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油气渗流研究中心
Center of Multiphase Flow in Porous Media

中国石油大学（华东）
CHINA UNIVERSITY OF PETROLEUM

Micro-Continuum Simulation of

Pore-Scale Mineral Dissolution

Pore-Space Structure & Dissolution Regimes

Jinlei Wang · Yongfei Yang · Branko Bijeljic · Martin J. Blunt

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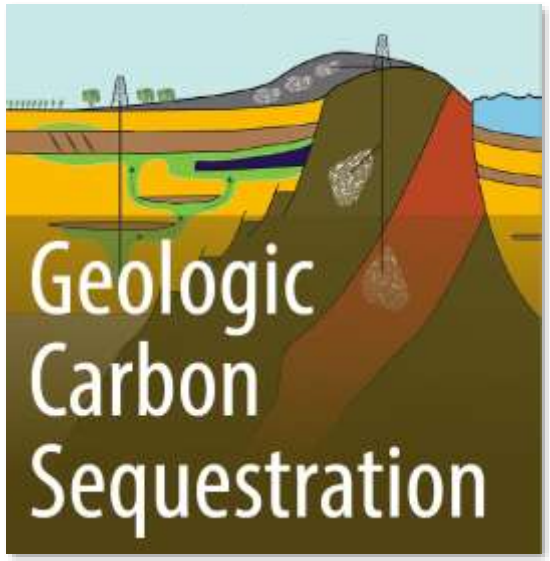
Why Pore-Scale Mineral Dissolution Matters

Reactive transport in porous media couples fluid flow with mineral dissolution

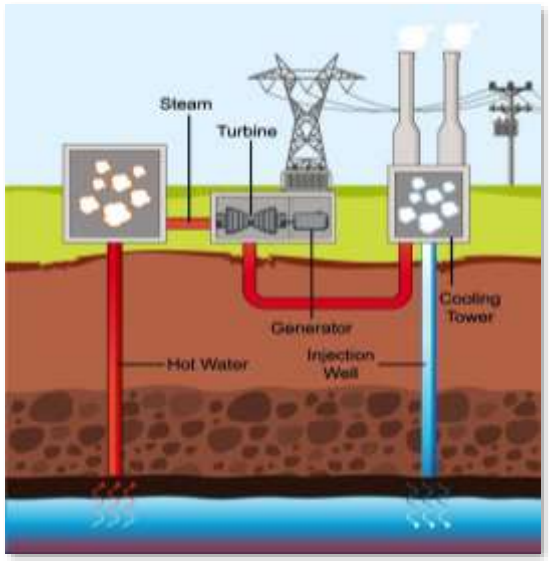
— a fundamental process spanning natural and industrial subsurface systems

Pore-space evolution dictates macroscopic transport

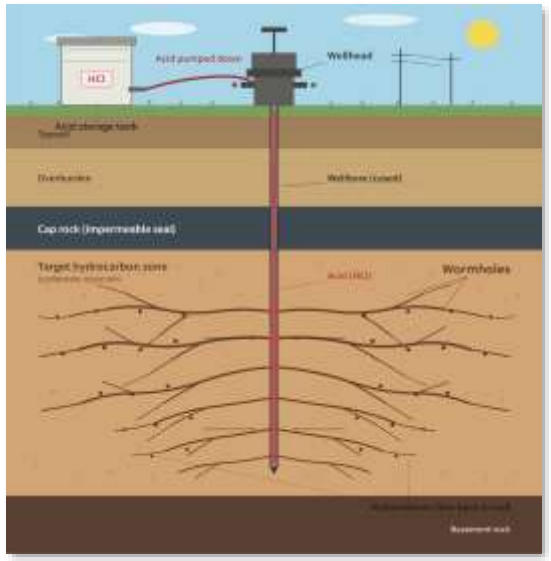
—predicting it requires resolving fluid–mineral interactions at pore scale



CO_2 Storage



Geothermal



Oil & Gas Recovery

Karst Formation

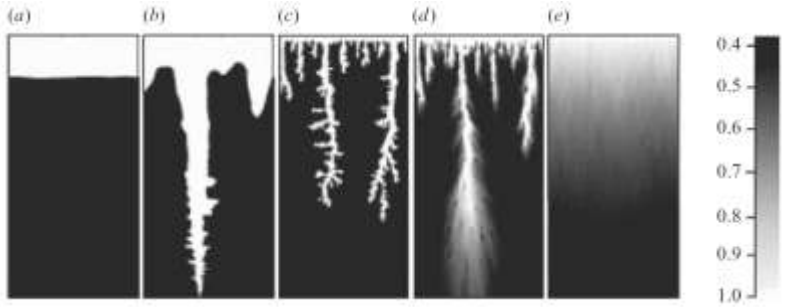
Static *Pe–Da* Diagrams Miss the Real Behavior

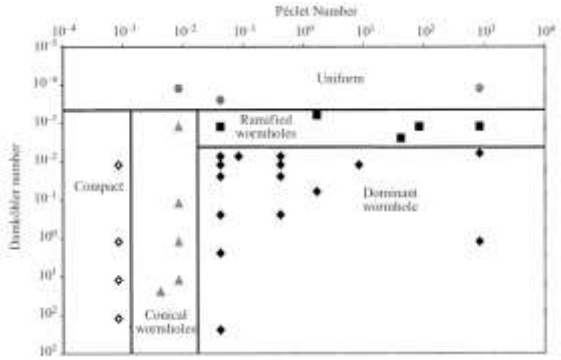
Classical mineral dissolution regimes in the Péclet–Damköhler plane: ***face, wormhole, uniform***

Real rocks defy the classification :

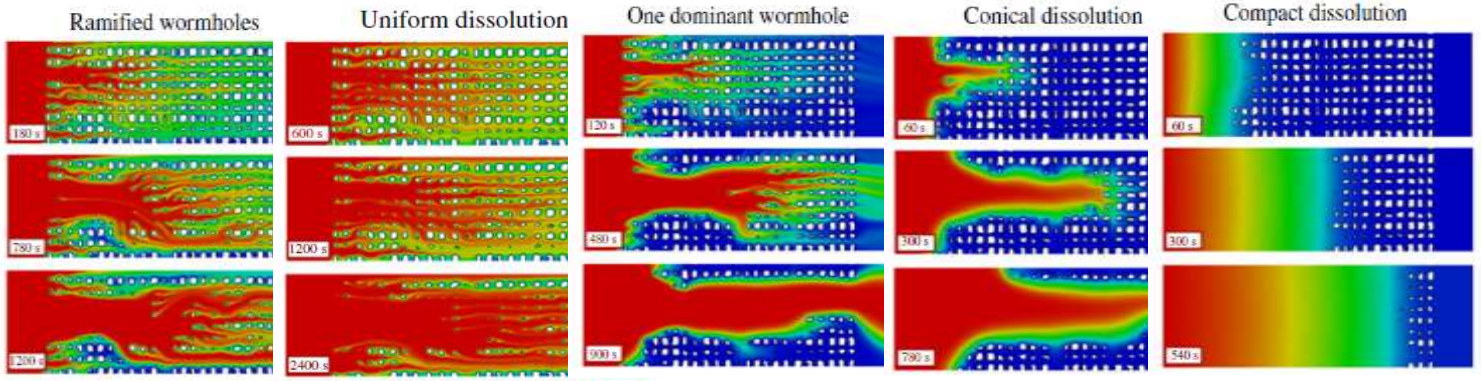
— *Boundaries derived from **homogeneous media**, they cannot capture pore-scale heterogeneity*

— *Treats regime as a **fixed label**, not a process that evolves with pore-structure changes*

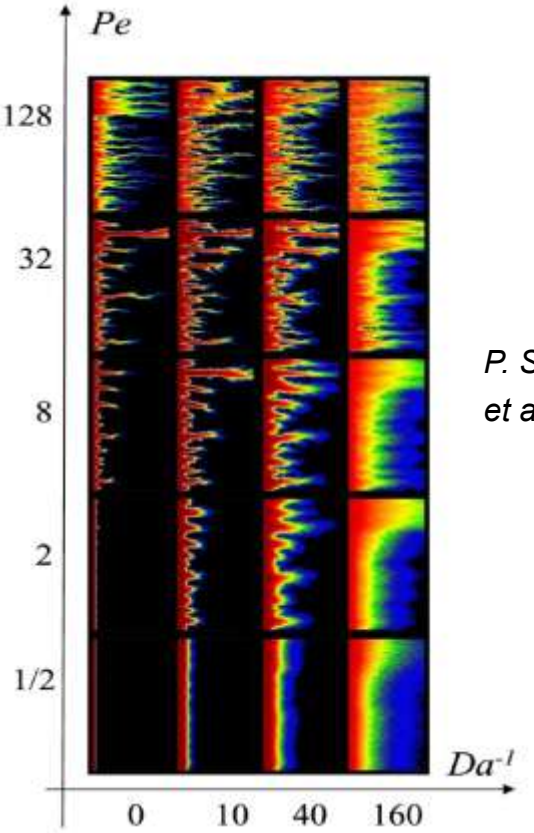




F. Golfier, et al., 2002



C. Soulaine, et al., 2017



P. Szymczak, et al., 2002

How do structure and flow evolve to set the dissolution regime?

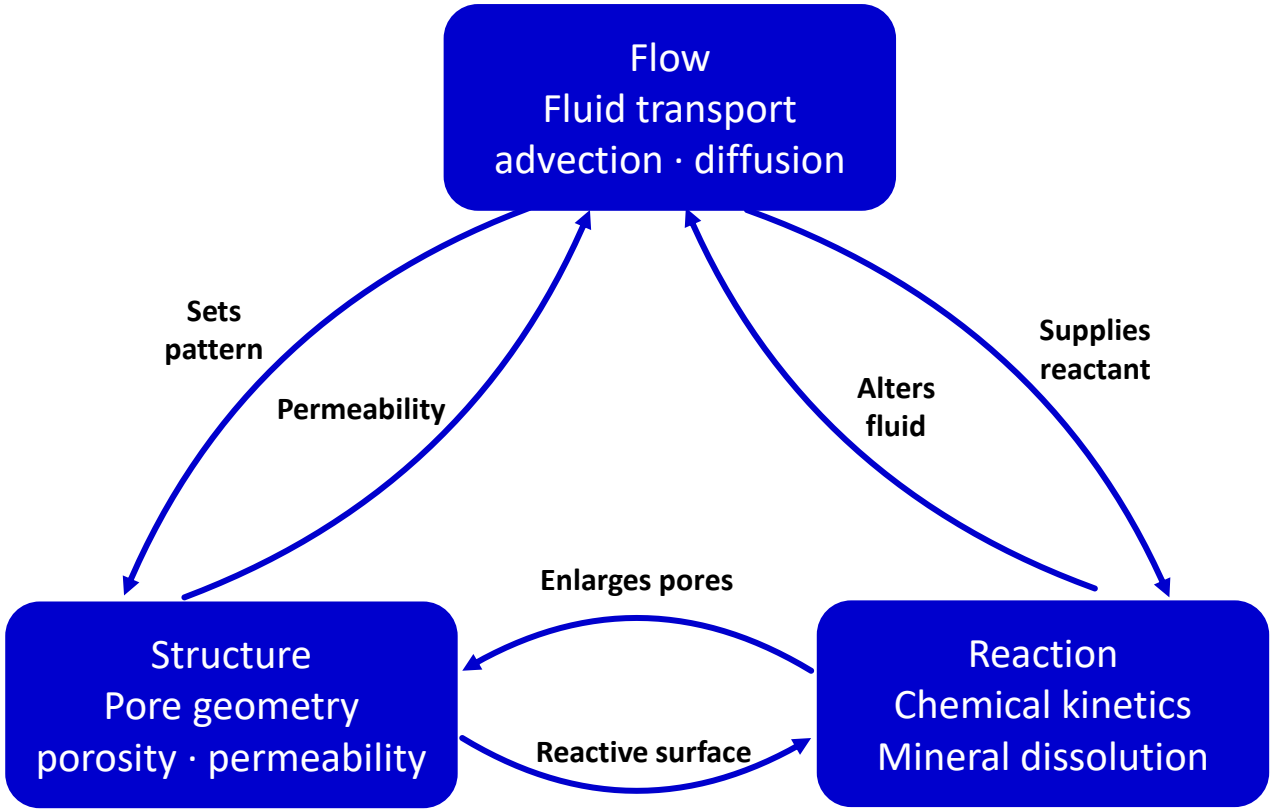
Objectives:

i ***Establish a methodology for quantifying the impact of heterogeneity on dissolution regimes and their transitions***

ii ***Identify which media sustain uniform dissolution and what initial flow heterogeneity is needed to produce channeling***

iii ***Examine the dependence of the permeability–porosity relationship on heterogeneity and transport conditions***

iv ***Quantify the reduction in effective reaction rate from heterogeneity-induced mass-transfer limitations across regimes***



Three Samples Spanning a Wide Heterogeneity Range

Pore-scale Heterogeneity order : Beadpack < Ketton limestone < Estaillades limestone

Pore structure heterogeneity is super-linearly amplified into ***flow heterogeneity***

$$CV = \sqrt{\sum_{i=1}^{n} (v_i - 1)^2 \cdot p(v_i) \cdot \Delta v_i}$$

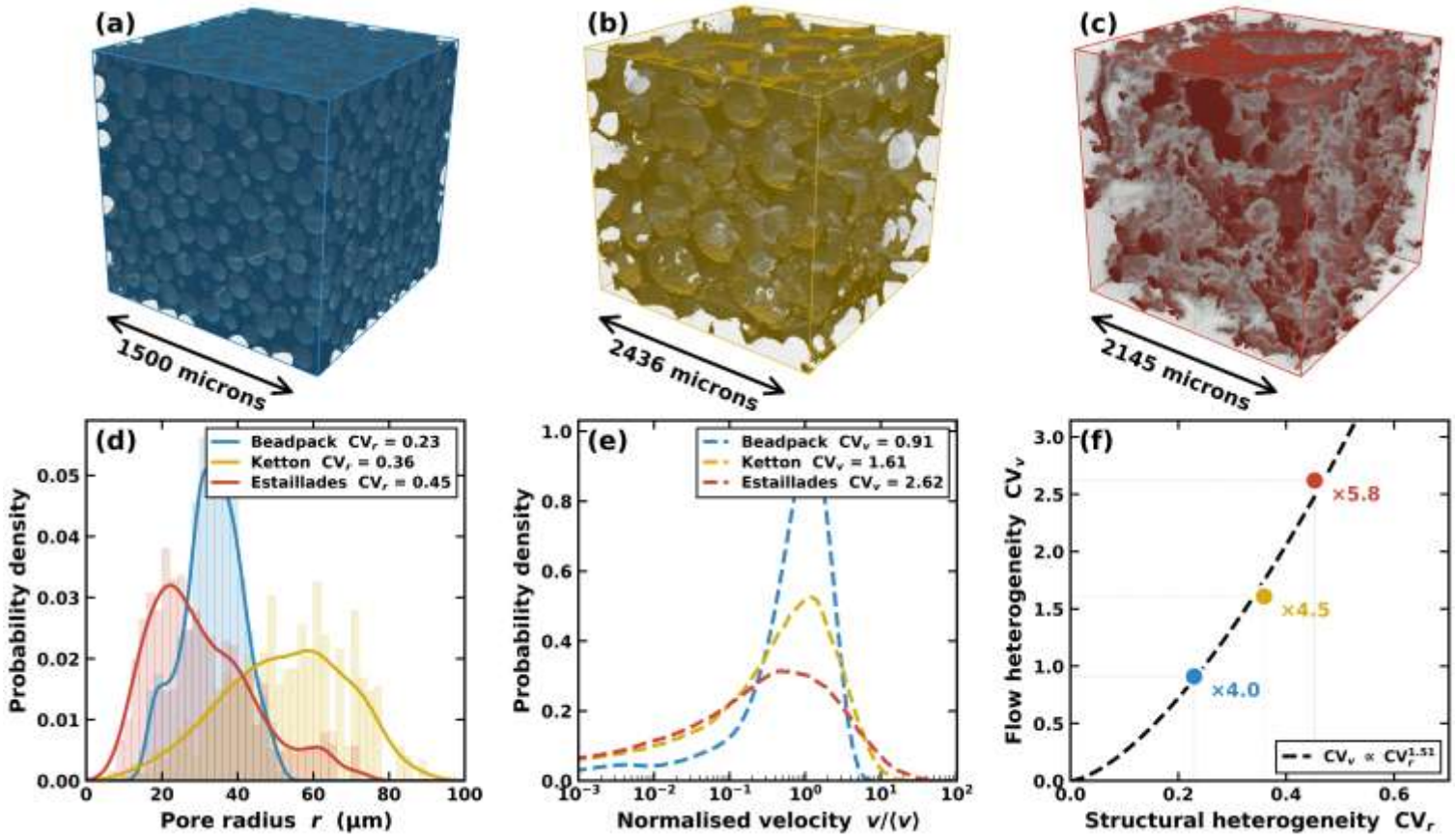


Figure 1. 3D pore visualizations and pore radius / velocity PDFs across the three samples.

Beadpack (a)

CV_v = 0.91

φ = 0.362 **K = 13.9 D**

Homogeneous benchmark — random close packing of identical spheres

Ketton limestone (b)

CV_v = 1.61

φ = 0.140 **K = 2.7 D**

Oolitic limestone — moderate pore-size variability

Estaillades limestone (c)

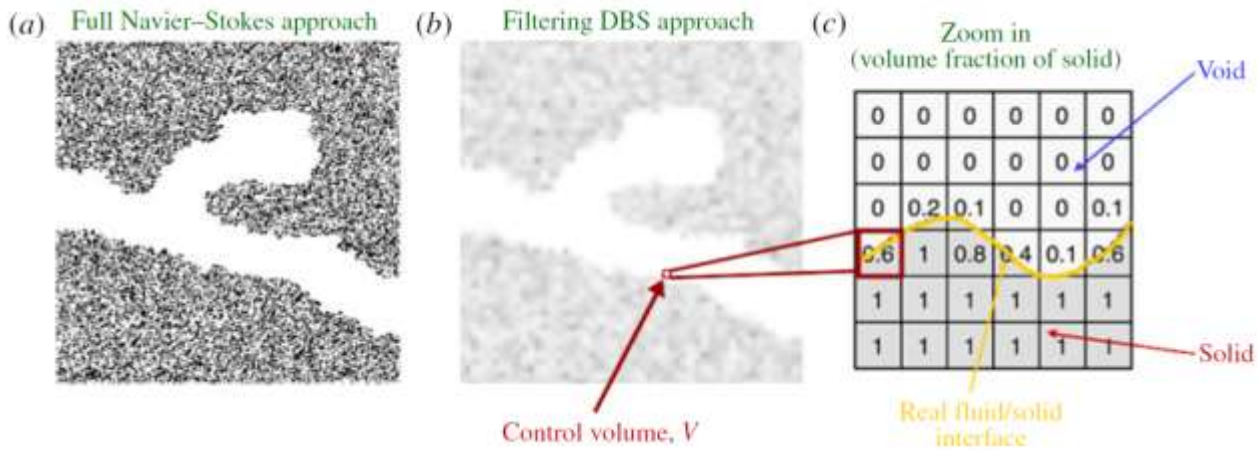
CV_v = 2.62

φ = 0.119 **K = 0.5 D**

Bioclastic limestone — strong heterogeneity, complex pore Sructure

3D Micro-Continuum Modeling of Reactive Transport

Governing Approach : Micro-Continuum method with improved Volume-of-Solid (*iVOS*) on micro-CT images



$$\nabla \cdot \mathbf{v} = 0$$

$$-\nabla p + \nu \nabla^2 \mathbf{v} = 0$$

$$\frac{\partial(\epsilon c)}{\partial t} + \nabla \cdot (c\,\mathbf{v}) = \nabla \cdot (\epsilon\, D_m\, \nabla c) - R$$

$$R = \epsilon \nabla \cdot \mathbf{\Phi}_R - \nabla \cdot (\epsilon\, \mathbf{\Phi}_R) \qquad \mathbf{\Phi}_R = -k_c\, c\, \frac{\nabla \epsilon}{|\nabla \epsilon|} \qquad \frac{\partial \epsilon}{\partial t} = \frac{R\, M_s}{\rho_s}$$

Figure 2. Full N-S approach and filtering DBS approach. (C. Soulaine, et al., 2017)

https://github.com/GeoChemFoam, by J. Maes & H. Menke

Simulation Design : *Pe* = 1 - 1000,
2000 Pore Volume Injection (PV)
CO_2-saturated brine at 10 MPa, 50 °C , with calcite
reaction-limited regime (*Pe·Da_adv < 0.05*)

Dimensionless numbers : $Pe = v_{avg} \cdot L_c / D_m$ $Da = k_c \cdot L_c / D_m$

Result 1: Permeability - Porosity Exponent Evolves Over time

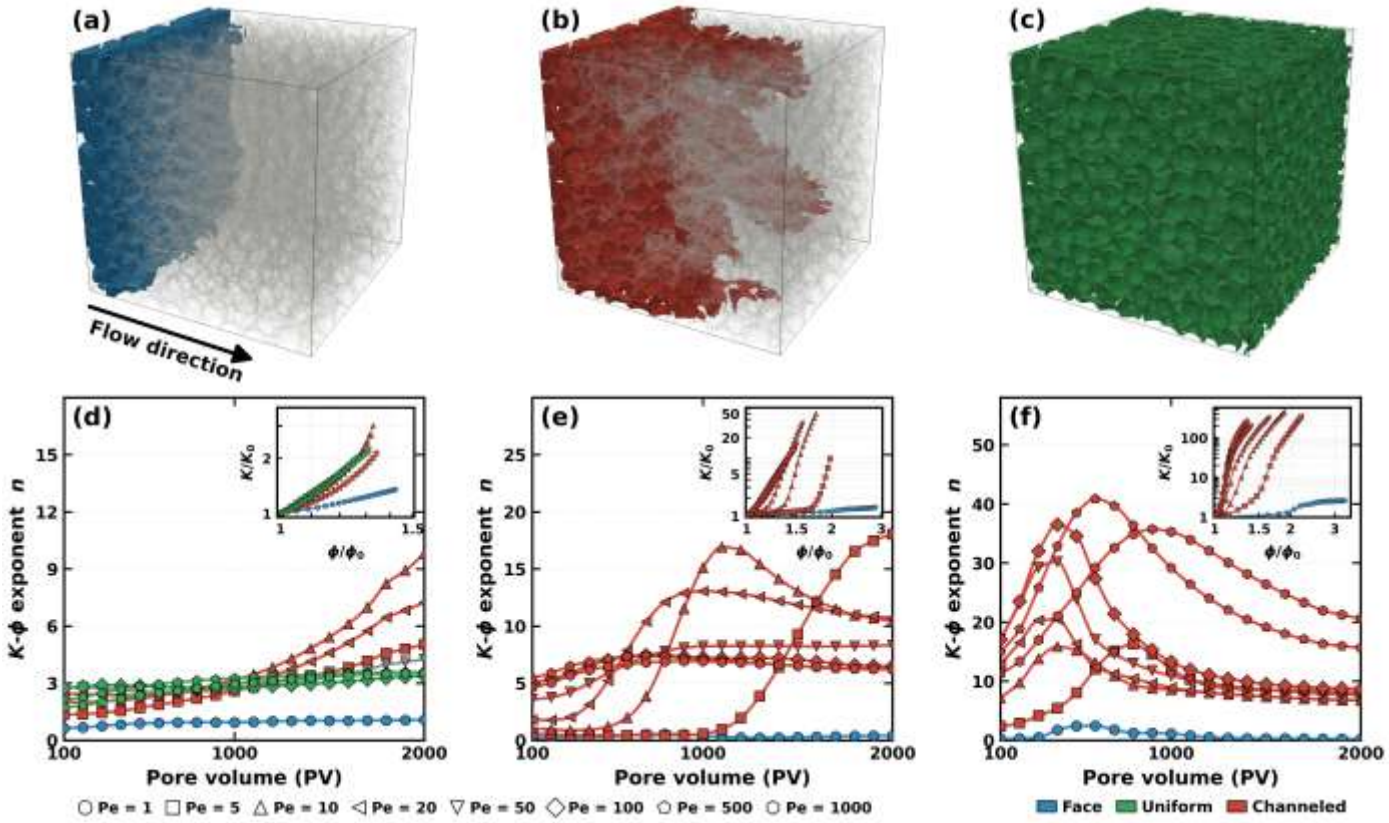
Beadpack: monotonic rise, *n* stays ≤ 10 — pore enlargement without flow focusing

Ketton: transient peak at intermediate *Pe*, plateau at high *Pe*

Estaillades: sharp single peak, then pronounced decay — channel widens, flow focuses

Instantaneous Exponent

$$n = d \ln K / d \ln \phi$$



- ✓ ***n_max*** **increases with increasing heterogeneity**
- ✓ **No single power-law exponent describes *K–φ* trajectory once channeled dissolution sets in**

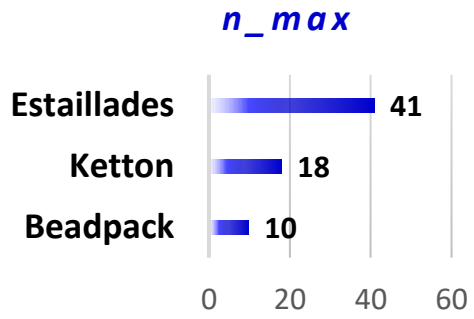
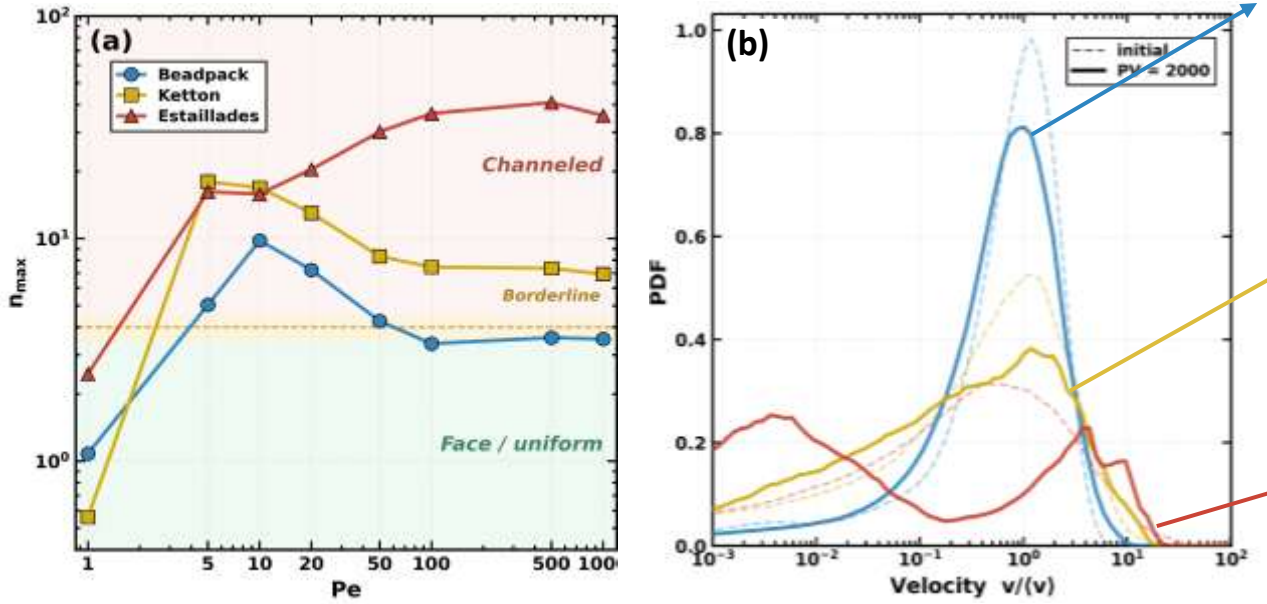


Figure 3. (a-c) 3D visualizations of the dissolved solid with semi-transparent pore space in the beadpack (face, channeled, uniform). Evolution of the instantaneous K–φ exponent n(PV) for (d) the beadpack, (e) Ketton, and (f) Estaillades.

Result 2: Flow Heterogeneity Determines Feasible Regimes

Whether a rock reaches uniform dissolution at any *Pe* depends on ***pore-scale heterogeneity***

Pore-scale heterogeneity selects the transport condition with highest level of preferential channels



beadpack: narrow & unimodal

Ketton: broadens to lower velocities

Estaillades: Bimodal

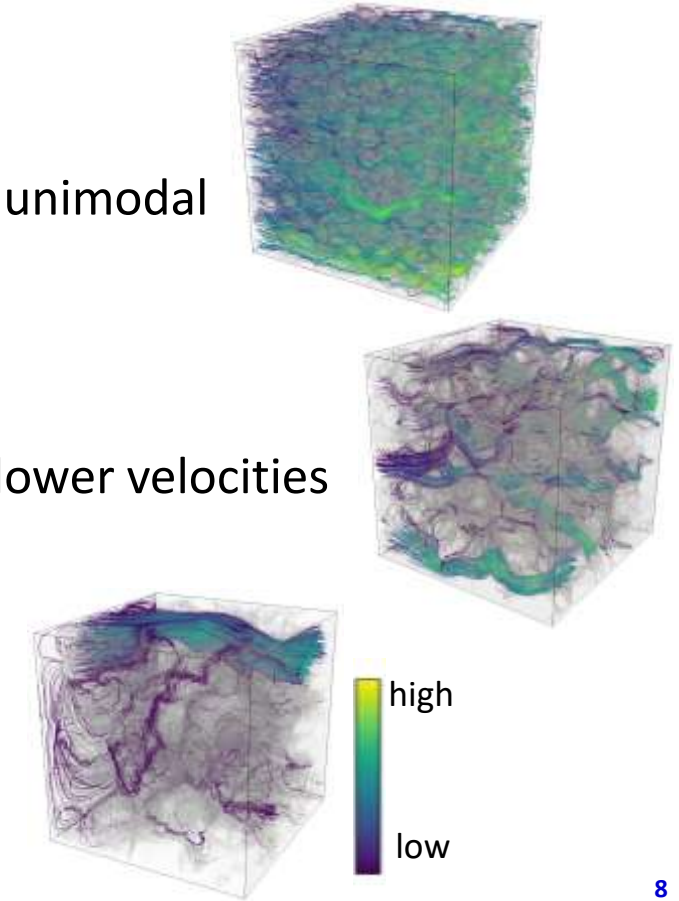


Figure 4. (a) n_max vs Pe and (b) velocity PDFs.

Result 3: Mechanism of Channeled Dissolution

Estaillades, Pe=500 (*n_max* for all the *Pe* numbers)

n and CV_v reach maximum ***synchronously***

Channel emergence is a ***localized dynamical event*** rather than a gradual reclassification

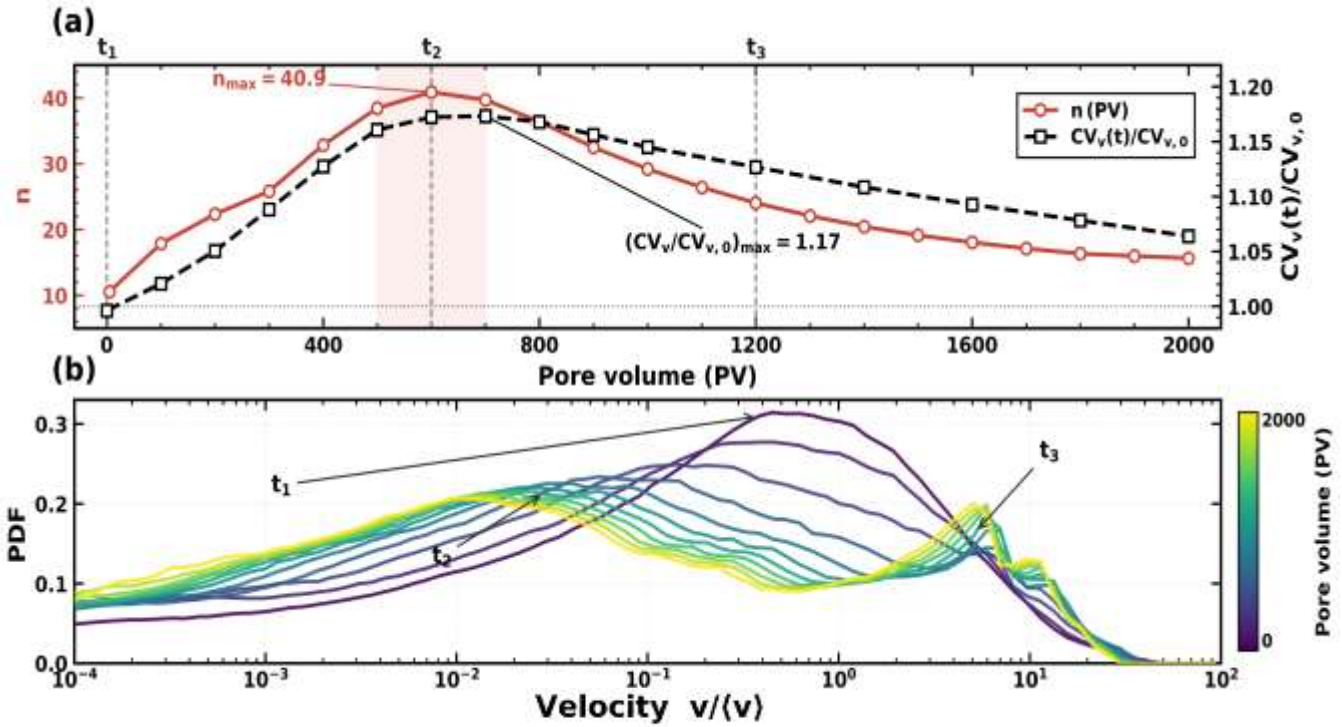
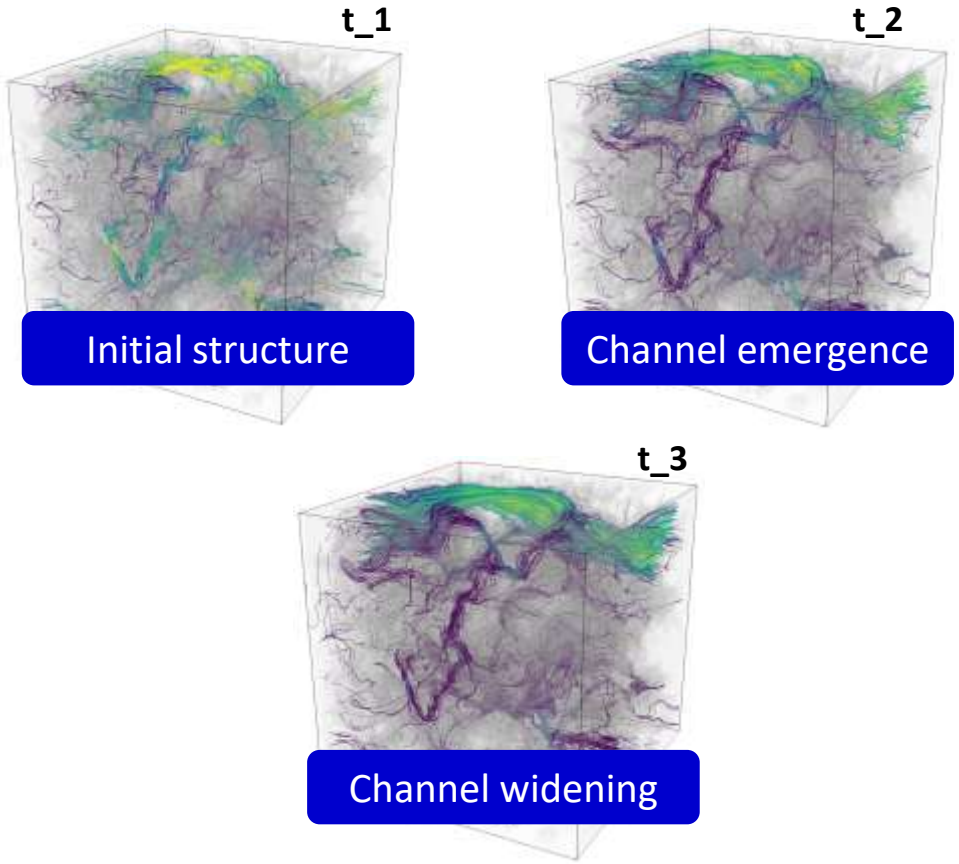


Figure 5. (a) Coevolution of n and CVv(t)/$CV_{v,0}$ and (b) Evolution of velocity PDFs.



Result 4: Suppression of Effective Reaction Rate

1 to 3 orders of magnitude below the uniform dissolution prediction

The gap between the initial and post-dissolution curves widens with CV_v

The additional suppression introduced by ***dissolution-driven flow field reorganization*** from the intrinsic geometric suppression of the pore structure

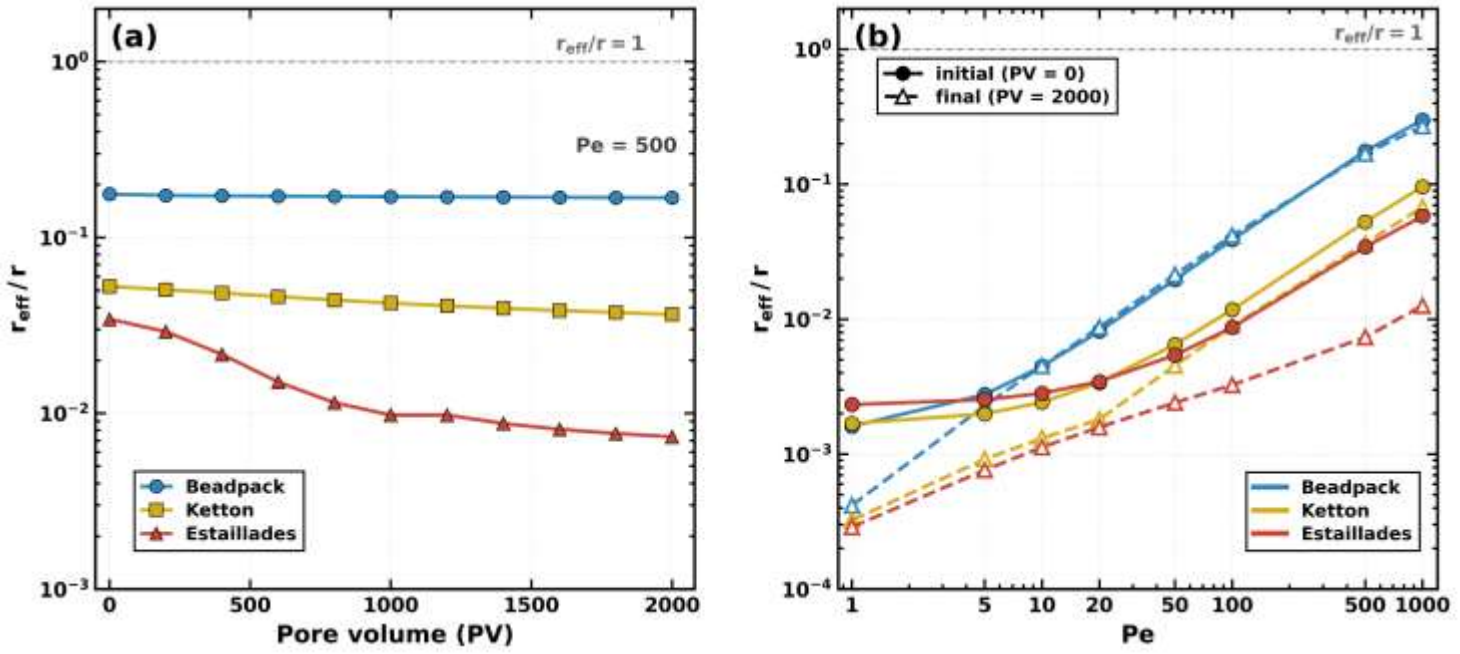


Figure 6. (a) Normalized reaction rate r_{eff}/r vs PV and (b) r_{eff}/r vs Pe.

Intrinsic calcite reaction rate

$r = 8.1 \times 10^{-4}$ mol m^{-2} s^{-1}

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Thank you

Linkedin

Wechat

Email: *jwang1@imperial.ac.uk*




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