Supporting Information

Simultaneous Evaluation of Reaction and Diffusion over Molecular Sieve for Shape Selective Catalysis

Jingfeng Han^a, Zhiqiang Liu^b, Hua Li^a, Jiawei Zhong^{a,c}, Wenna Zhang^a, Jindou

Huang^a, Anmin Zheng^b, Yingxu Wei^{a,*}, and Zhongmin Liu^{a,d*}

a National Engineering Laboratory for Methanol to Olefins, State Energy Low Carbon Catalysis and Engineering R&D Center, Dalian National Laboratory for Clean Energy, iChEM (Collaborative Innovation Center of Chemistry for Energy Materials), Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning, China b State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, National Center for Magnetic Resonance in Wuhan, Key Laboratory of Magnetic Resonance in Biological Systems, Wuhan Institute of Physics and Mathematics, Innovation Academy for Precision Measurement Science and Technology, Chinese Academy of Sciences, Wuhan 430071, P.R. China

c University of Chinese Academy of Sciences, Beijing 100049, China

d State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning, China

*E-mail: liuzm@dicp.ac.cn (Z. L.), weiyx@dicp.ac.cn (Y. W.),



Scheme S1. Homemade setup for combined MTO reaction and diffusion evaluation and the feeding procedure of methanol and the probe molecules onto working catalyst bed to conduct catalytic reaction and diffusion measurement. Catalyst: 60-80 mesh pellets fixed by quartz cotton, bed length: 4 mm, bed inner diameter: 4 mm.

TOS(min)	3	30	60	90	120	150	180	210
Con.(%)	99.9	100.	100.	99.9	98.4	47.9	3.37	2.49
CH4	1.12	2.34	3.21	3.54	3.87	7.31	60.5	69.7
C ₂ H ₄	37.3	50.6	51.8	52.5	52.7	55.7	26.3	17.9
C ₂ H ₆	0.35	0.46	0.55	0.49	0.50	0.81	4.35	4.81
C3H6	41.9	32.9	30.7	29.5	28.4	25.3	6.94	5.50
C ₃ H ₈	2.23	1.09	1.01	0.94	0.85	0.96	0.41	0.50
C4 ⁺	16.9	12.5	12.6	12.8	13.5	9.80	1.46	1.40
C ₃ =/C ₂ =	1.12	0.64	0.59	0.56	0.53	0.45	0.26	0.30
HTI	0.05	0.03	0.03	0.03	0.03	0.03	0.05	0.09

 Table S1. Product distribution of MTO reaction over SAPO-34.

The hydrogen transfer index (HTI) is calculated as the propane selectivity divided by propene selectivity.



Figure S1. Comparison of continuous-flow MTO reaction (a) and MTO

reaction with interval alkane pulsing for diffusion measurement (b)



Figure S2. The splitting of E(t)-curves of C₂H₆ diffusion through the fresh
(a), methanol-reacted catalyst bed after reaction for 30 min (b), 60 min (c), 90 min (d), 120 min (e), 150 min (f), 180 min (g) and 210 min (h).



Figure S3. The splitting of E(t)-curves of C₃H₈ diffusion through the fresh
(a), methanol-reacted for 30 min (b), 60 min (c), 90 min (d), 120 min (e), 150 min (f), 180 min (g) and 210 min (h) catalyst bed.