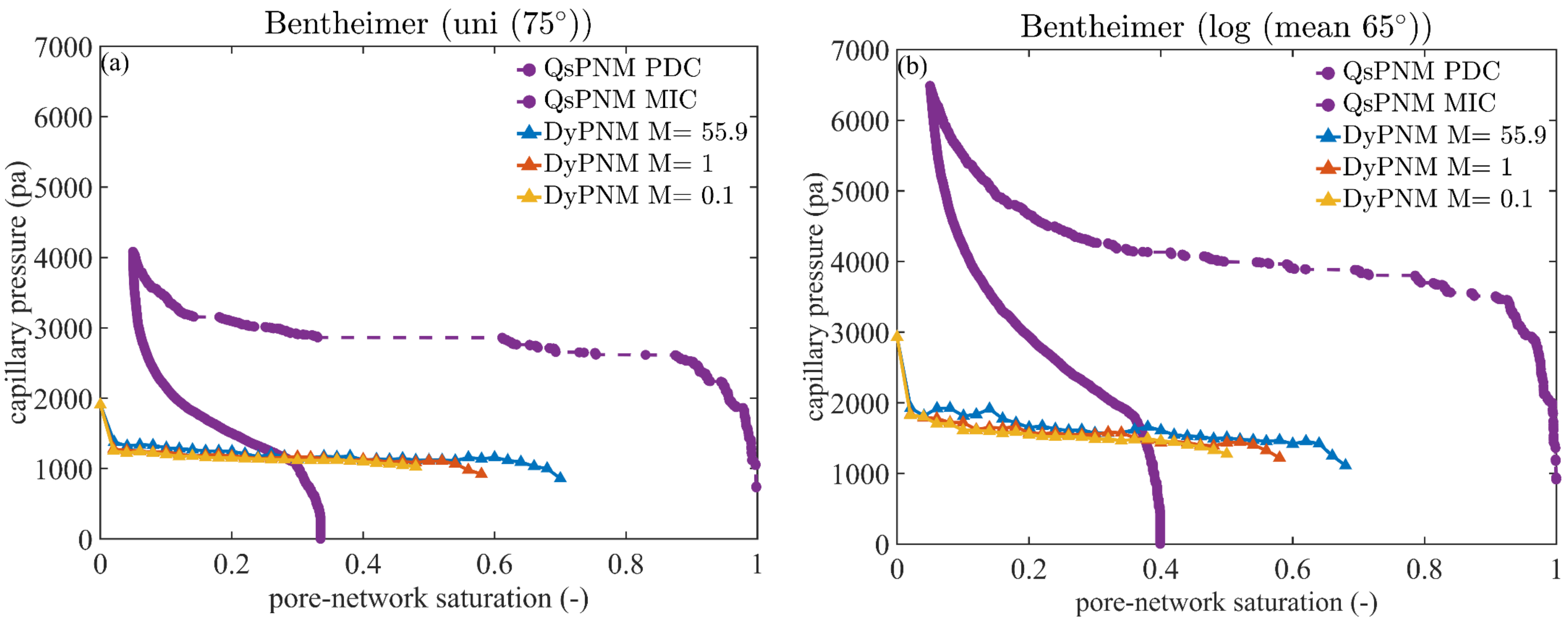


为什么达西模型不能有效模拟正向自发渗吸？

如何提高模型预测？

- 修改控制方程？
- **修改材料参数？**

自发渗吸的毛管力与相渗曲线：毛管力曲线



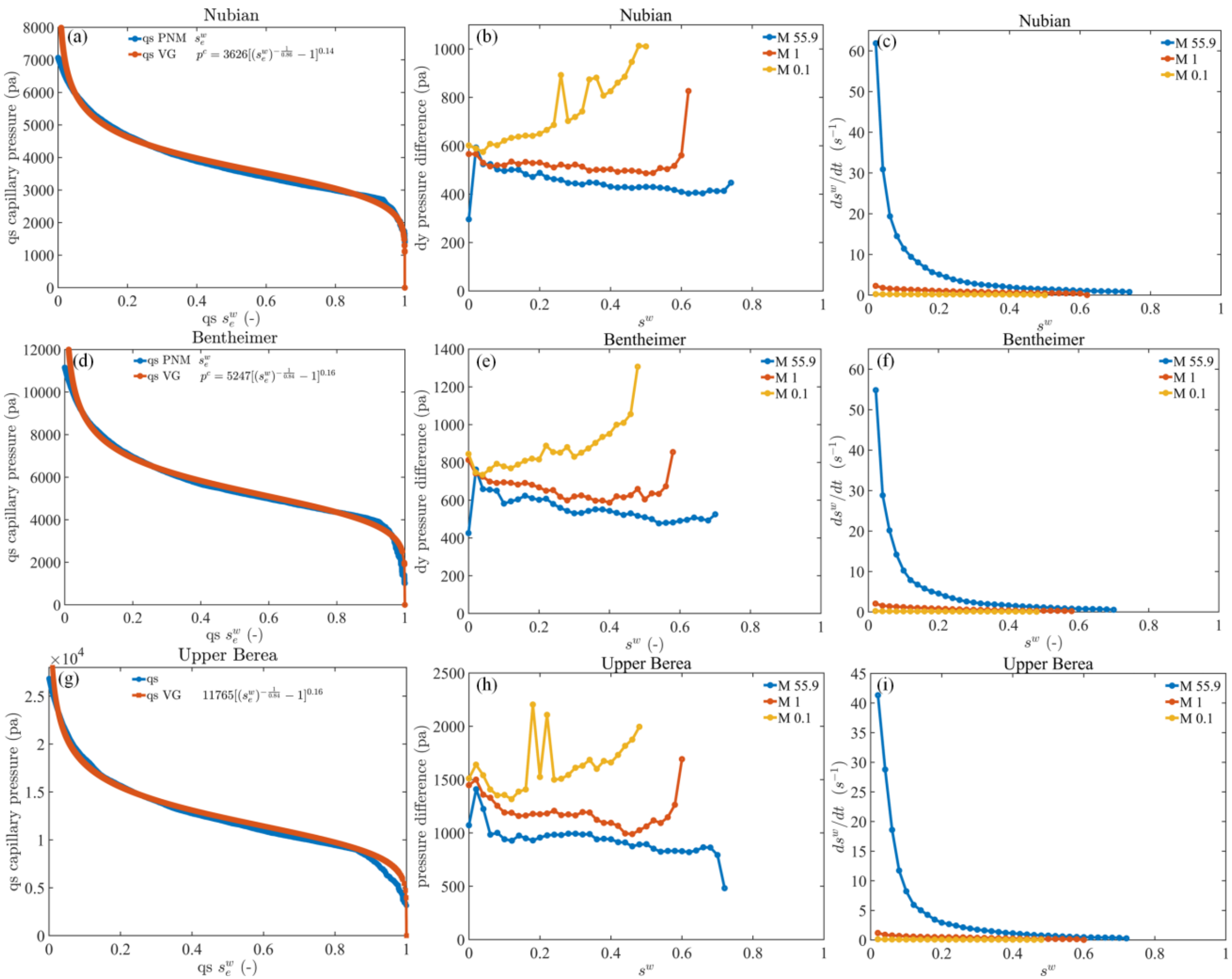
- 自发渗吸毛细压力-饱和度曲线呈水平，呈现强动力学特性。
- 分布式接触角预测的准静态毛细压力跨度更大，动态毛细压力曲线也更高。
- 基于平均孔径的Young-Laplace方程高估自发渗吸中的毛细管力约50%。

$$\overline{p}^c = \frac{\sum_{i=1}^{N_{pb}} \left(2\pi r_i^2 (1-\sin\theta)/\cos^2\theta\right)\left(2\cos\theta\sigma/r_i\right)}{\sum_{i=1}^{N_{pb}} 2\pi r_i^2 (1-\sin\theta)\Big/\cos^2\theta}$$

自发渗吸的毛管力与相渗曲线：tau term

$$k_0(\text{Upper Berea}) < k_0(\text{Bentheimer}) < k_0(\text{Nubian })$$

$$\tau(\text{Upper Berea}) > \tau(\text{Bentheimer}) > \tau(\text{Nubian })$$



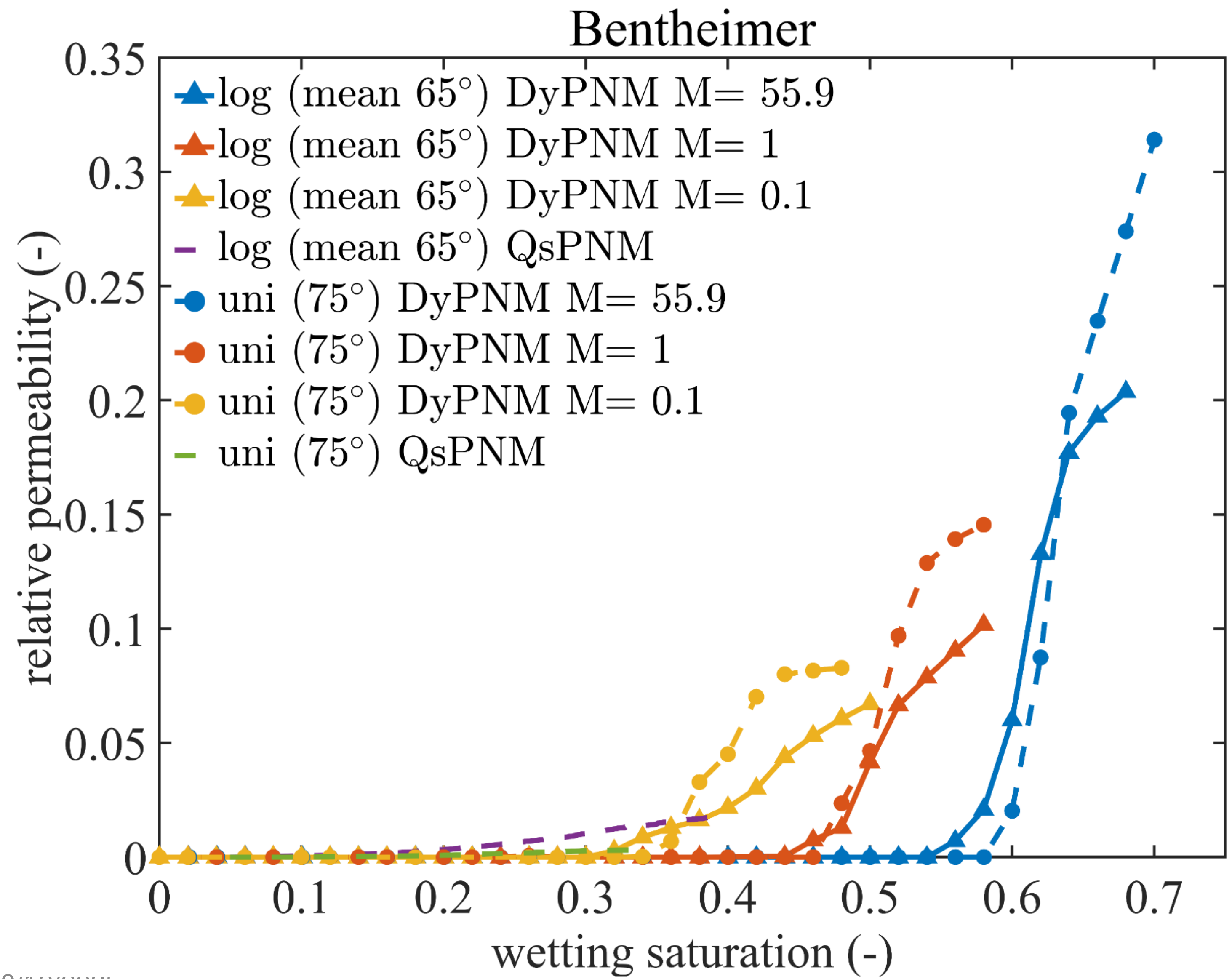
毛管力的动力学特性

$$p^n - p^w = p^c(s^w) - \tau \frac{\partial s^w}{\partial t}$$

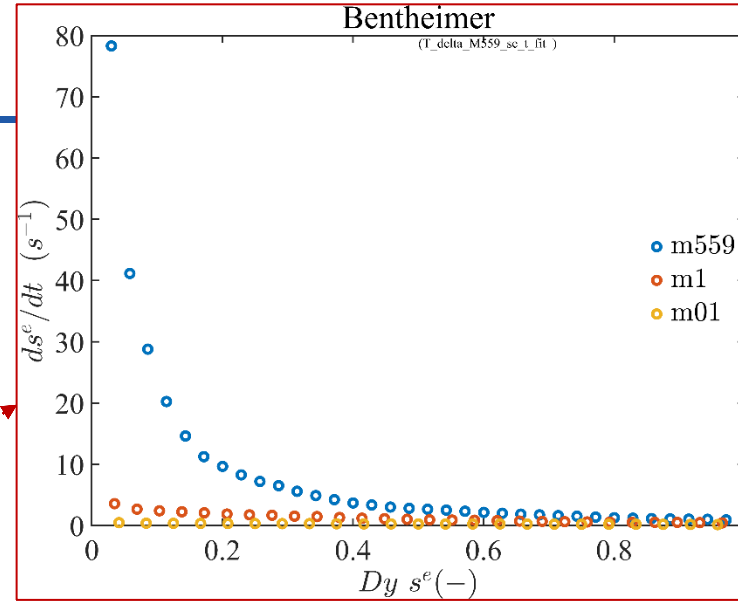
$$\tau = a \times s^w + b$$

τ	a	b
Nubian	3805	128
Bentheimer	7432	80
Upper Berea	13388	517

自发渗吸的毛管力与相渗曲线：润湿相的相渗曲线



自发渗吸的毛管力与相渗曲线：

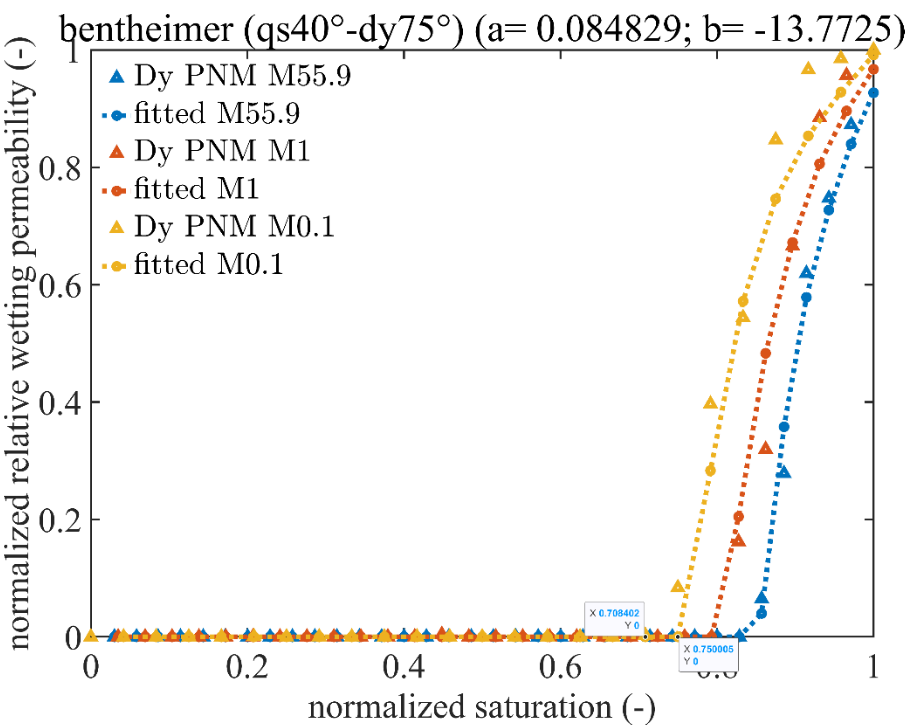


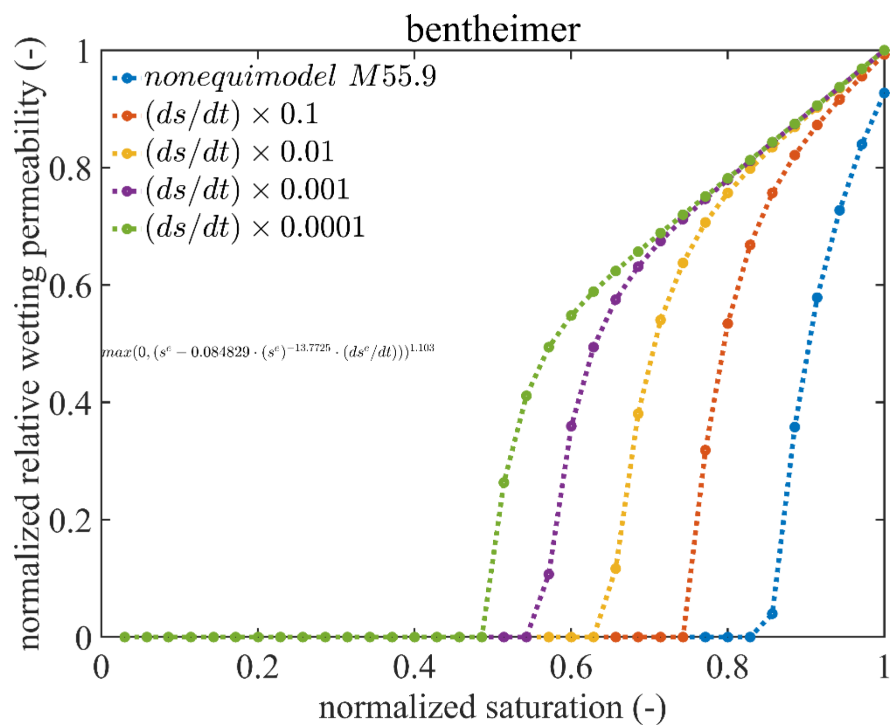
非平衡相渗模型

normalized K_r^w =

$$max(0, (s^e - m(s^e)^n\,(ds^e)/dt))^\alpha$$

表征微观动力学特性





Outline

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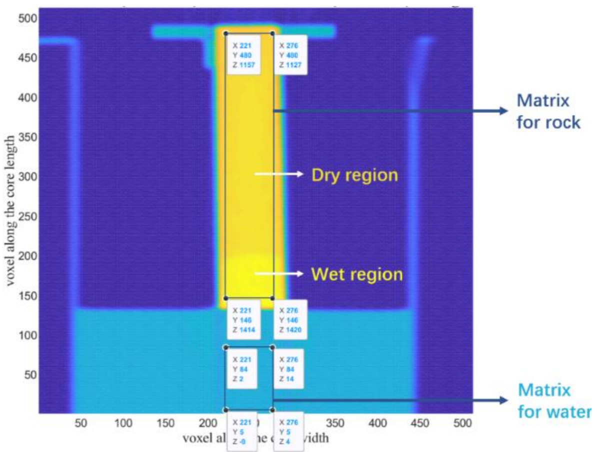
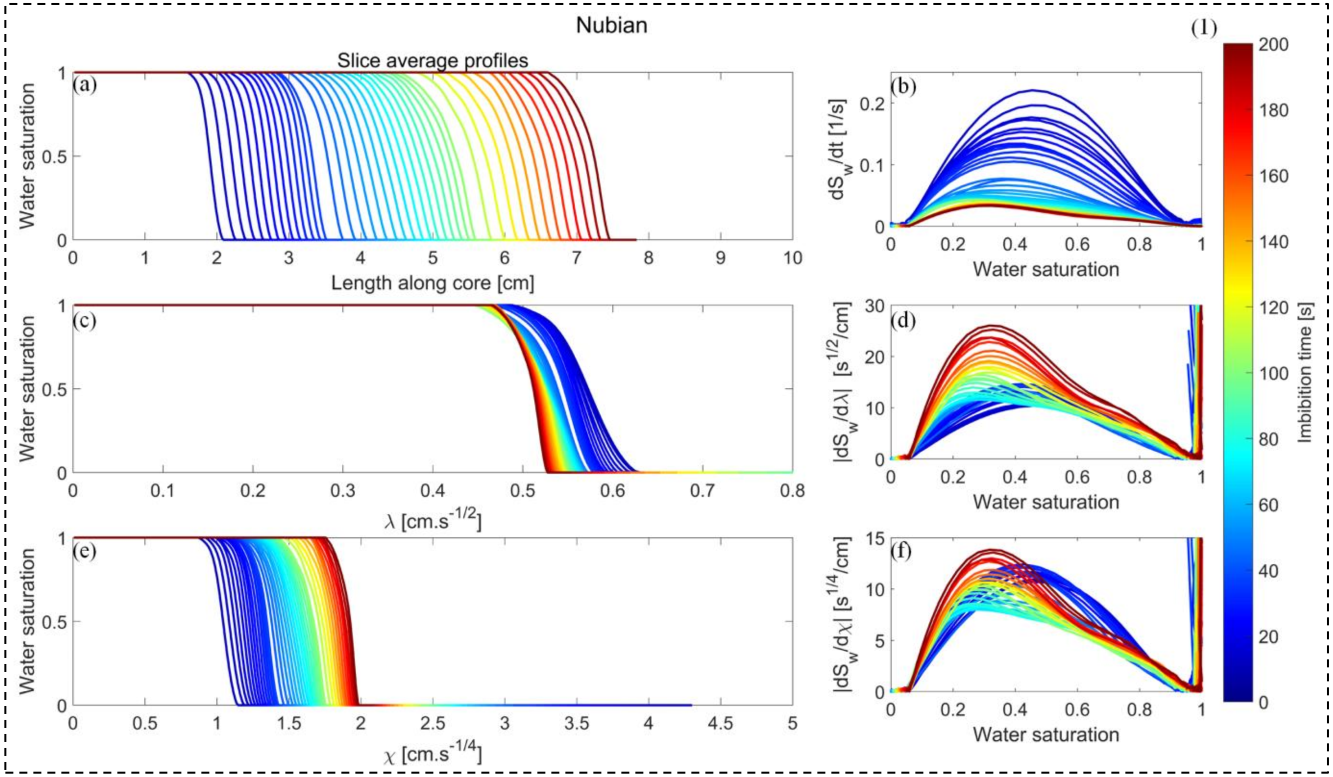
2. （正向）自发渗吸动态孔隙网络模型
3. 自发渗吸的毛管力与相渗曲线
4. 自发渗吸达西尺度数值模拟
5. 结论与展望

自发渗吸达西尺度数值模拟：基准实验数据



医学CT参数	X射线球管电流（mA）	X射线球管电压（kV）	CT切片厚度（mm）	像素大小（mm）	单张曝光时间（s）
	250	130	0.48	0.02	1

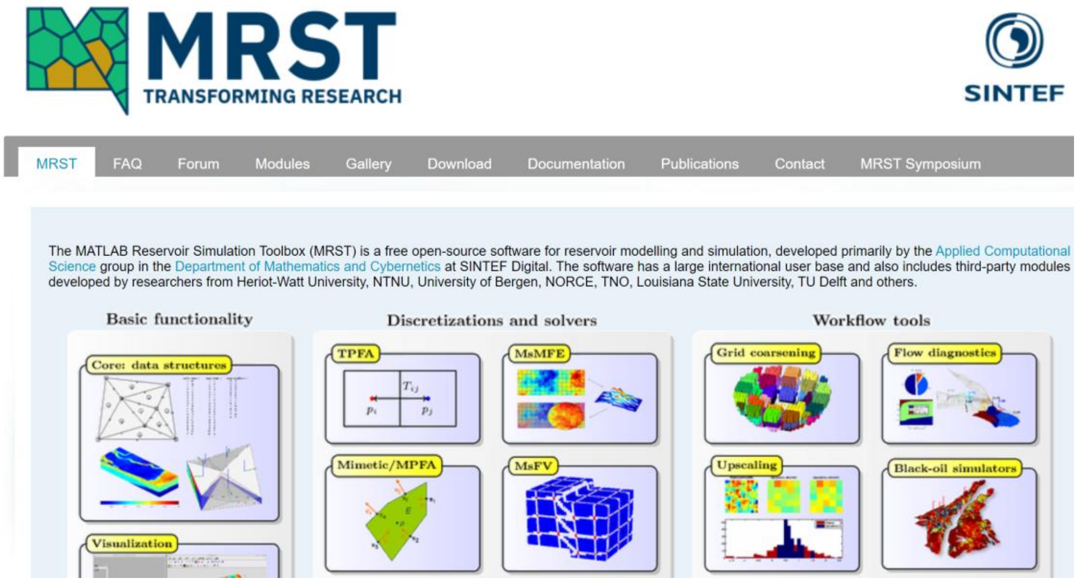


$$\frac{ds^w}{dt} = \frac{s^w(\zeta, t_n) - s^w(\zeta, t_{n-1})}{t_n - t_{n-1}}$$

$$\lambda = x/\sqrt{t}$$

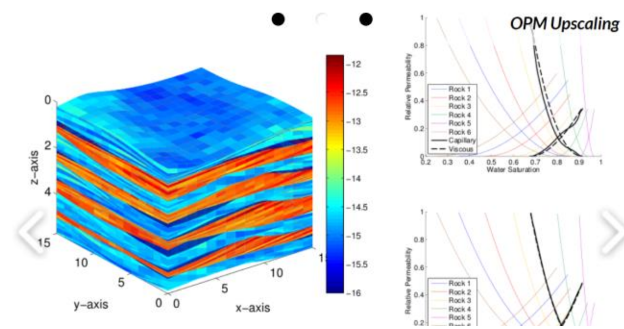
$$\chi = x/t^{1/4}$$

自发渗吸达西尺度数值模拟：控制方程



OPEN POROUS MEDIA

The Open Porous Media (OPM) initiative encourages open innovation and reproducible research for modeling and simulation of porous media processes.



$$\varepsilon\frac{\partial s^w}{\partial t}+\frac{\partial}{\partial x}\left[-\frac{k^w(s^e)}{\mu^w}\left(\frac{\partial p^w}{\partial x}-\rho^w g_x\right)\right]=0$$

$$-\varepsilon\frac{\partial s^w}{\partial t}+\frac{\partial}{\partial x}\left[-\frac{k^n(s^e)}{\mu^n}\left(\frac{\partial p^n}{\partial x}-\rho^n g_x\right)\right]=0$$

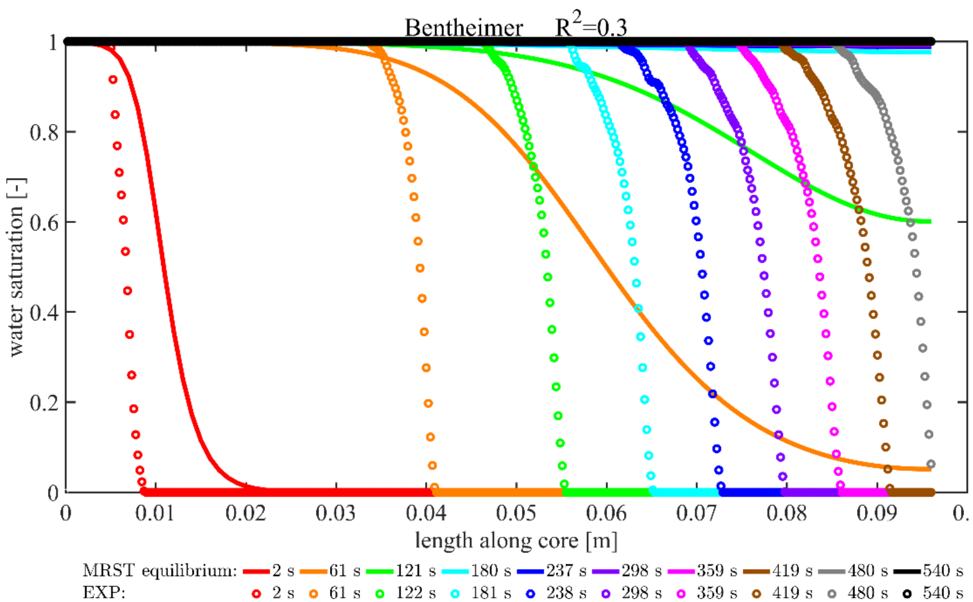
+

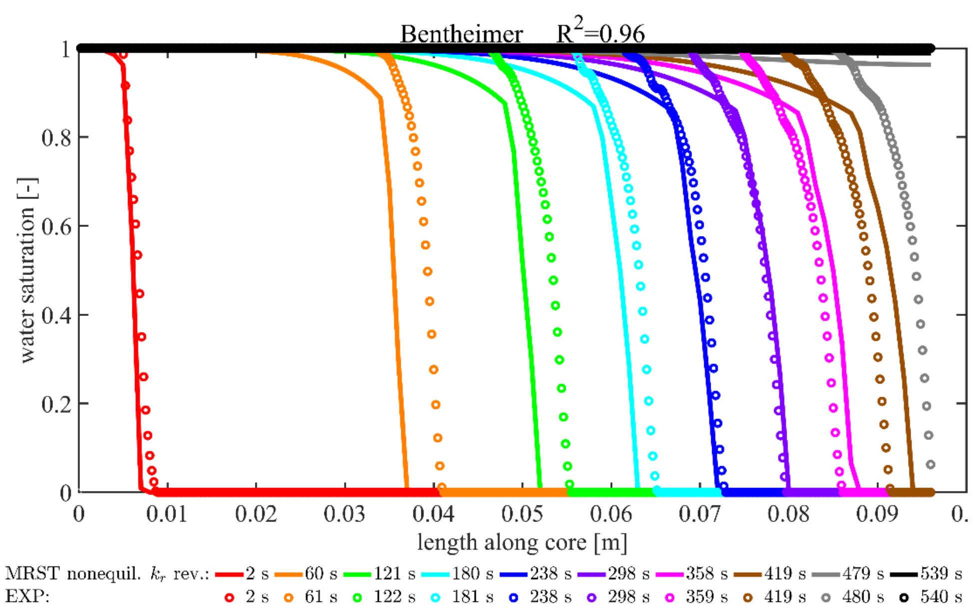
$$K_r^w = max(0,(s^e-m(s^e)^n\,(ds^e)/dt))^\alpha$$

$$p^n - p^w = p^c(s^w) - \tau\frac{\partial s^w}{\partial t}$$

$$\tau = a\times s^w + b$$

自发渗吸达西尺度数值模拟：饱和度剖面



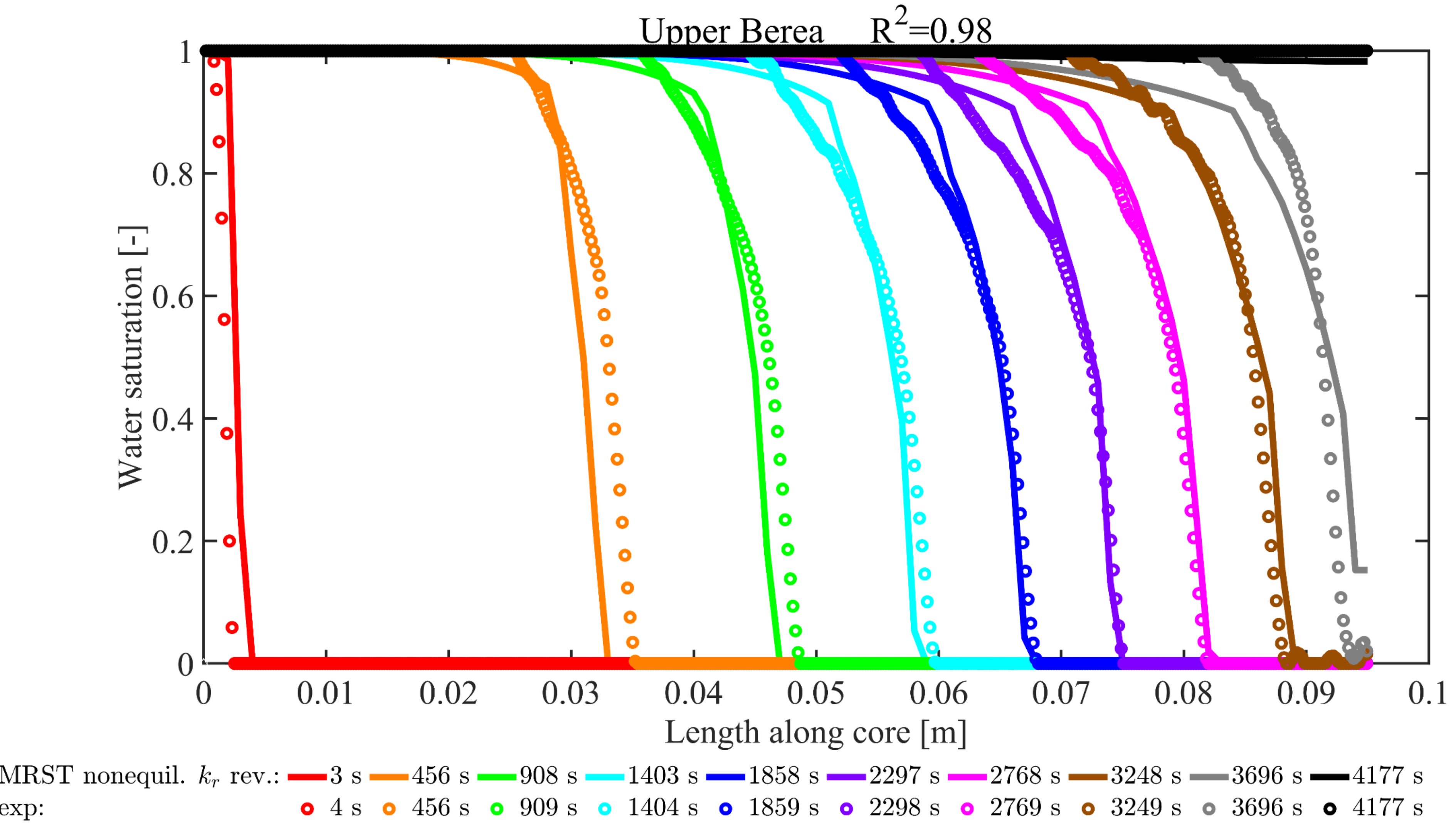


传统两相达西模型无法捕捉前缘位置与形态；

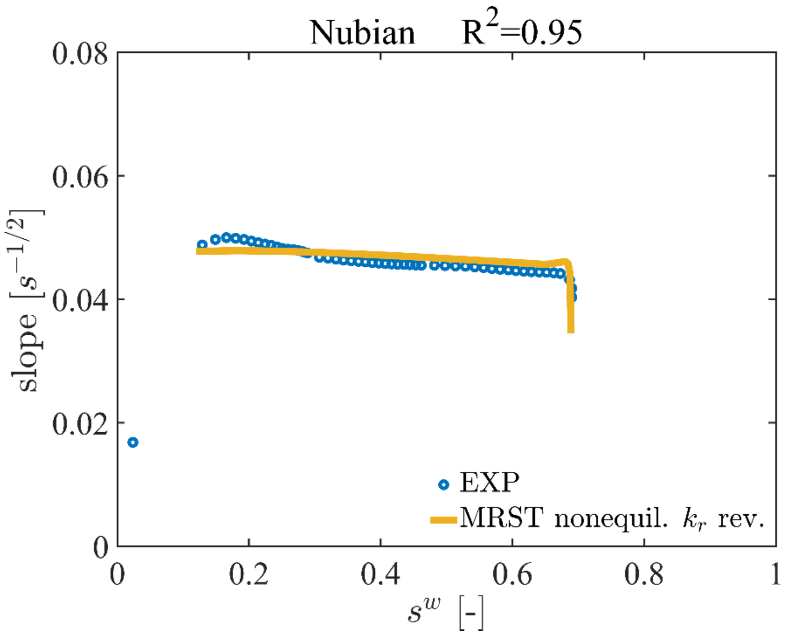
修正的传统两相达西模型仍无法重现尖锐渗吸前缘；

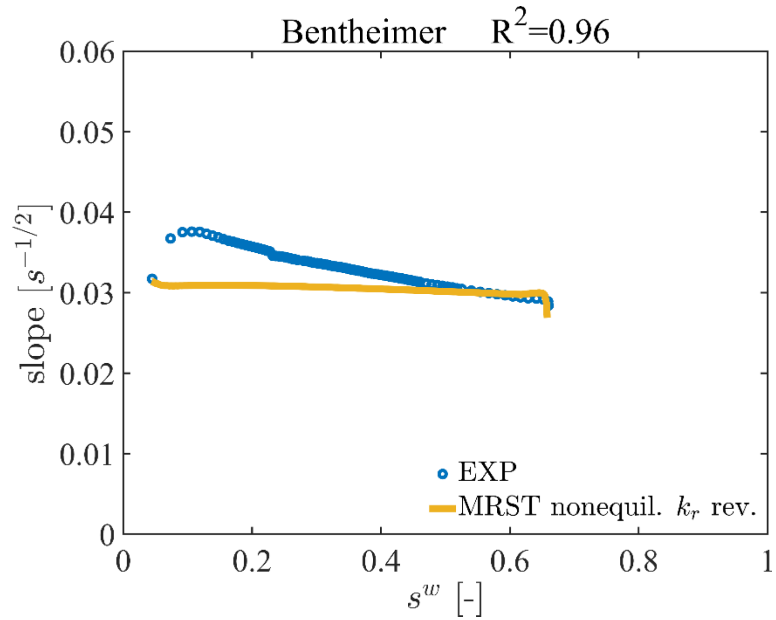
利用提出的相渗模型可以预测尖锐渗吸前缘

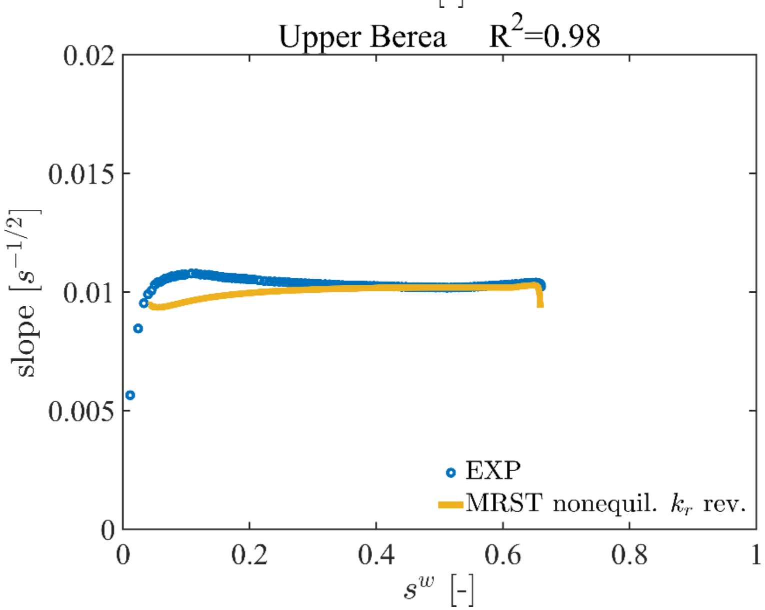
自发渗吸达西尺度数值模拟：饱和度剖面



自发渗吸达西尺度数值模拟：渗吸速率







模型可以**匹配渗吸速率**包括重力影响，**进口边界的影响**在岩心渗吸实验中比较显著

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结论与展望

- Our dynamic pore-network model of SI is **predictive**;
- The crucial uncertainty arises from the determination of **effective contact angles**;
- Dynamics causes **the deviation** of capillary pressure and relative permeability away from their quasi-static counterparts.
- We are formulating non-equilibrium relative permeability and capillary pressure, to **bridge the gas** between pore-scale and Darcy-scale SI.

- We need **an implicit scheme** for modeling low capillary number and unfavorable imbibition processes (ongoing);
- Further lab experiments are needed to determine **effective contact angles** for the pore-network modeling.

References

1. X. Wang et al., Experimental Validation of a Dynamic Pore-Network Model for Spontaneous Imbibition in Sandstone Rocks, ***Advances in Water Resources***, 104859, 2025.

2. B. Shi, H. Jiang, B. Guo, J. Tian, and C.Z. Qin. Modeling of flow and transport in multiscale digital rocks aided by grid coarsening of microporous domains. ***Journal of Hydrology***, 633: 131003, 2024.

3. C.Z. Qin, H. van Brummelen, M. Hefny, and J. Zhao. Image-based modeling of spontaneous imbibition in porous media by a dynamic pore network model. ***Advances in Water Resources***, 152: 103932, 2021.

4. C.Z. Qin, X. Wang, M. Hefny, J. Zhao, S. Chen, and B. Guo. Wetting dynamics of spontaneous imbibition in porous media: from pore scale to Darcy scale. ***Geophysical Research Letters***, 49, e2021GL097269, 2022.

5. Chen, S., Qin, C.Z., & Guo, B. (2020). Fully implicit dynamic pore-network modeling of two-phase flow and phase change in porous media. ***Water Resources Research***, 56, e2020WR028510, 2020.

6. C.Z. Qin and H. van Brummelen. A dynamic pore-network model for spontaneous imbibition in porous media. ***Advances in Water Resources***, 133: 103420, 2019.

Our new journal

Thank you for your attention!

Lab data: sample information

Core label	Diameter (mm)	Length (mm)	Weight of $core^{dry}$ (g)	Weight of $core^{si}$ (g)	Imbibed water weight (g)	Weight of $core^{sat}$ (g)	Saturated water weight (g)	Water saturation after SI	Porosity
NS1	25.2	45.5	45.715	49.367	3.652	50.978	5.263	0.6939	0.2320
NS2	25.1	45.1	45.598	49.219	3.621	50.831	5.233	0.6920	0.2346
NL1	25.1	81.6	79.397	85.795	6.398	88.637	9.240	0.6924	0.2290
NL2	25.2	82.4	79.413	86.116	6.703	89.061	9.648	0.6948	0.2349
TL3	24.9	100.2	95.368	102.731	7.363	106.484	11.116	0.6624	0.2279
TL4	24.8	100.1	94.847	101.991	7.144	105.645	10.798	0.6616	0.2234
TL5	24.9	100.3	95.533	102.863	7.330	106.574	11.041	0.6639	0.2262
TS1	24.9	49.8	47.404	51.174	3.770	53.085	5.681	0.6636	0.2344
TS2	24.7	49.8	47.049	50.697	3.648	52.550	5.501	0.6632	0.2306
TS3	25	50	47.51	51.285	3.775	53.198	5.688	0.6637	0.2319
TS4	24.9	49.7	47.169	50.858	3.689	52.731	5.562	0.6633	0.2299
TS5	24.9	50	47.199	50.876	3.677	52.743	5.544	0.6632	0.2278
US1	24.9	49.7	50.284	53.523	3.239	55.171	4.887	0.6628	0.2020
US2	25	49.8	50.338	53.559	3.221	55.175	4.855	0.6634	0.2020
US3	24.9	49.6	49.906	53.104	3.198	54.741	4.835	0.6614	0.2003
US5	24.9	49.8	50.117	53.336	3.219	54.977	4.860	0.6623	0.2005
UL1	24.7	100.1	100.298	106.819	6.521	110.119	9.821	0.6640	0.2049
UL2	24.9	100.1	100.453	107.058	6.605	110.416	9.963	0.6630	0.2045

Lab data: Geometrical and physical parameters used in the case studies

Digital core samples		NS2	TL3	US2
µCT data				
Number of voxels in X, Y, and Z directions		900×900×900		
Voxel resolution (um)		4	3	2
Pore network information				
Number of pores / pore throats		9913/ 20455	9091/ 17863	8750/ 16955
Numbers of inlet/ outlet pores		304/ 285	256/ 238	272/ 263
Volume averaged mean pore size (um)		31	23	12
Porosity (excluding isolated pores)		0.2056	0.2023	0.1482
Porosity (including isolated pores)		0.2058	0.2031	0.1506
Porosity by MIP		0.2127	0.2271	0.2084
Intrinsic permeability by the pore-network model (md)		5635	2212	212
Permeability by Avizo software (md) in X, Y, and Z directions within a 600-voxel cubic	x	7152	2183	184
	y	6287	2208	186
	z	5945	2173	178
physical parameters in the modeling				
surface tension at 21 ℃ (N/m)		0.073		
water/ air dynamic viscosity (Pa s)		1.0×10^{-3} / 1.83×10^{-5}		
Inlet/ outlet reservoir pressure (Pa)		0/0		
pre-wetting film capillary pressure (Pa)		1.0×10^{-6}		

In the validation, we checked the core **permeability**.

Lab data: residual saturations

Nubian	EXP	Dy (v 55.9)	Dy (v 1)	Dy (v 0.1)	Qs
Uni 75°	0.69	0.74008	0.62001	0.50000	0.31777
Log 70°		0.70000	0.62005	0.56000	0.44271

Bentheimer	EXP	Dy (v 55.9)	Dy (v 1)	Dy (v 0.1)	Qs
Uni 75°	0.66	0.70016	0.58007	0.48003	0.33842
Log 70°		0.68005	0.58004	0.54000	0.42599

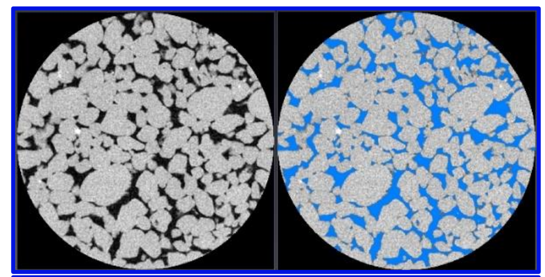
Upper Berea	EXP	Dy (v 55.9)	Dy (v 1)	Dy (v 0.1)	Qs
Uni 75°	0.66	0.72008	0.60001	0.48006	0.38326
Log 70°		0.68000	0.58006	0.54000	0.44923

基本概念的理解

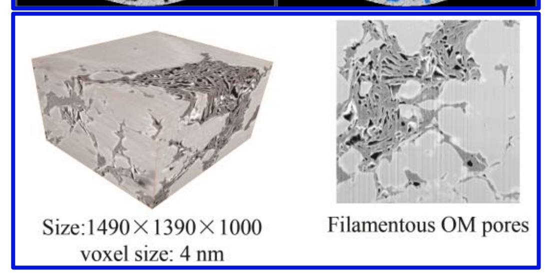
1. 数字岩心（digital rocks）
2. 孔隙网络模型（pore-network model）
3. 连续介质（continuum-scale）
4. 直接数值模拟（direct numerical simulation）
5. 多尺度渗流（multiscale）

常规岩心

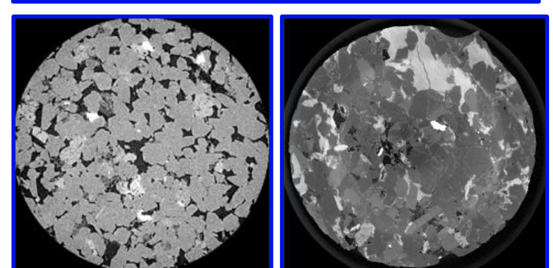
微纳米CT/FIB-SEM/MAPS



均质、固体与孔隙界限清晰



亚分辨有机质难以表征



各类粘土孔隙难以识别

基本概念的理解

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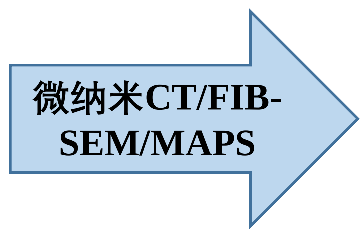
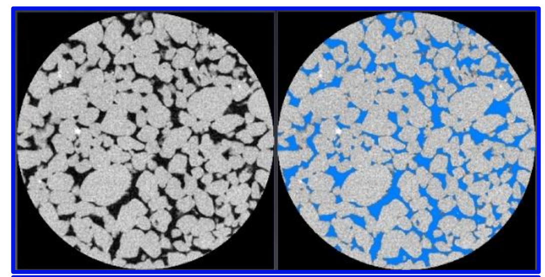
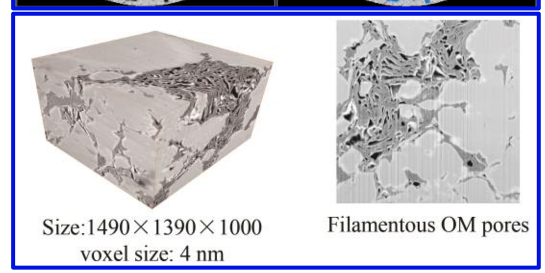
2. 孔隙网络模型（**pore-network model**）
3. 连续介质（**continuum-scale**）
4. 直接数值模拟（**direct numerical simulation**）
5. 多尺度渗流（**multiscale**）





均质、固体与孔隙界限清晰



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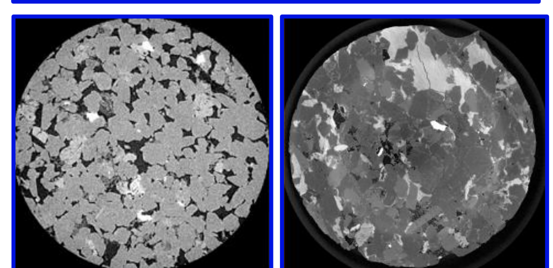

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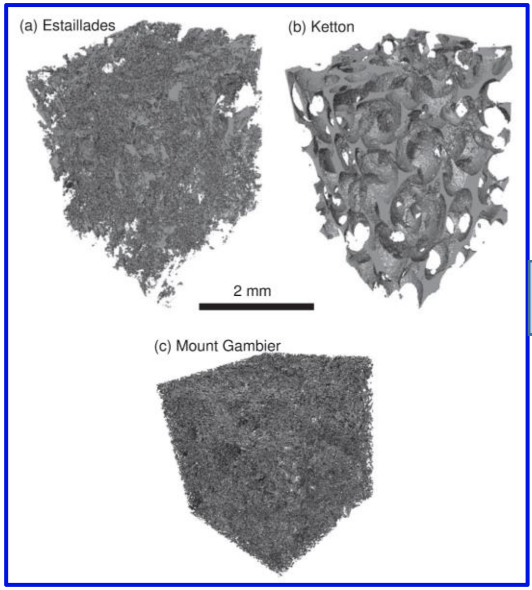
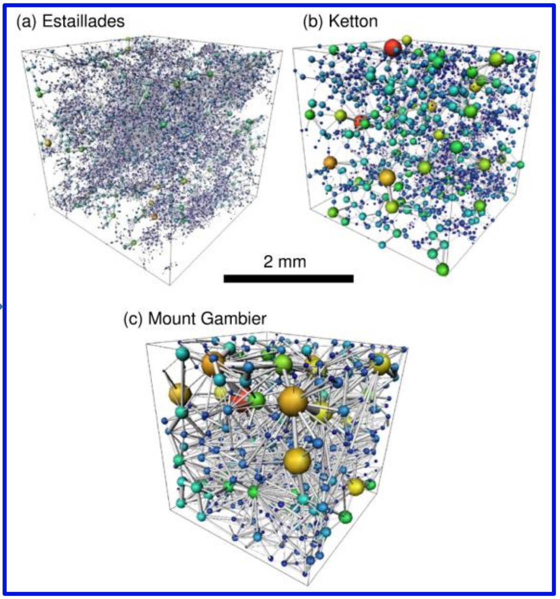


孔隙网络提取



流动与传输：

- ❑ 准静态两相驱替、渗吸
- ❑ 动态两相驱替、渗吸
- ❑ 反应流动与传输
- ❑ 非牛顿流体流动
- ❑ 矿物质溶解、沉淀
- ❑ 。。。。。。

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Advances in Water Resources 51 (2013) 197–216
Contents lists available at SciVerse ScienceDirect
Advances in Water Resources
journal homepage: www.elsevier.com/locate/advwatres

Pore-scale imaging and modelling

Martin J. Blunt [a,*], Branko Bijeljic [a], Hu Dong [b], Oussama Gharbi [a], Stefan Iglauer [c], Peyman Mostaghimi [a], Adriana Paluszny [a], Christopher Pentland [a]

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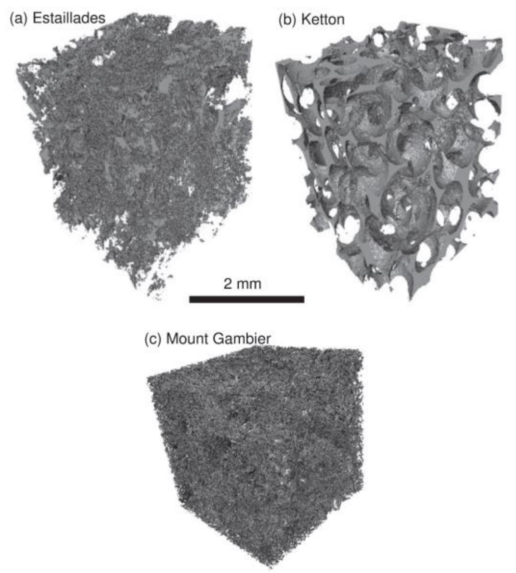
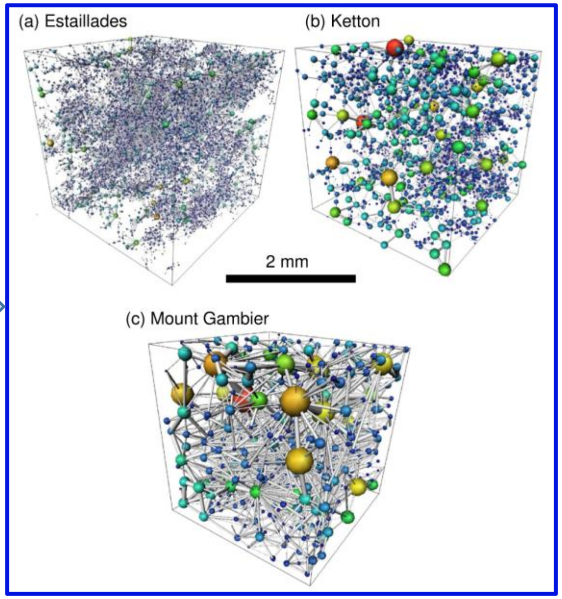
[c] Department of Petroleum Engineering, Curtin University, 6151 Perth, Australia

it is difficult to resolve thin wetting layers that control many processes in two and three-phase flow [1,7,8]; this limitation is discussed further at the end of the paper. In the literature to date, the most computationally efficient and successful predictions of multiphase flow come from network modelling, described below.



孔隙网络提取



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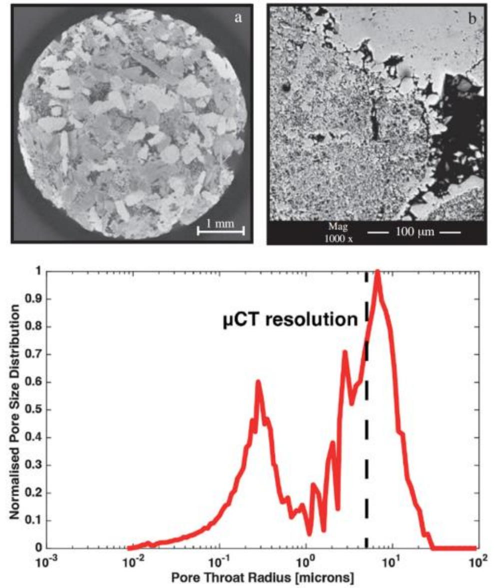
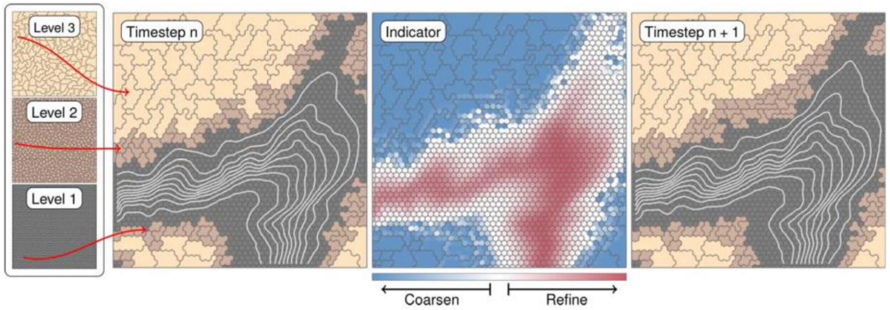


(Menke et al., 2022)

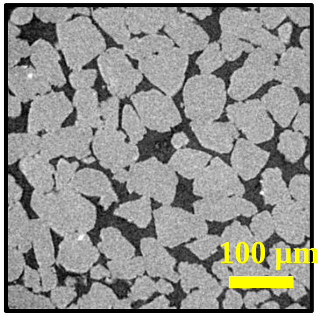
- **孔隙结构的多尺度：**孔径有明显的尺度分离，如页岩、碳酸盐岩和催化剂。注意与非均质性的异同。
- **数学模型的多尺度：**分子动力学模拟（MD）、直接数值模拟（DNS或micro）、孔隙网络模拟（PNM）、连续介质模拟（如Darcy），两个或多个耦合形成混合模型。
- **计算网格的多尺度：**如自适应网格技术，储层尺度下的multiscale modeling

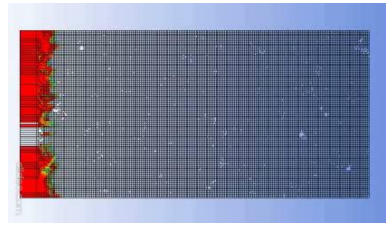


(Klemetsdal et al., 2021, SPE J)

数字岩心渗流模拟

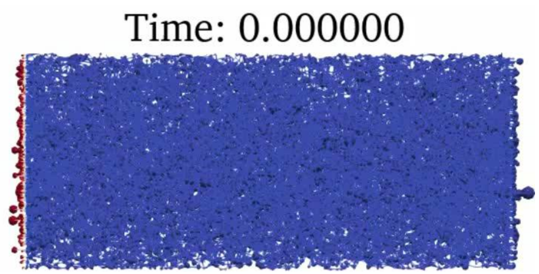
Nubian砂岩





自发渗吸数值模拟, 100×100×200 图像

(*Qin et al., AWR, 2021*)

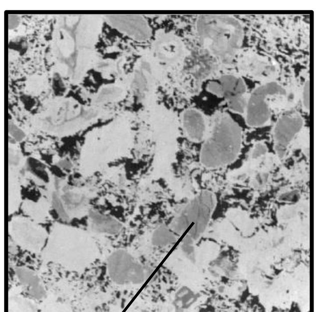


900×900×2000 image

自发渗吸动态孔隙网络模拟

Digital rock core

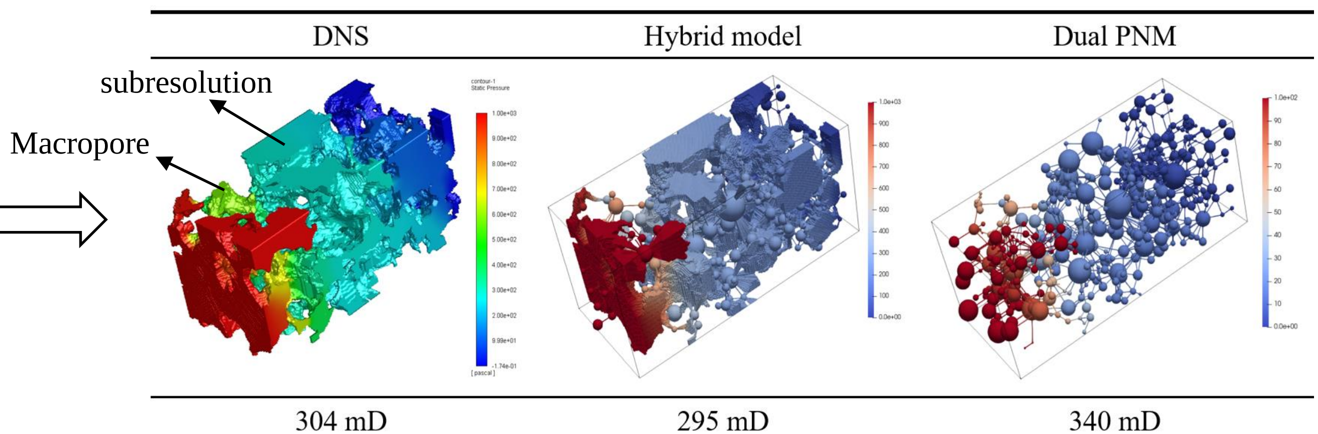
Estaillades碳酸盐岩



亚分辨率微孔区

微观-连续介质模型

(*Koch et al., TiPM, 2021*)



(*Zhang, Guo, Qin, and Xiong, AWR, 2024*)

多尺度渗流力学团队

秦朝中

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- 2016.11~2019.10，荷兰埃因霍温理工大学（机械工程），达西研究中心，执行主管
- 2005.09~2016.10，西安交通大学学士、中国科学技术大学硕士、荷兰乌特列支大学/通用汽车欧洲研究院博士、博后
- 从事数字岩心分析技术、多尺度渗流力学等方面的研究，主持（研）国家自然科学基金面上、联合重点基金、中比国际合作与交流、通用汽车工业应用研究项目、荷兰科学研究组织项目、欧盟研究委员会项目和瑞士国家科学基金，在Geophysical Research Letters、Water Resources Research、Advances in Water Resources、Journal of Petroleum Science and Engineering等国际渗流力学杂志发表论文50多篇

蒋 函

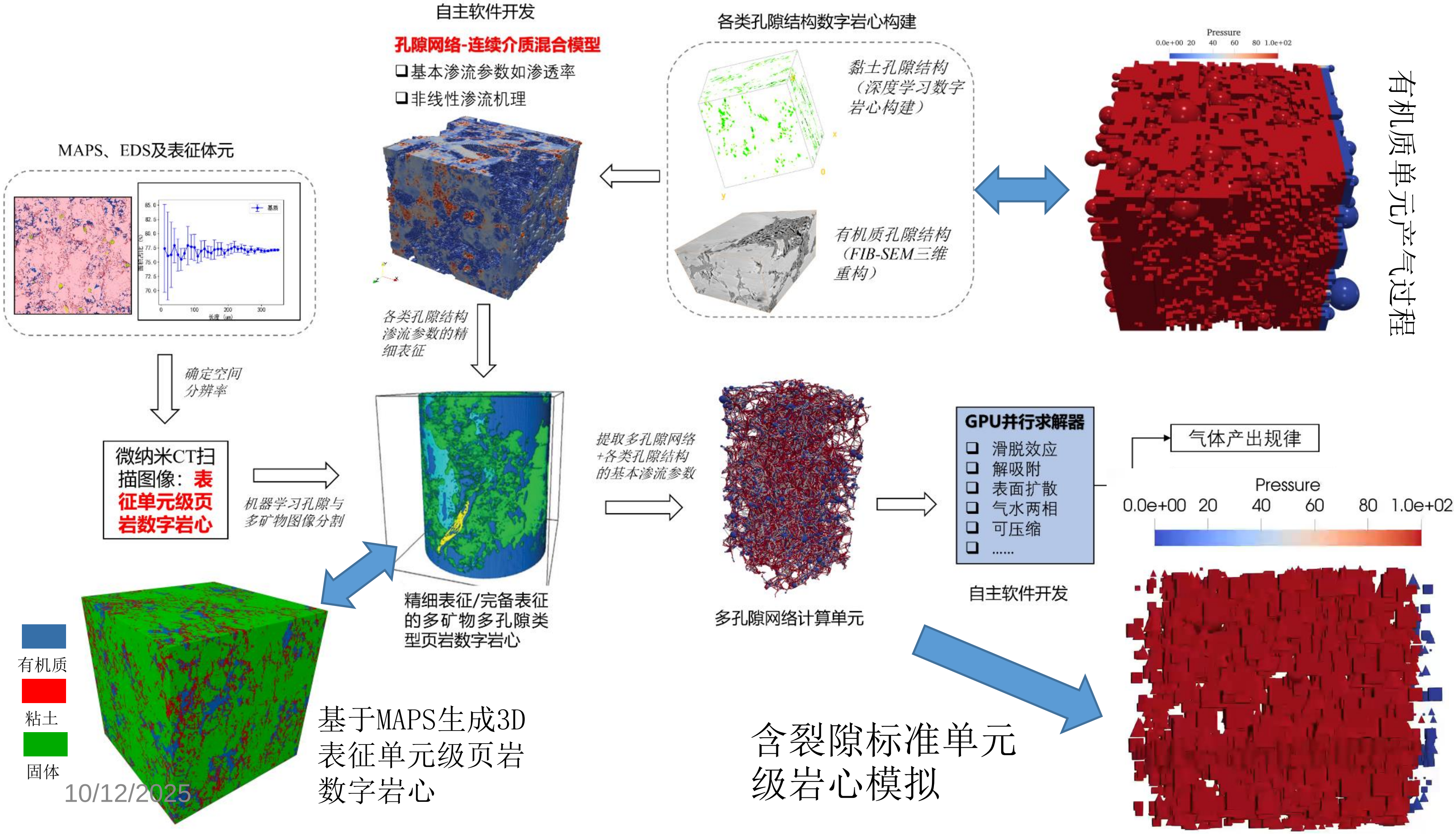
- 重庆大学资源与安全学院，讲师、助理研究员
- 2021年，博士毕业于澳大利亚新南威尔士大学石油工程专业，从事数字岩心分析技术与渗流理论研究
- 主持（研）国家自然科学基金、博士后基金等多项科研项目，在Water Resources Research、Physical Review E、Journal of Petroleum Science and Engineering等顶级期刊发表论文10余篇

田 键

- 重庆大学资源与安全学院，讲师、助理研究员
- 2021年，博士毕业于西南石油大学油气井工程，从事油气储层保护与开发，致密油气藏提高采收率理论与技术
- 主持（研）国家自然科学基金、博士后基金等多项科研项目，在石油学报、Physics of fluids、Journal of Petroleum Science and Engineering等顶级期刊发表论文20余篇

二、页岩多尺度孔隙结构表征与微纳尺度流动模拟

构建了跨尺度信息融合的页岩孔隙结构定量表征技术，建立了页岩多尺度数字岩心渗流模拟技术包括孔隙网络-连续介质模型和多重孔隙网络模型。

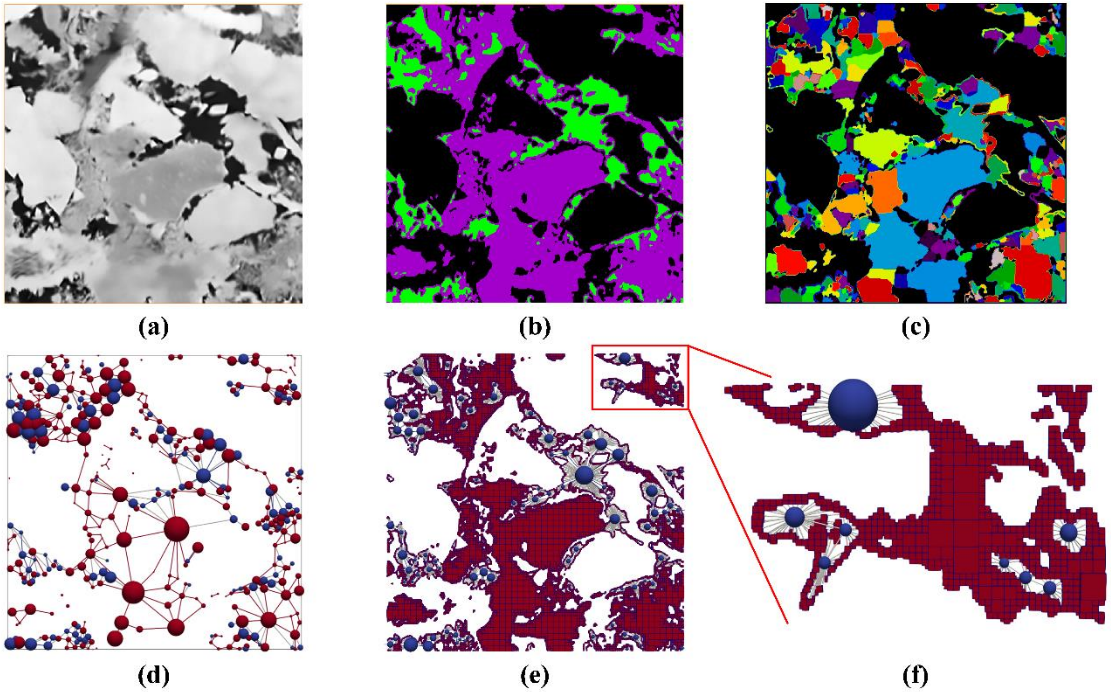


三、多尺度数字岩心渗流模型对比研究

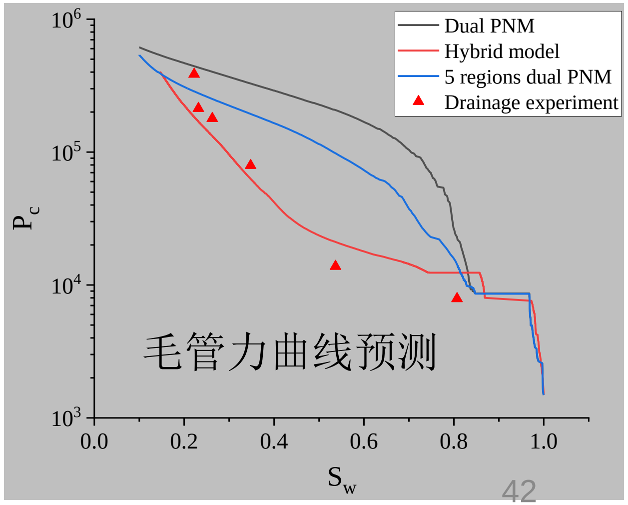
相比孔隙网络-连续介质模型，更加高效的多重孔隙网络模型不可以较好地处理非均质微孔区（亚分辨率区域），需要开展微孔区单元流动参数的升尺度研究。

单相渗透率预测对比

Sample number	Dual-PNM (mD)	PNM-continuum (mD)	Reference model (mD)
ES3.1	109	116	117
ES3.6	34	37	37
ES6.5	28	18	18
ES6.5 (Heterogeneity)	12	128	174

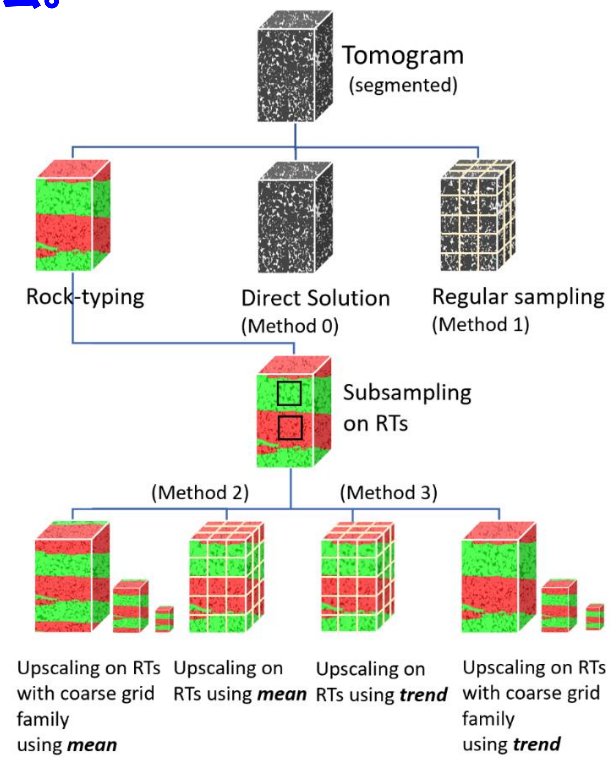


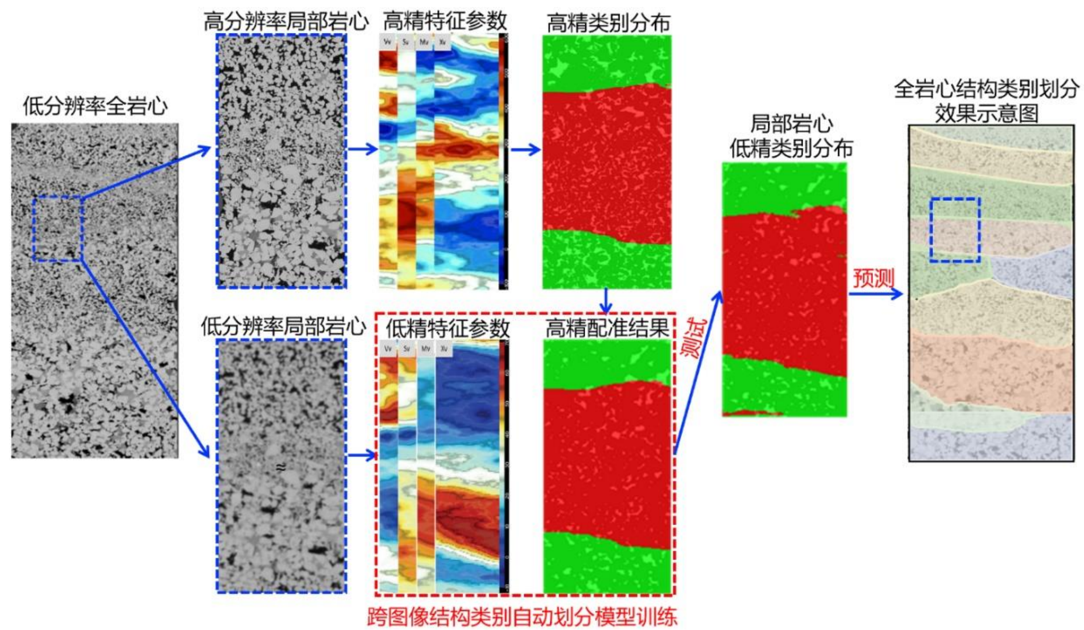
基于图像生成两种模型的计算单元或网格

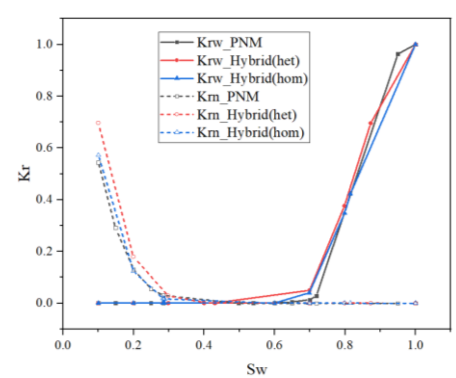


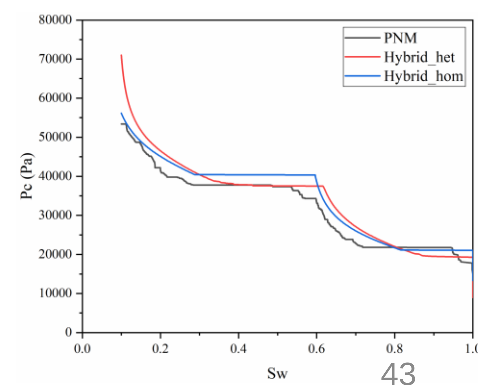
四、大尺度非均质数字岩心渗流模拟技术

发展了跨图像孔隙结构类别自动划分技术，提出了渗流参数升尺度高效计算方法。









（PRE 2020, WRR 2020, 2021, AWR 2024）

五、多物理场耦合数字岩心渗流模拟技术与高效求解器