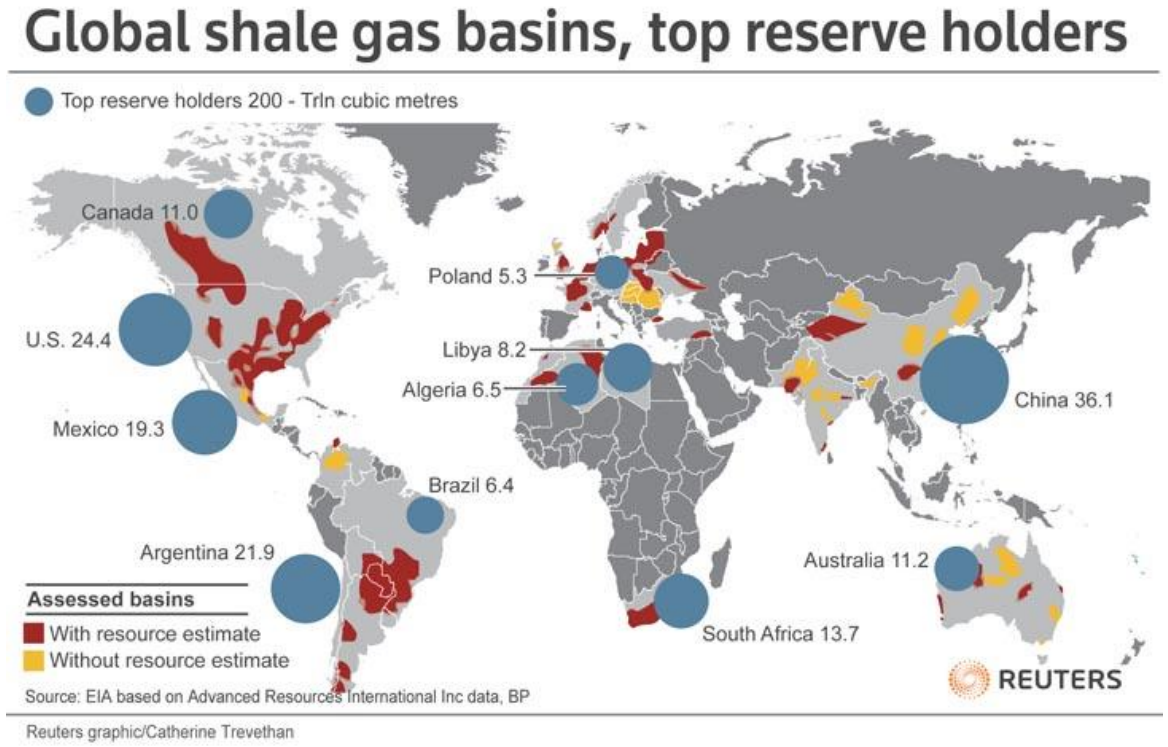
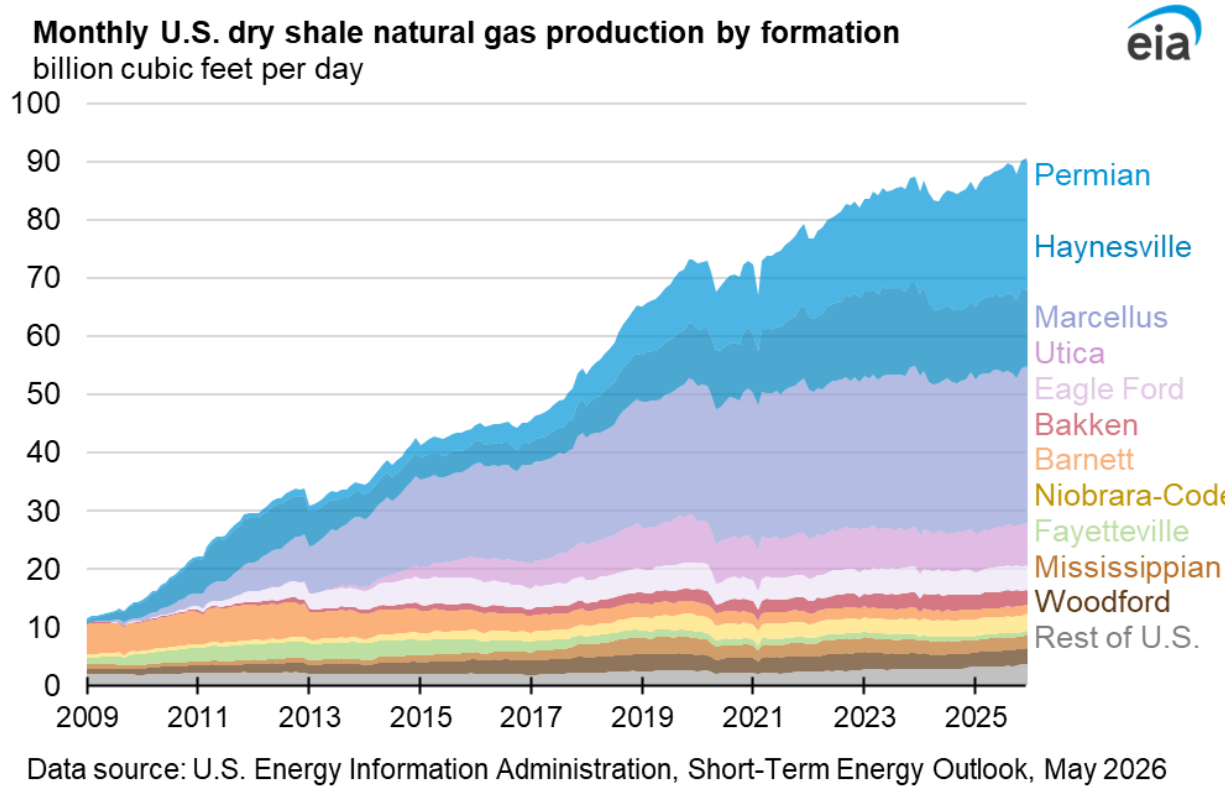
Dynamic migration and recovery mechanism of multi-component shale gas within intra-connected kerogen nanopores

Mingshan Zhang

2026/05/21

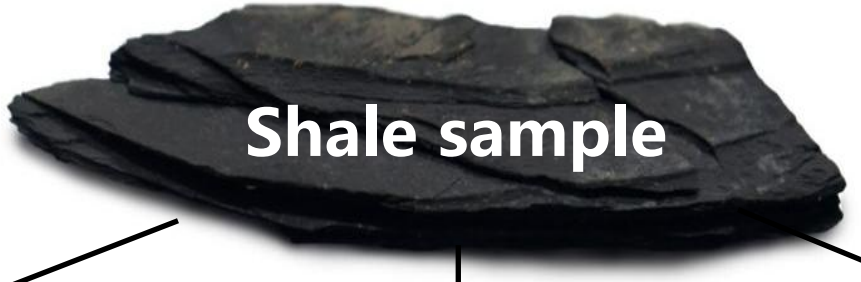




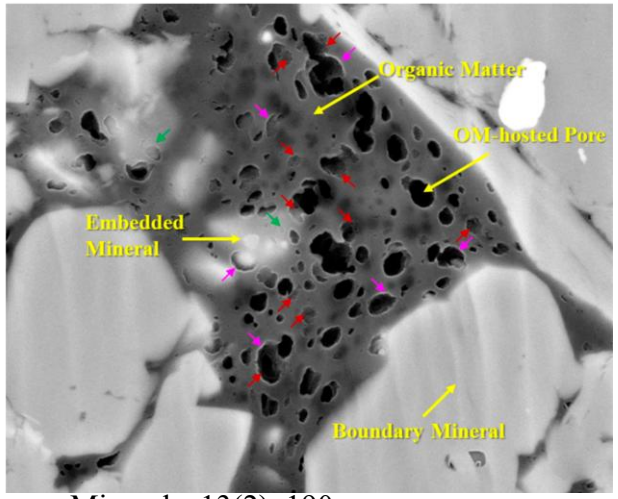
Abundant reserves and great development potential of shale gas worldwide.

In 2025, about 76% of total U.S. dry natural gas production was from shale formations.

Shale gas plays a crucial role in global natural gas supply

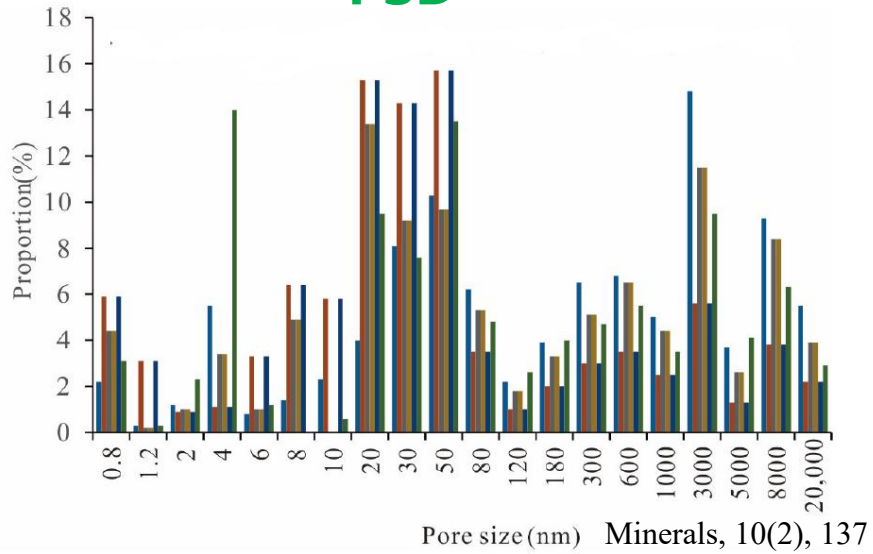


SEM Image



Minerals, 13(2), 190

PSD

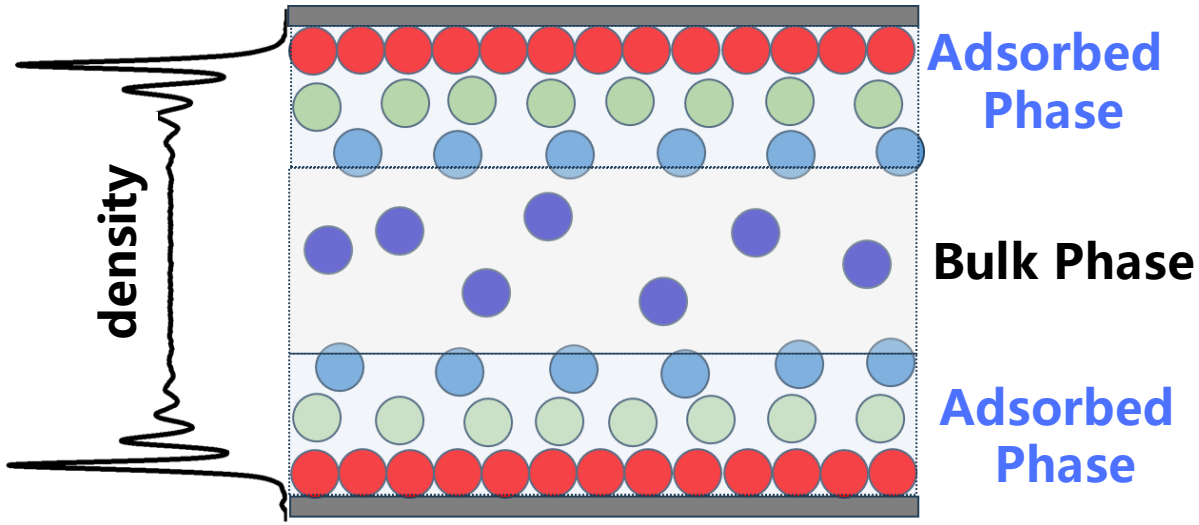


Minerals, 10(2), 137

Component

#	CH_4	C_2H_6	C_3H_8
1	80.3	**8.1**	**2.3**
2	81.2	**11.8**	**5.2**
3	91.8	**4.4**	**0.4**

- **Rich in organic mater (kerogen)**
- **Well-developed nanopores**
- **Complex fluid component**

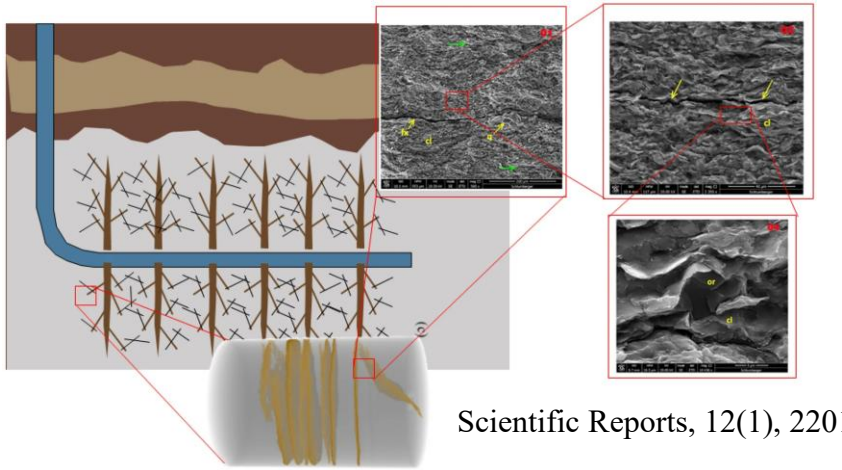


◆ Ordered structure
(adsorption effect)

◆ Heterogeneous distribution

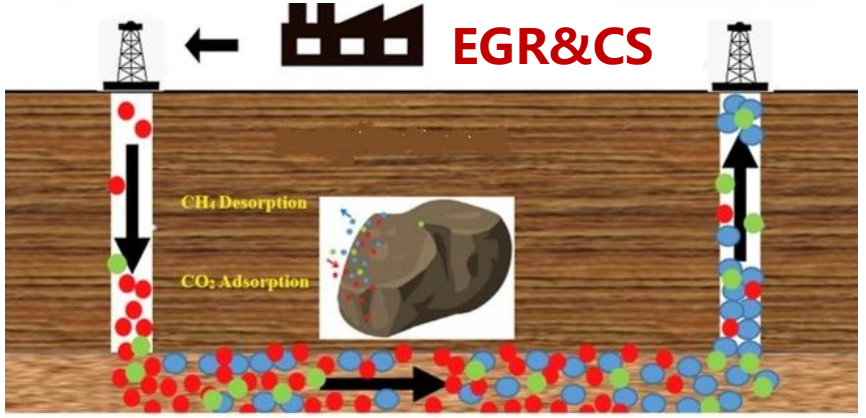
High ratio adsorbed gas leads to low recovery

Hydraulic fracturing (pressure drop)

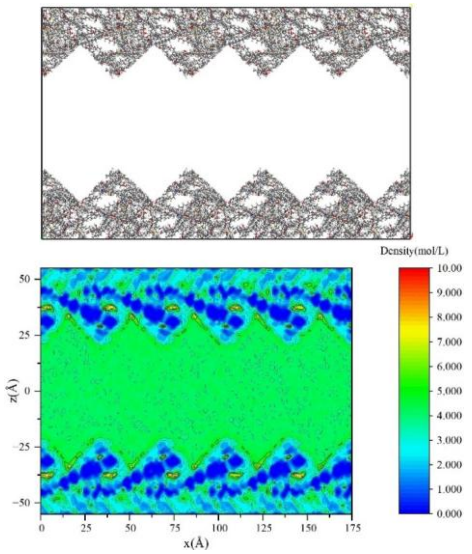


Scientific Reports, 12(1), 22018

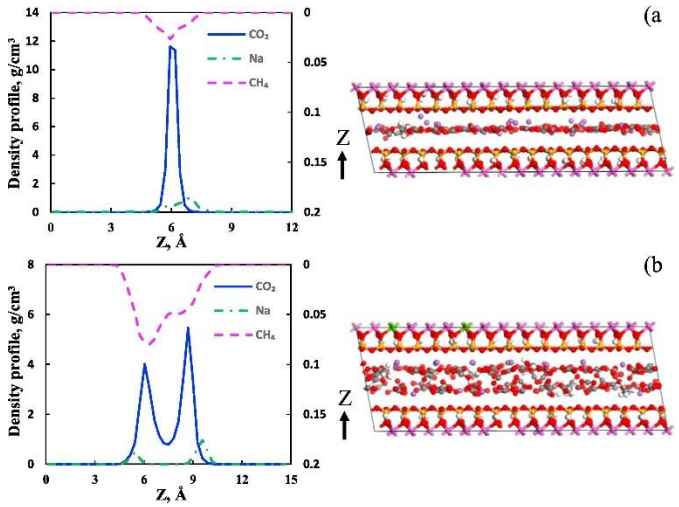
CO_2 injection (competitive adsorption)



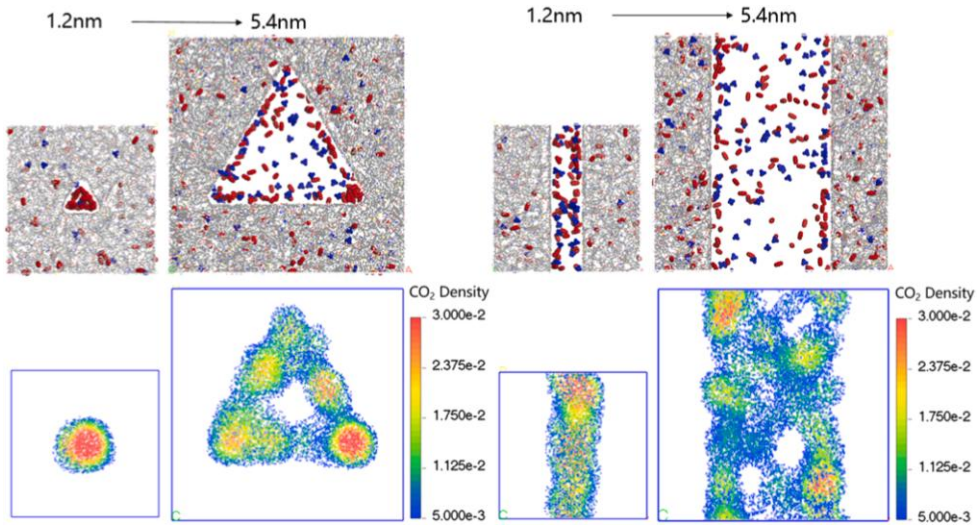
It is urgent to clarify the dynamic mass transfer and recovery mechanism of multi-component shale gas under different development patterns.



CEJ, 2024, 500: 156784



CEJ, 2021, 411: 128423

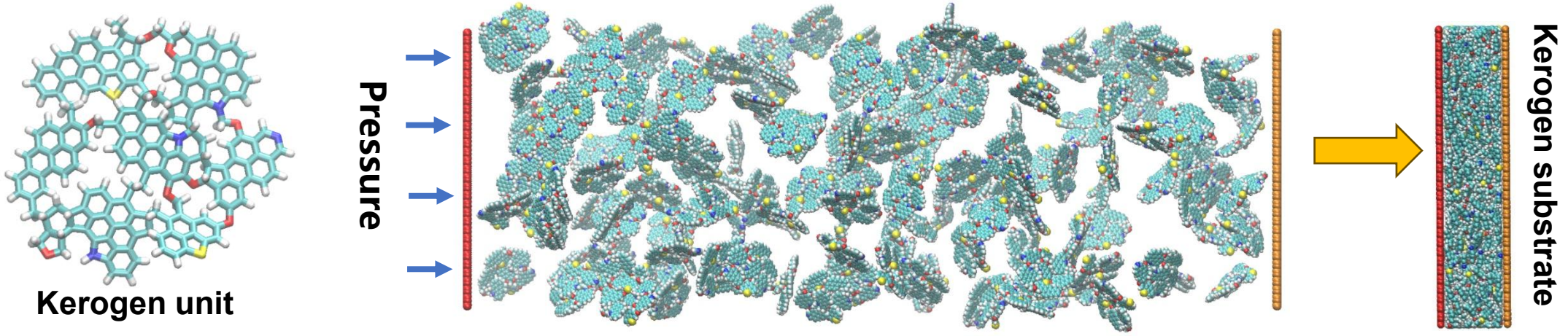


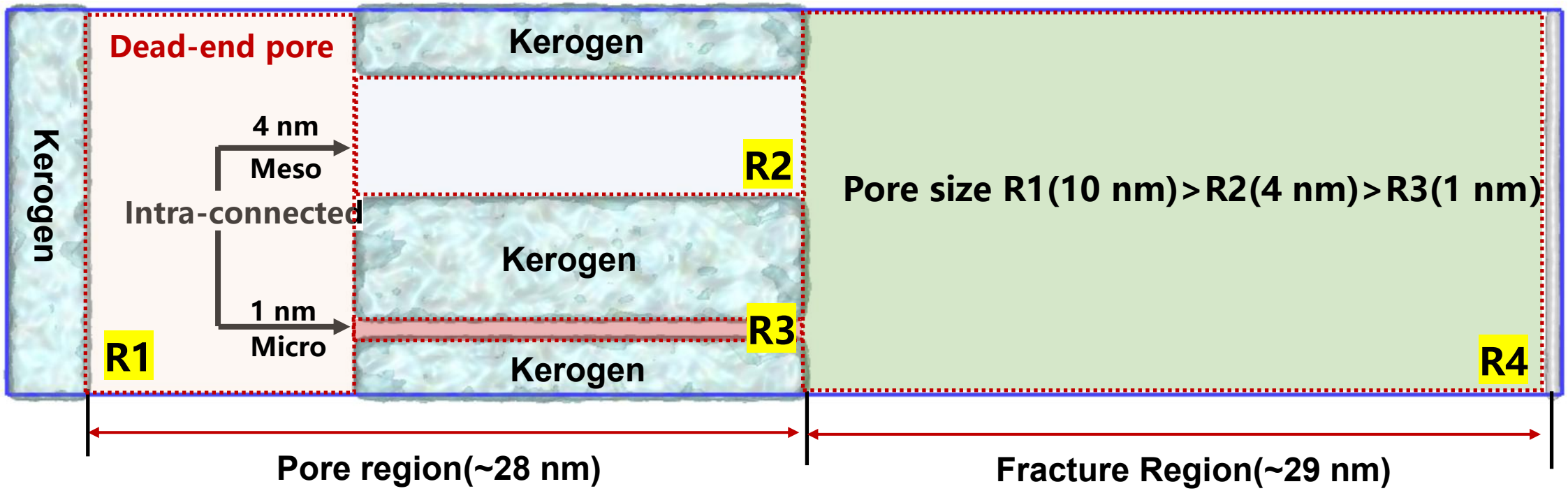
GSE, 2026: 214454

The adsorption behaviors of shale gas and its mixture with CO_2 in various shale nanopores have been extensively explored.

Limitations

- **Focus on the equilibrium state and ignore the dynamic process**
- **Pore is relatively simple without considering pore connectivity**
- **Pure CO_2 injection involves inherent shale gas chemical potential difference**


Kerogen unit
Pressure
Kerogen substrate


Dead-end pore
Kerogen
4 nm
Meso
Intra-connected
1 nm
Micro
Kerogen
R1
R2
R3
R4
Kerogen
Kerogen
Pore size R1(10 nm)>R2(4 nm)>R3(1 nm)
Pore region(~28 nm)
Fracture Region(~29 nm)

Simulation Workflow

Hybrid GCMC+MD

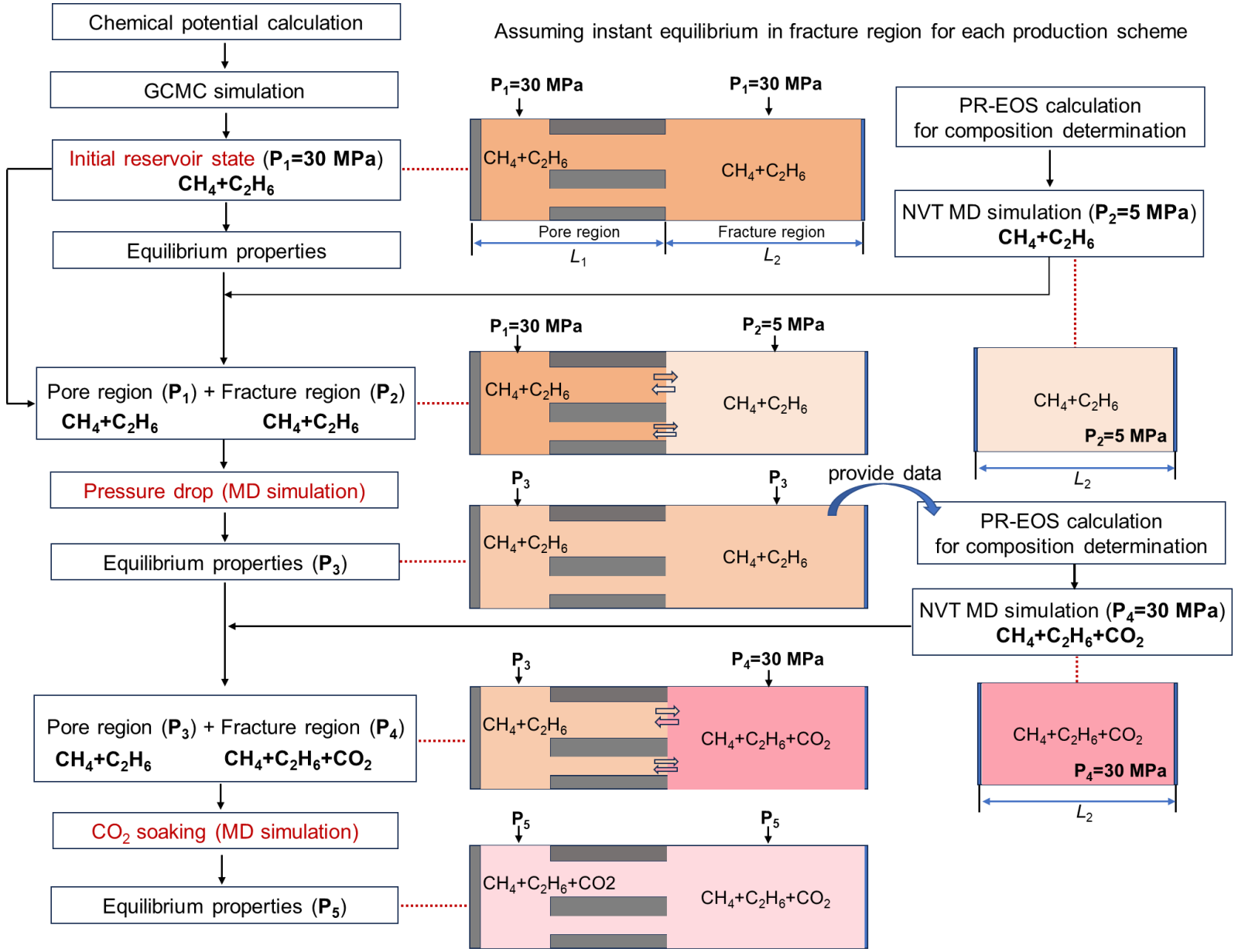
Initial state=30 MPa

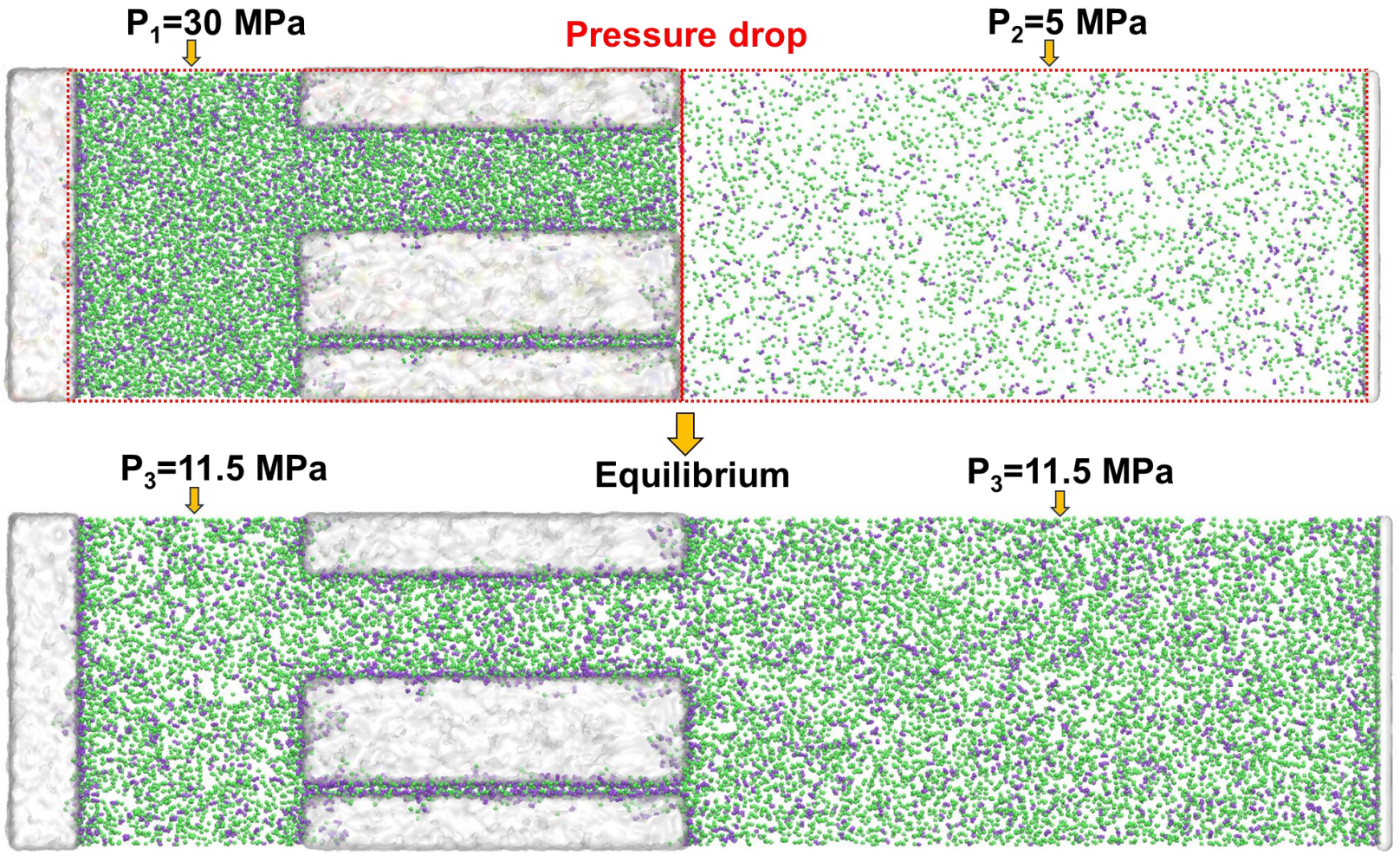
↓

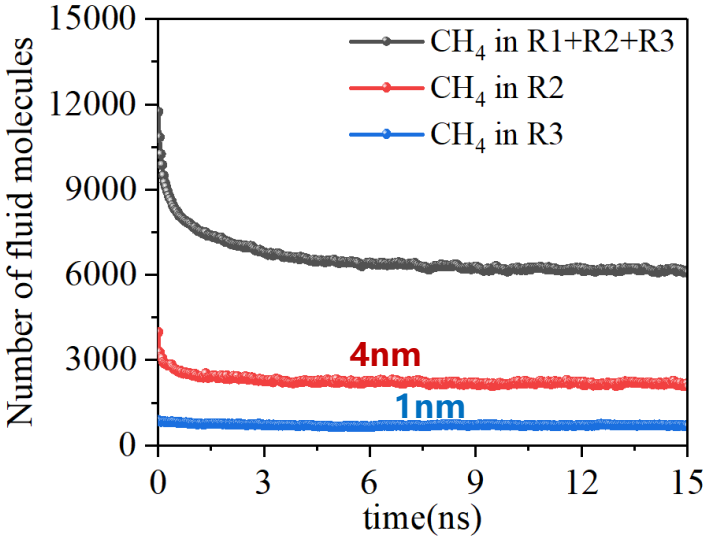
Pressure drop to 5 MPa

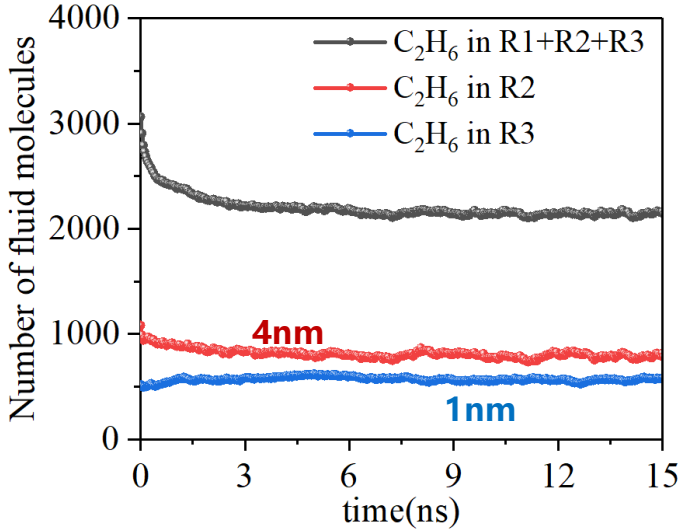
↓

CO_2 soaking=30 MPa





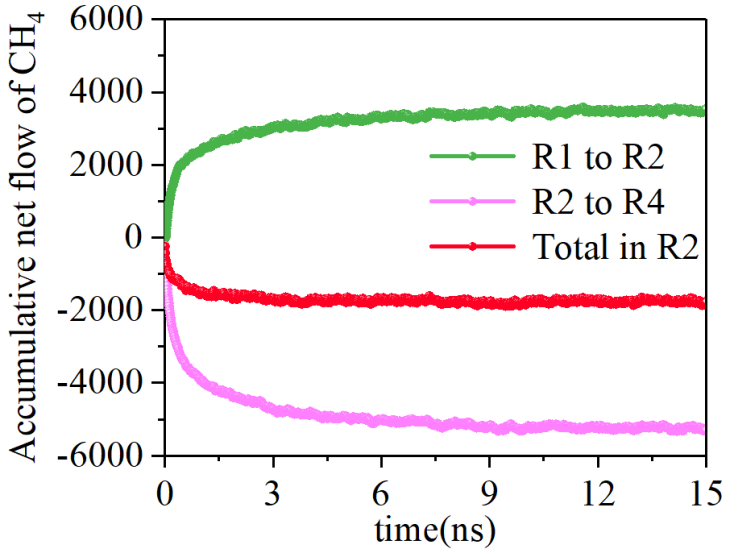




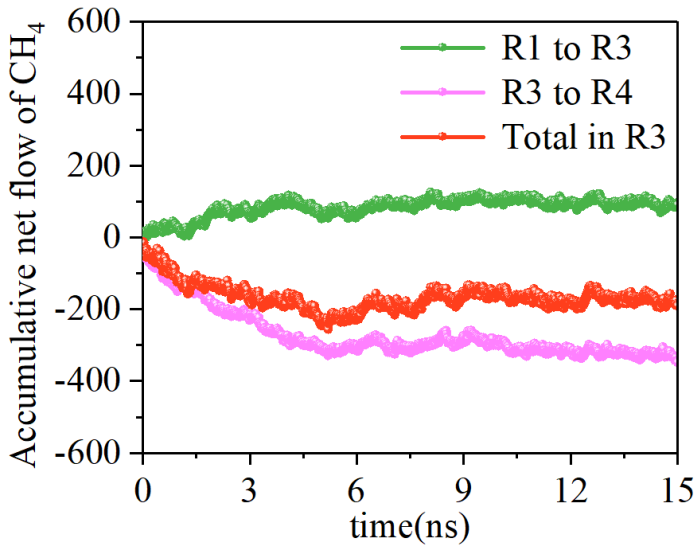
CH_4 : C_2H_6 = 85 : 15

C_2H_6 in micropores (1 nm) gradually increases during pressure drop

CH_4 production dynamics during pressure drop

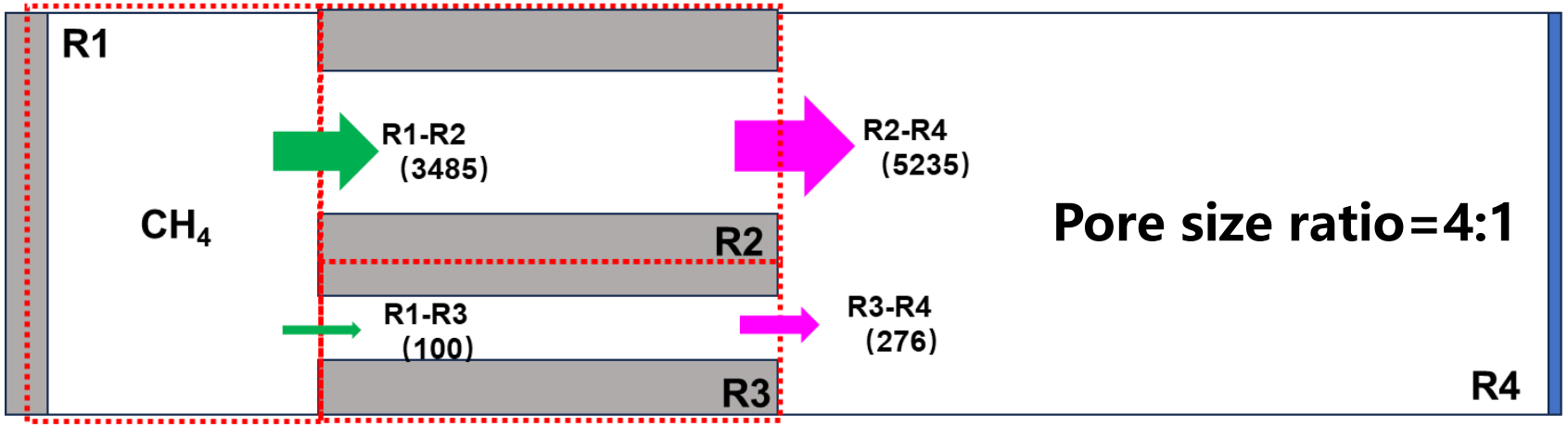


P_1=30 MPa



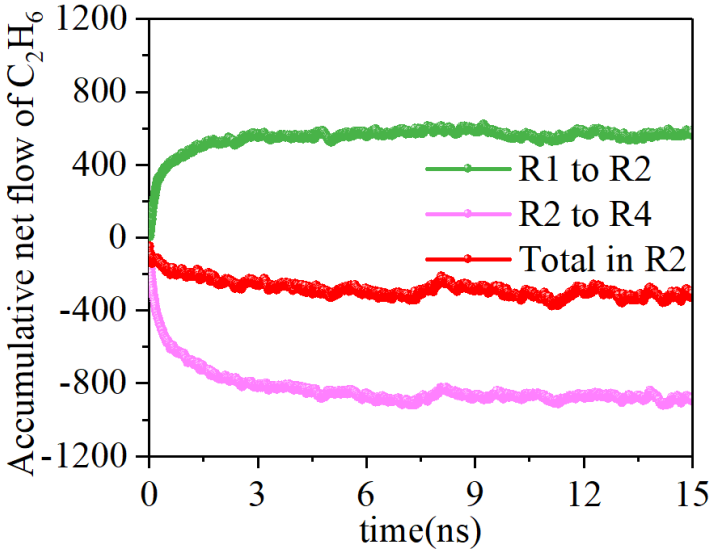
P_1=5 MPa

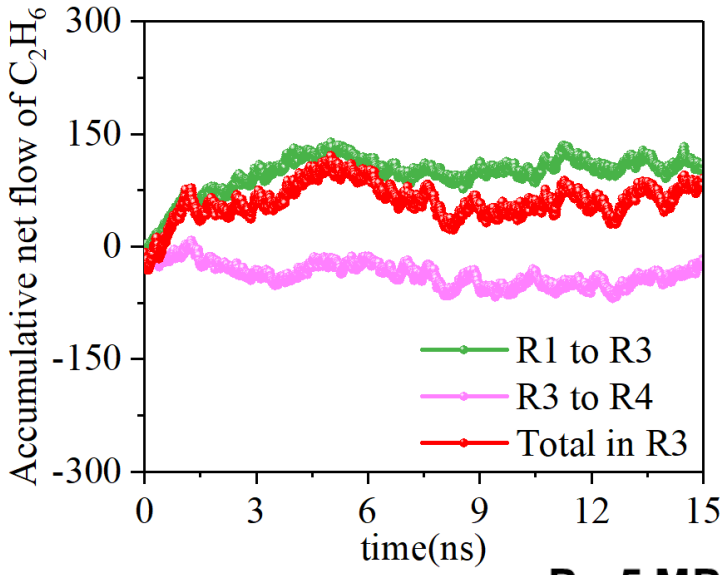
Path	Ratio	Partition Coefficient
R1 - R2	97%	32:1 (Primary)
R1 - R3	3%	
R2 - R4	95%	19:1 (Secondary)
R3 - R4	5%	



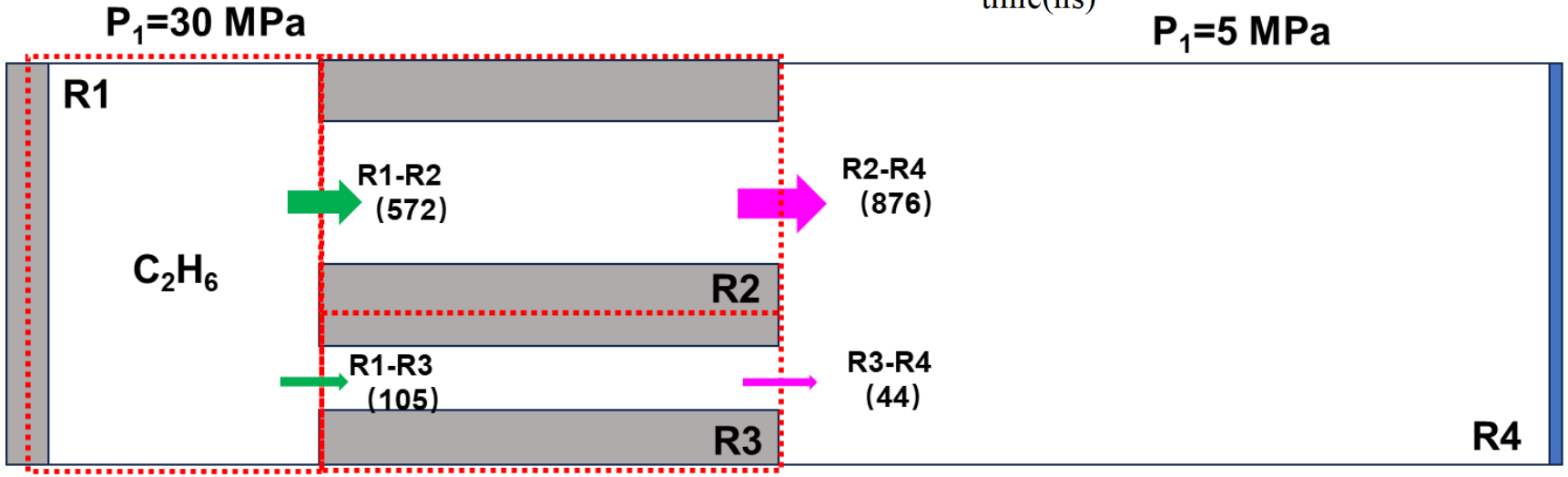
Mesopore is the dominant channel for CH_4 production

C_2H_6 production dynamics during pressure drop

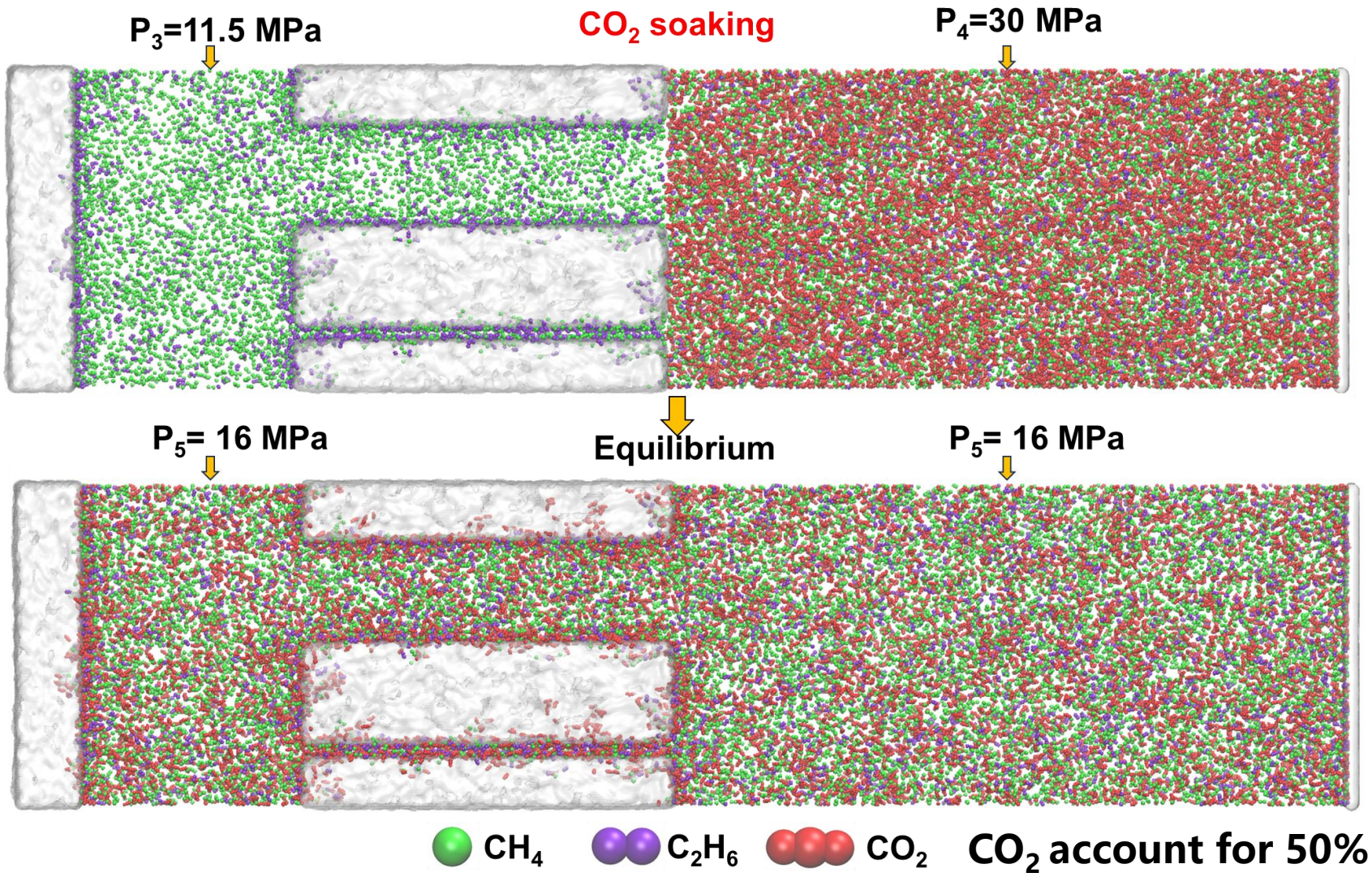


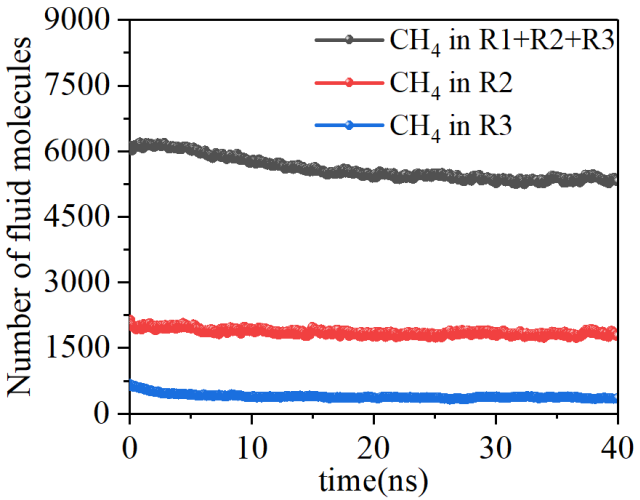


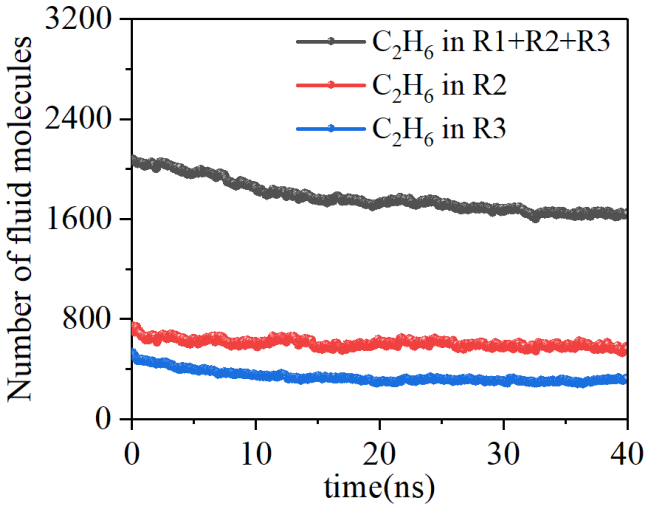
Path	Ratio	Partition Coefficient
R1 - R2	85%	5.6:1 (Primary)
R1 - R3	15%	
R2 - R4	95%	19:1 (Secondary)
R3 - R4	5%	



C_2H_6 accumulate and is trapped in micropores

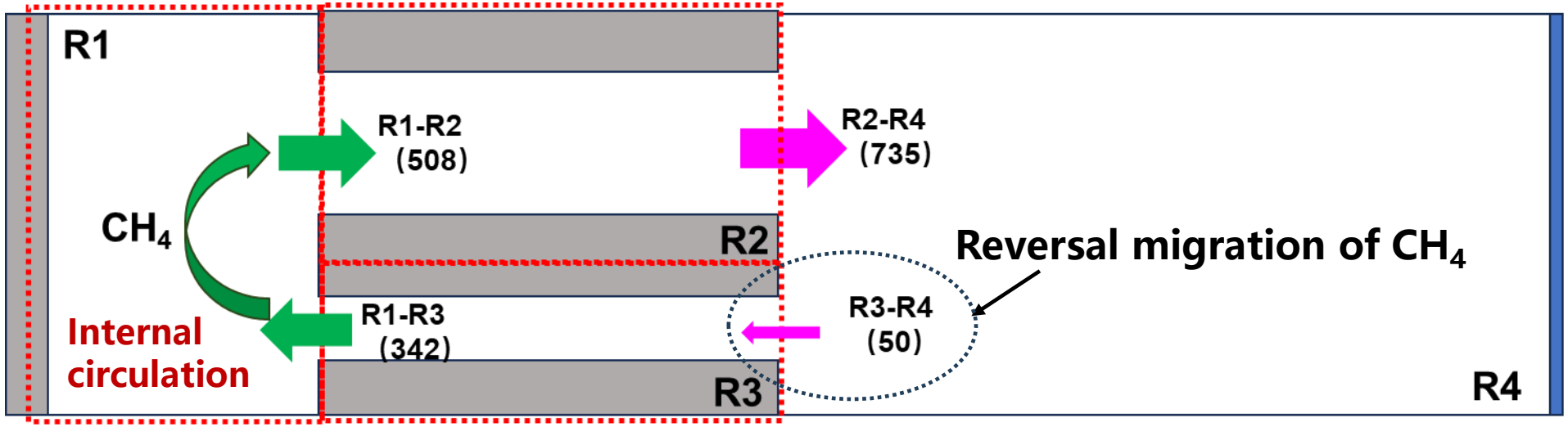




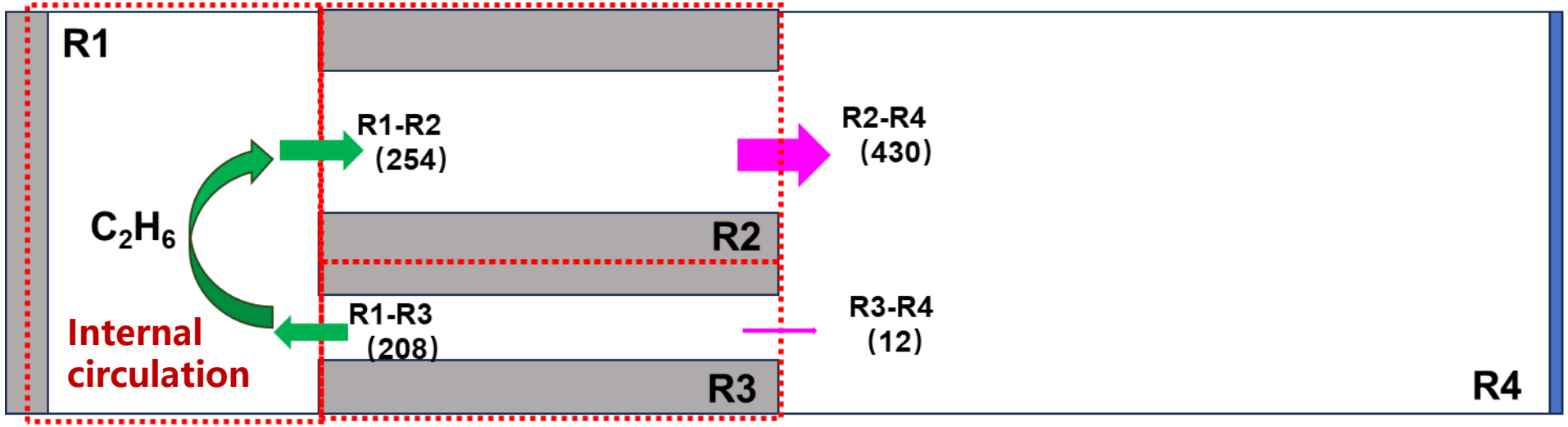


During CO_2 soaking, both CH_4 and C_2H_6 gradually decrease in all regions.

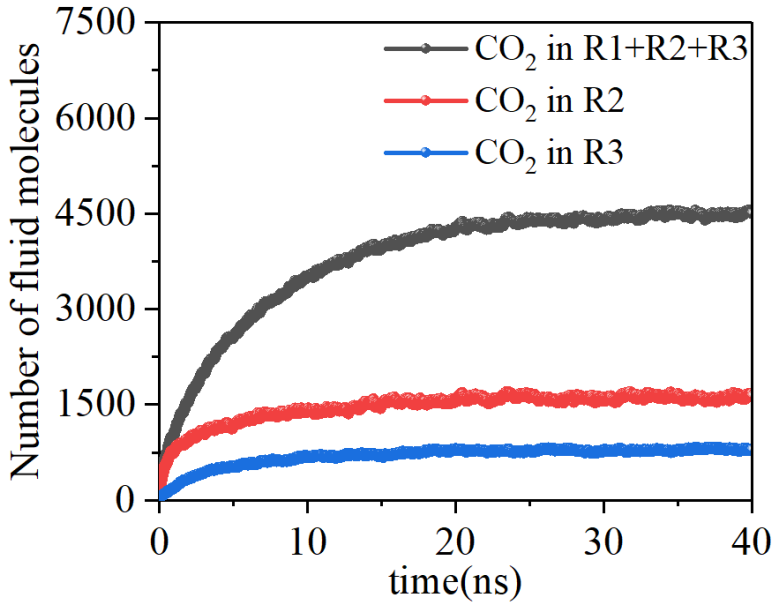
CH_4 and C_2H_6 production dynamics during CO_2 soaking



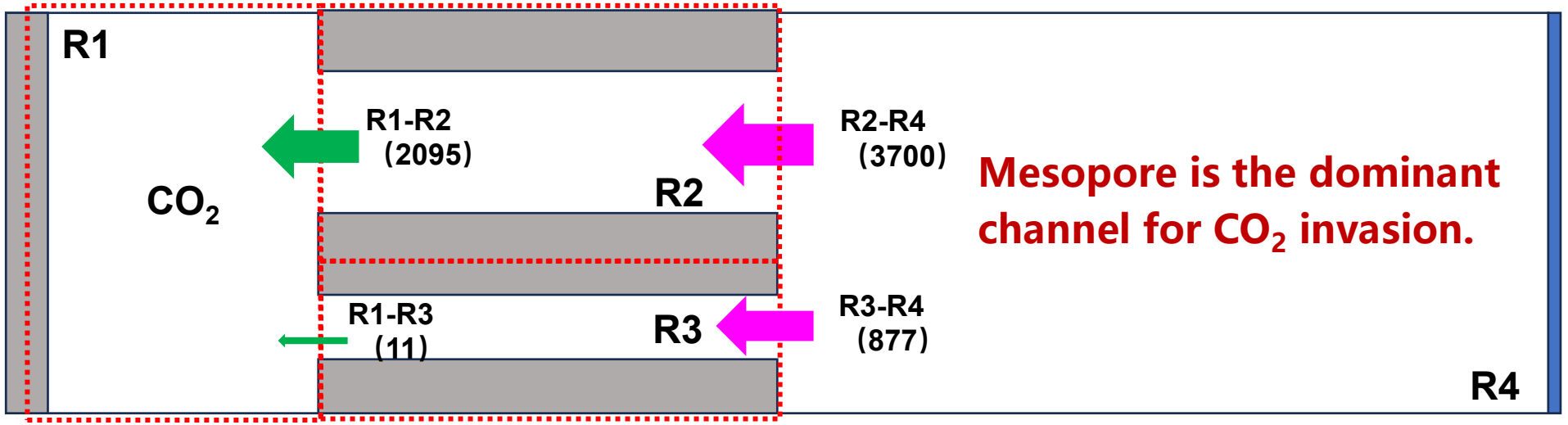
Shale gas in micropores is recovered through mesopores



CO_2 invasion dynamics during CO_2 soaking



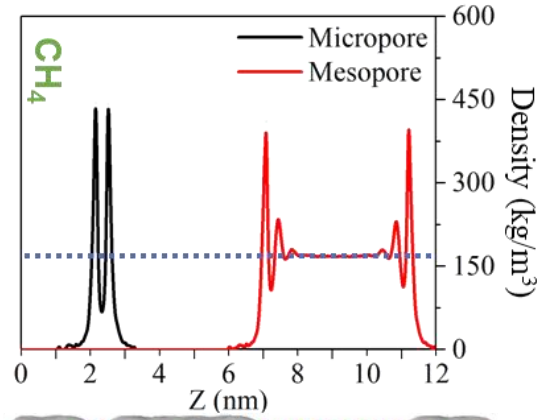
Path	CO_2	Partition Coefficient
R1 - R2	99%	99:1 (Secondary)
R1 - R3	1%	
R2 - R4	81%	4:1 (Primary)
R3 - R4	19%	

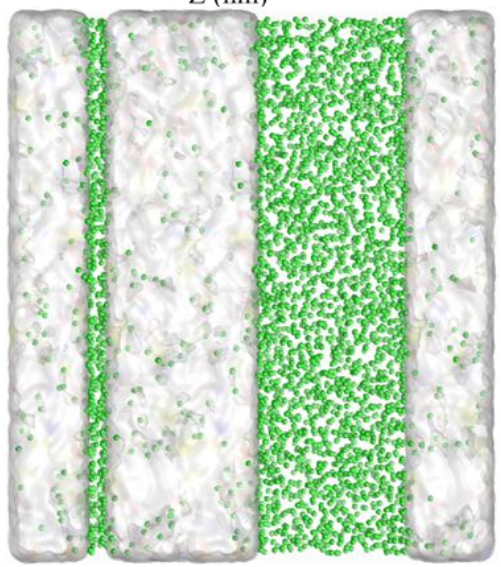


Mesopore is the dominant channel for CO_2 invasion.

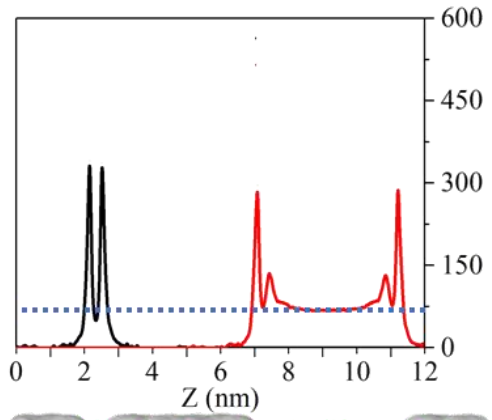
CH_4 distribution at equilibrium

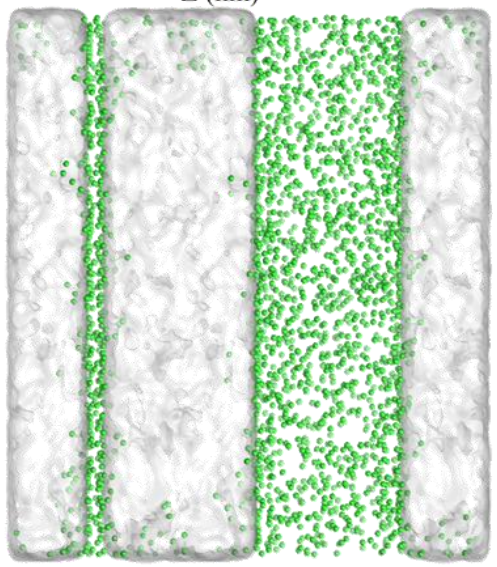
Initial



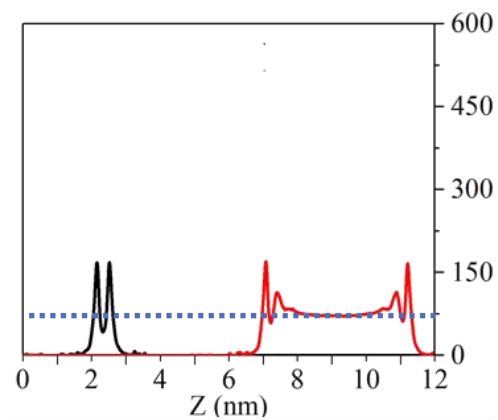


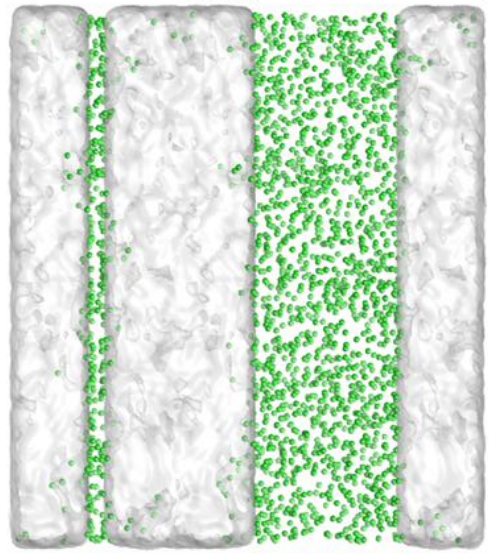
Pressure drop





CO_2 soaking

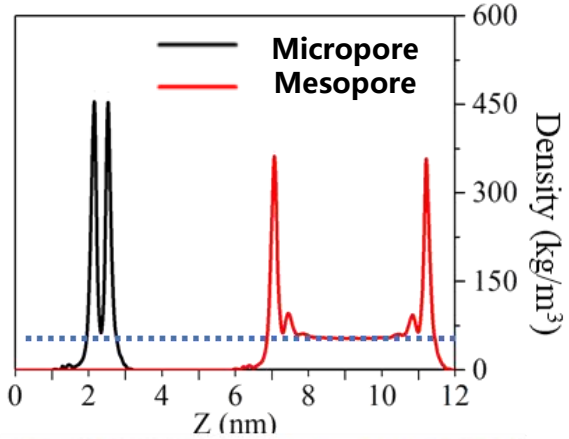


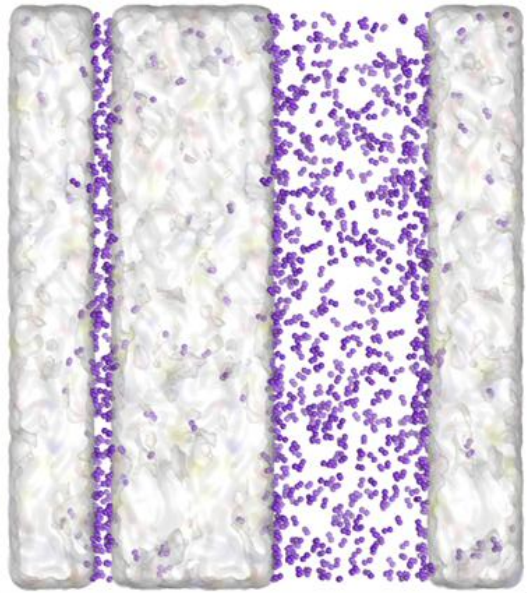


- Both adsorbed and bulk phase is recovered during pressure drop.
- Only adsorbed phase is further recovered during CO_2 soaking.

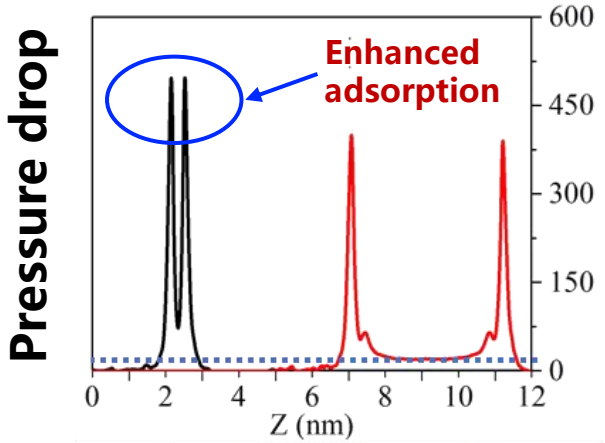
C_2H_6distribution at equilibrium

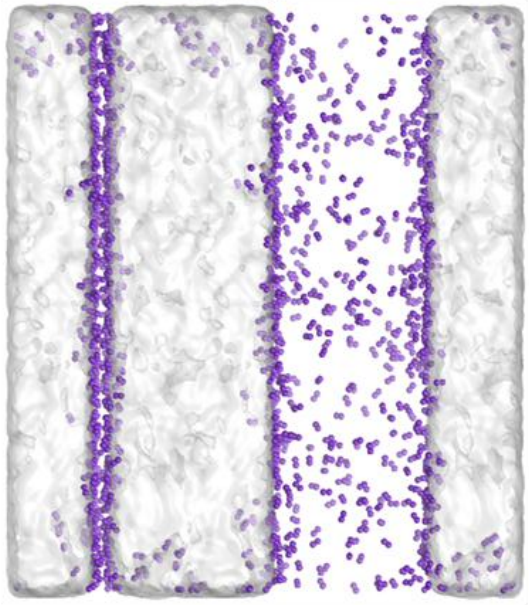
Initial



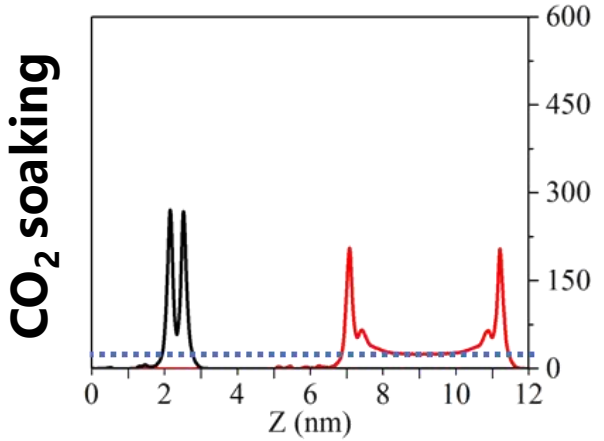


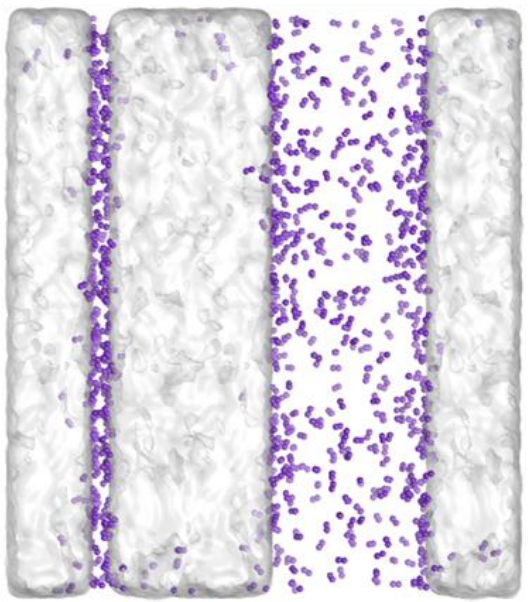
Pressure drop



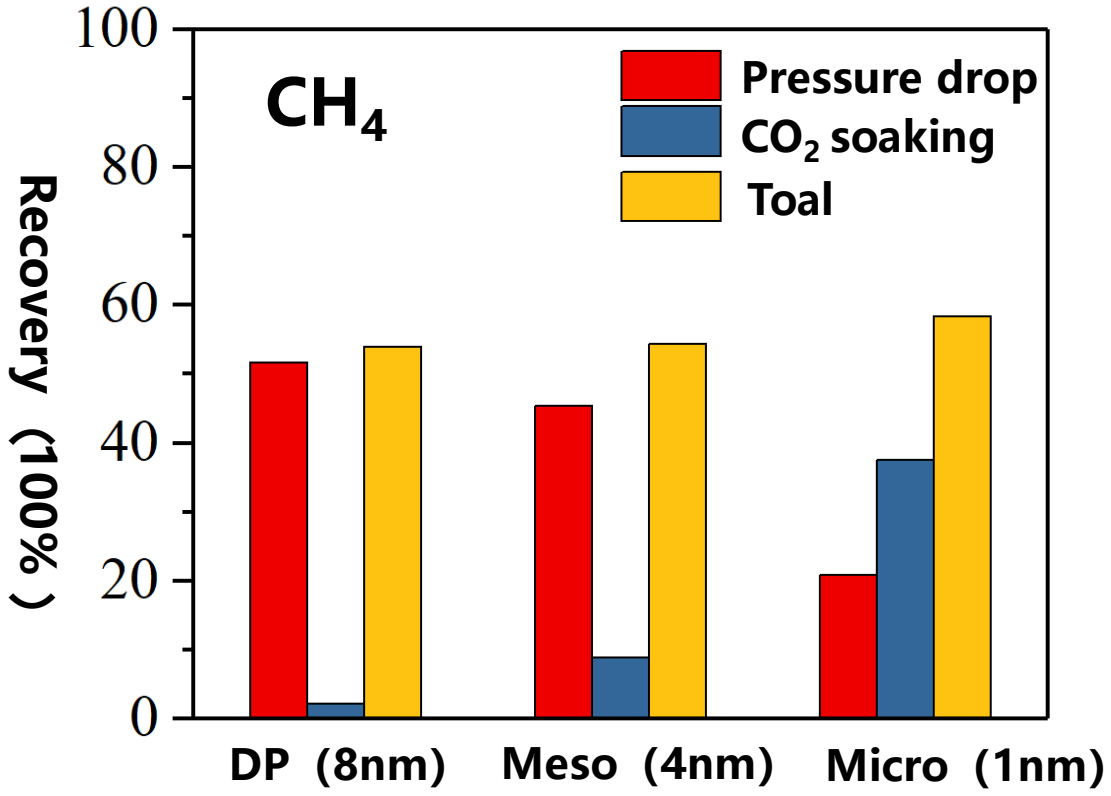


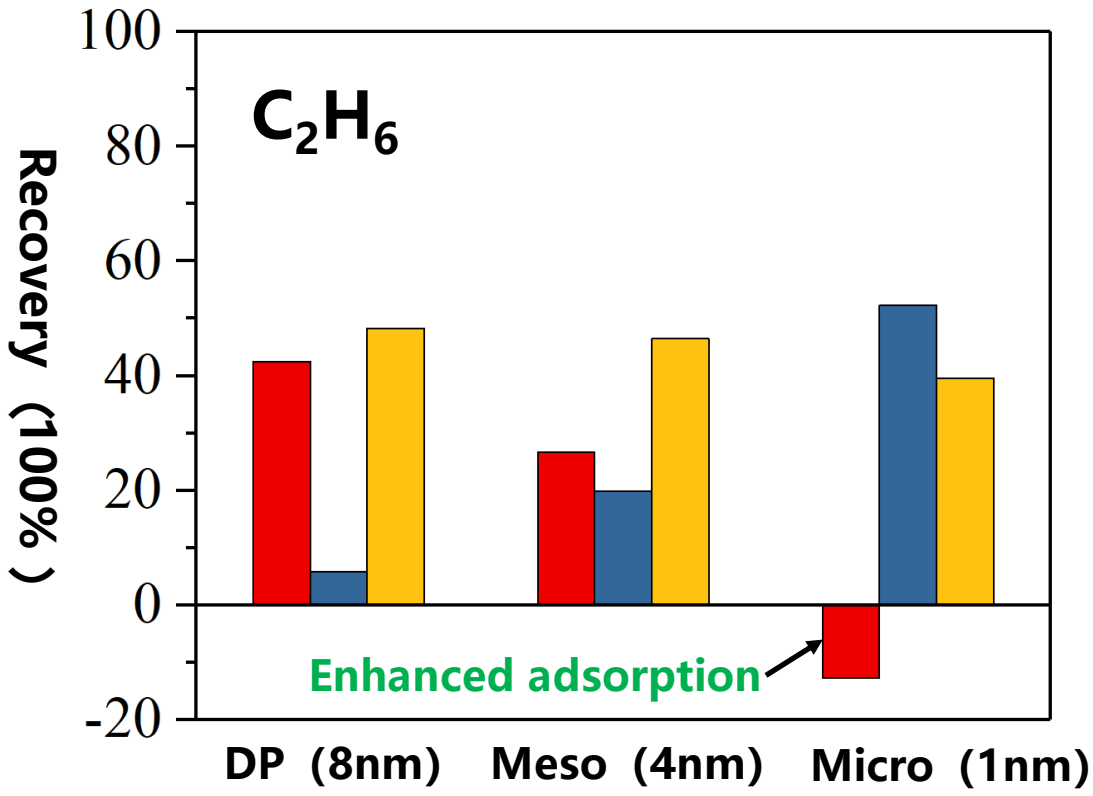
CO_2 soaking





Adsorbed phase can not be recovered during pressure drop





Pressure drop work poorly in small pores especially for heavier gas

CO_2 soaking work poorly for shale gas production in large pores

Conclusions

- Pressure drop is not favorable for C_2H_6 production in micropores
- Shale gas production present different mass transfer pathways during pressure drop and CO_2 soaking
- CO_2 soaking enhances gas recovery mainly by improving the mobilization degree of adsorbed phase.
- Smaller pore sizes and heavier gas component contribute to superior recovery efficiency during CO_2 soaking.

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ISSN: 2207-9963 e-ISSN: 2208-598X

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