Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Table S1 Experimental results of MTA reaction kinetics

T/K	τ/h	w(Methanol and DME)	w(Alkane and Olefin)	w(Aromatics (except PX))	w(PX)
	0.1	0.4009	0.0862	0.0898	0.4231
	0.15	0.2593	0.1106	0.0965	0.5336
623.15	0.2	0.1530	0.1278	0.1024	0.6167
	0.25	0.1158	0.1338	0.1212	0.6292
	0.3	0.0083	0.0886	0.1548	0.7483
	0.1	0.3949	0.0794	0.0830	0.4426
	0.15	0.2187	0.0463	0.1059	0.6291
648.15	0.2	0.0833	0.0536	0.1401	0.7231
	0.25	0.0321	0.0770	0.1881	0.7029
	0.3	0.0031	0.0675	0.2168	0.7126
	0.1	0.4609	0.0388	0.1038	0.3966
	0.15	0.0889	0.1016	0.1248	0.6847
673.15	0.2	0.0739	0.0443	0.1390	0.7428
	0.25	0.0419	0.1023	0.1440	0.7118
	0.3	0.0189	0.0375	0.1553	0.7884
	0.1	0.6739	0.0452	0.0556	0.2253
	0.15	0.3339	0.0744	0.1175	0.4743
698.15	0.2	0.2260	0.0857	0.1344	0.5539
	0.25	0.1173	0.0748	0.1658	0.6420
	0.3	0.0480	0.0413	0.1784	0.7323
	0.1	0.4053	0.0542	0.1064	0.4341
	0.15	0.2266	0.1082	0.1293	0.5358
748.15	0.2	0.0078	0.0581	0.1476	0.7865
	0.25	0.0565	0.0863	0.2664	0.5907
	0.3	0.0016	0.0310	0.2225	0.7449

Mass Transfer Calculations for aromatization of methanol upon 3Zn-3Si /ZSM-5 catalyst at 425 °C（0.3 h）

For reaction mode relative to methanol

If $\frac{-r_A^{'}\rho_b Rn}{k_c C_{Ab}}$ <0.15, then external mass transfer effects can be neglected.

$-r_A'$ = reaction rate, kmol/kg-cat · s = 2.89×10^{-05}

n = reaction order = 2

R = catalyst particle radius, m = 4.5×10^{-5}

ρ_b = bulk density of catalyst bed, kg/m^3 = 950

ρ_c = solid catalyst density, kg/m^3 = 2.6×10^3

C_{Ab} = bulk gas concentration of A, kmol/m^3 = 2.59×10^{-2}

k_c = mass transfer coefficient, m/s = 0.066 m/s

$\frac{-r_A'\rho_b Rn}{k_c C_{Ab}}$ = [2.89×10^{-05} kmol /kg-cat.s] [950 kg/m^3][4.5×10^{-5} m][2]/([0.066 m/s] × [2.59×10^{-02} kmol/m^3])= **$1.45 \times 10^{-3} < 0.15$ {Mears for External Diffusion}**

Weisz-Prater Criterion for Internal Diffusion

If $\frac{-r_{A(obs)}^{'}\rho_c R^2}{D_e C_{As}}$ **<1, then internal mass transfer effects can be neglected.**

-r'$_{A(obs)}$ = observed reaction rate, kmol/kg-cat · s

R = catalyst particle radius, m

ρ_c = solid catalyst density, kg/m^3;

D_e = effective gas-phase diffusivity, m^2/s

C_{As} = gas concentration of A at the catalyst surface, kmol-A/m^3

$\frac{-r_{A(obs)}^{'}\rho_c R^2}{D_e C_{As}}$ = [2.89×10^{-05} kmol/kg-cat.s] × [2600 kg-cat/m^3] × [4.5×10^{-5} m]^2 / ([2.91×10^{-5} m^2/s] × [2.59×10^{-2} kmol/m^3]) = **$2.02 \times 10^{-4} < 1$**

{Weisz-Prater Criterion for Internal Diffusion}