

Supplementary material

New insights into synthesis of aromatics from syngas over hybrid FeMn Fischer-Tropsch catalyst and HZSM-5 zeolite: local environment effect and mechanism-directed tuning in the aromatic selectivity

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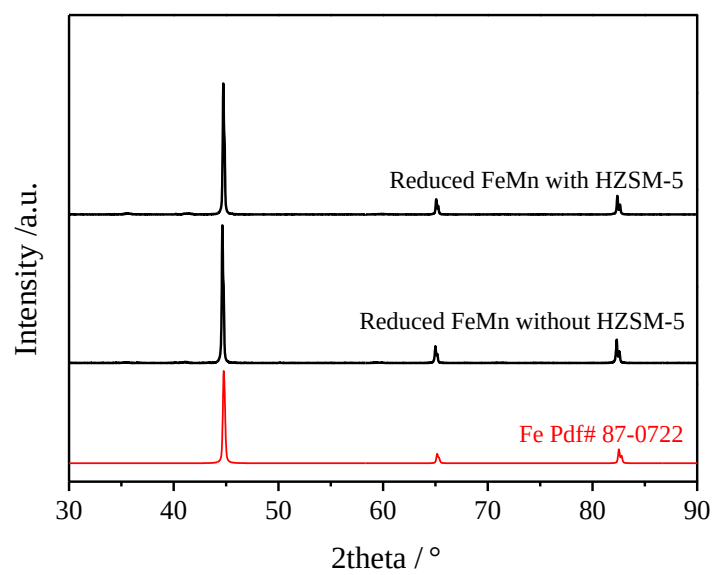


Fig. S1. XRD patterns of reduced FeMn catalyst samples with and without HZSM-5 zeolite at 450 °C for 3 h.

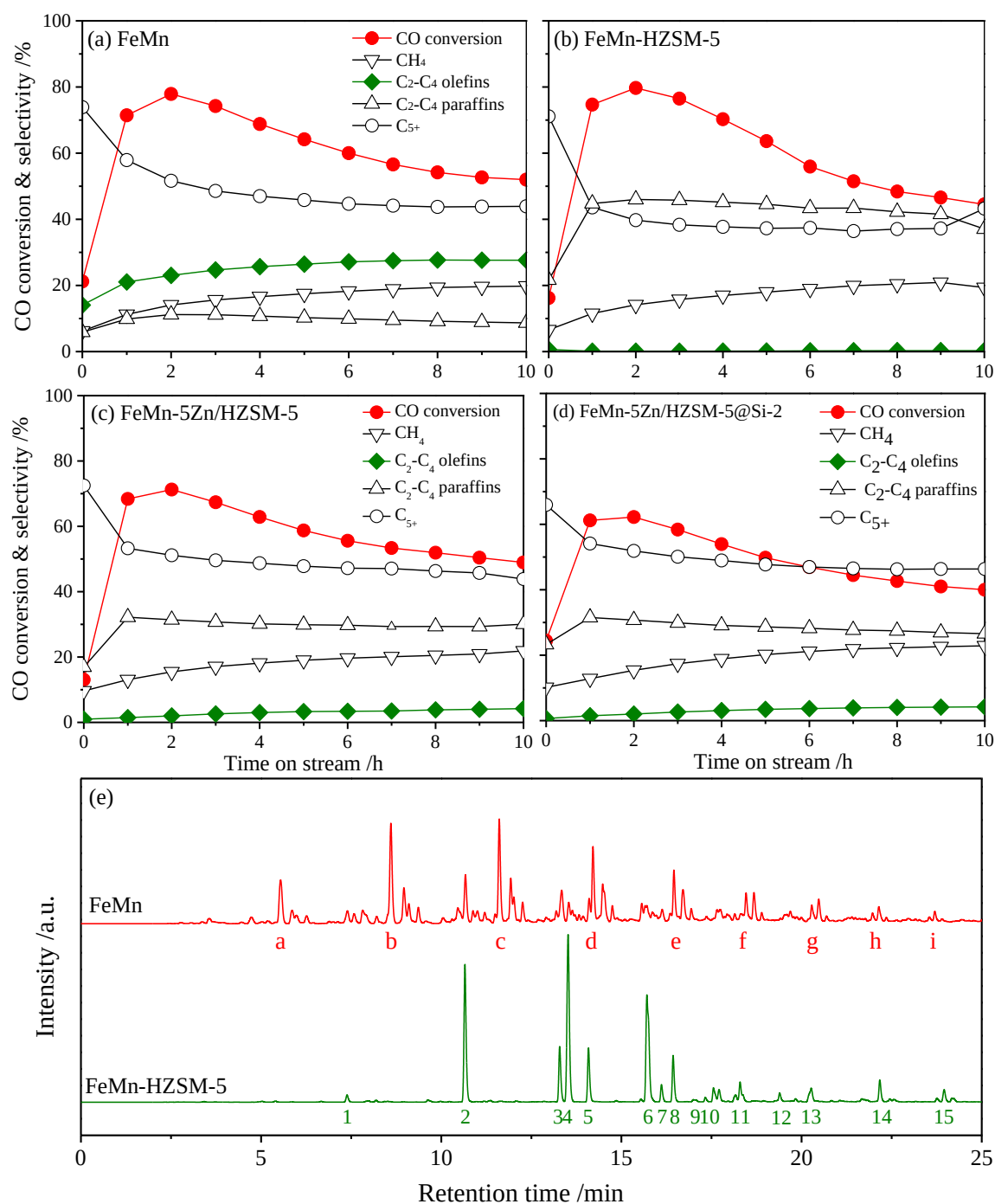


Fig. S2. (a)-(d) Time-dependences of CO conversion and the selectivities to hydrocarbons over selected catalysts at 320 °C, 1.0 MPa and 3600 mL/g/h; (e) GC spectra of liquid phases collected after tests (a) and (b). The peaks of a-i correspond to C₆-C₁₄ α-olefins, respectively, and the numbers 1-16 represent aromatics: 1) benzene; 2) toluene; 3) ethylbenzene; 4) *p*- and *m*-xylene; 5) *o*-xylene; 6) *p*- and *m*-ethyltoluene; 7) *o*-ethyltoluene; 8) 1,2,4-trimethylbenzene; 9) 1-isopropyl-2-methylbenzene; 10) *m*-diethylbenzene; 11) 1,3-dimethyl-5-ethyl-benzene; 12) *p*-diethylbenzene; 13) naphthalene; 14-15) naphthalene derivatives. The unlabeled peaks are assigned to normal, isomeric and cyclized paraffins.

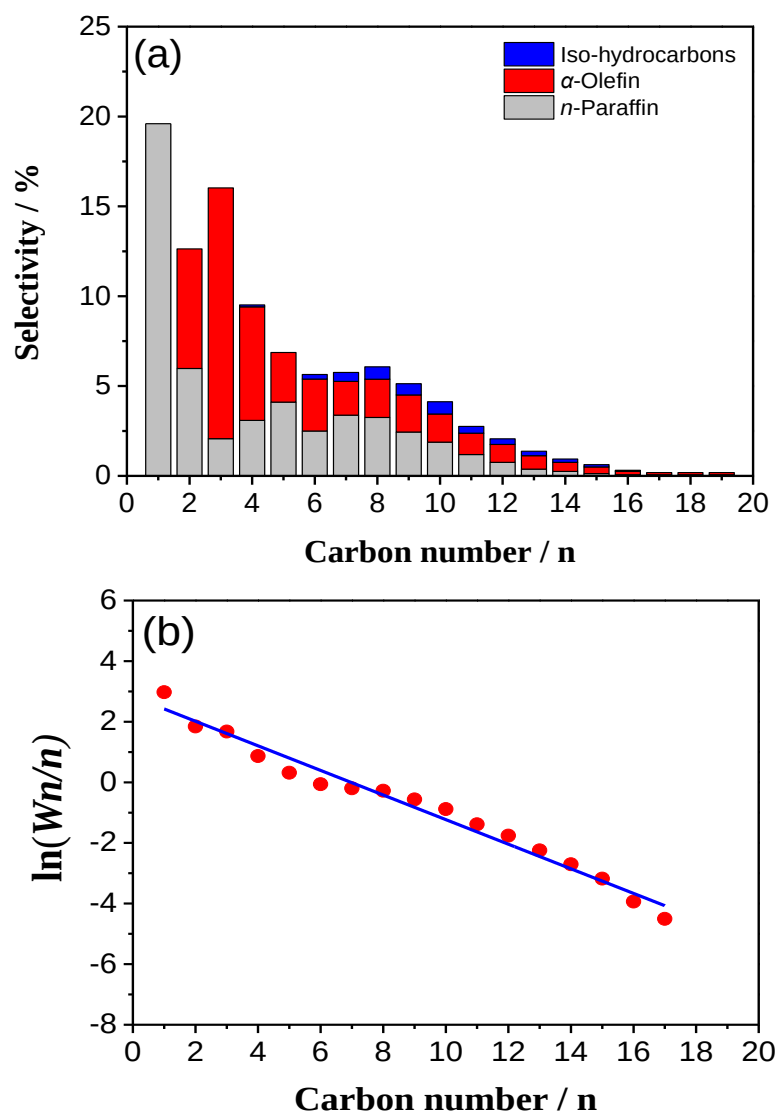


Fig. S3. The carbon number distribution of FTS products and the corresponding ASF plot over the FeMn catalyst under the conditions of 320°C, 1 MPa and 3600 mL/g/h.

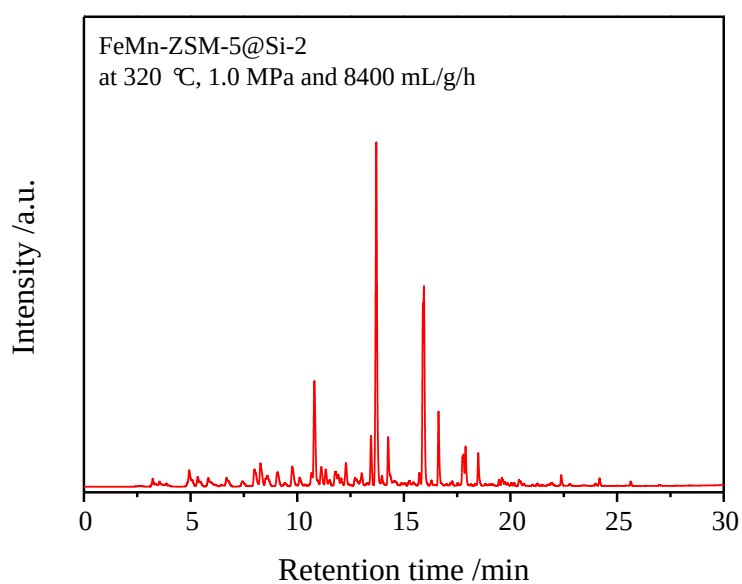


Fig. S4. GC spectrum of the liquid hydrocarbons obtained over FeMn-HZSM-5@Si-2 catalyst system at 320 °C, 1.0 MPa and 8400 mL/g/h.

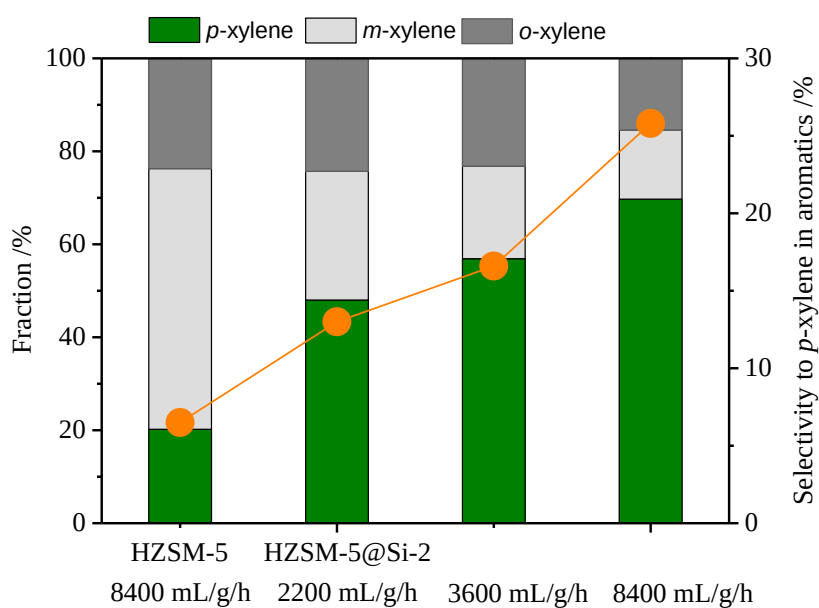


Fig. S5. The fractions of *p*-, *m*- and *o*-xylene in total xylene (bar) and the selectivity to *p*-xylene in total aromatics (point) obtained over FeMn-HZSM-5 and FeMn-HZSM-5@Si-2 catalyst systems at 320 °C, 1.0 MPa and various space velocities (2200-8400 mL/g/h).

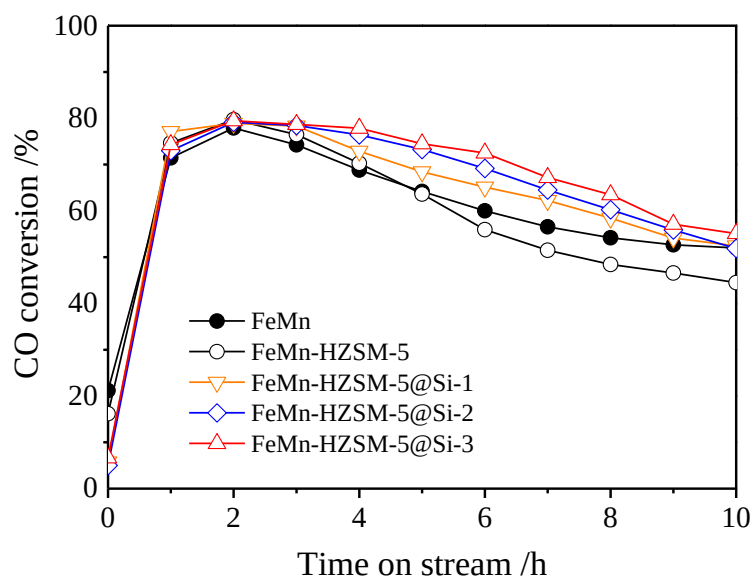


Fig. S6. Time-dependences of CO conversion over various catalysts at 320 °C, 1.0 MPa and 3600 mL/g/h.

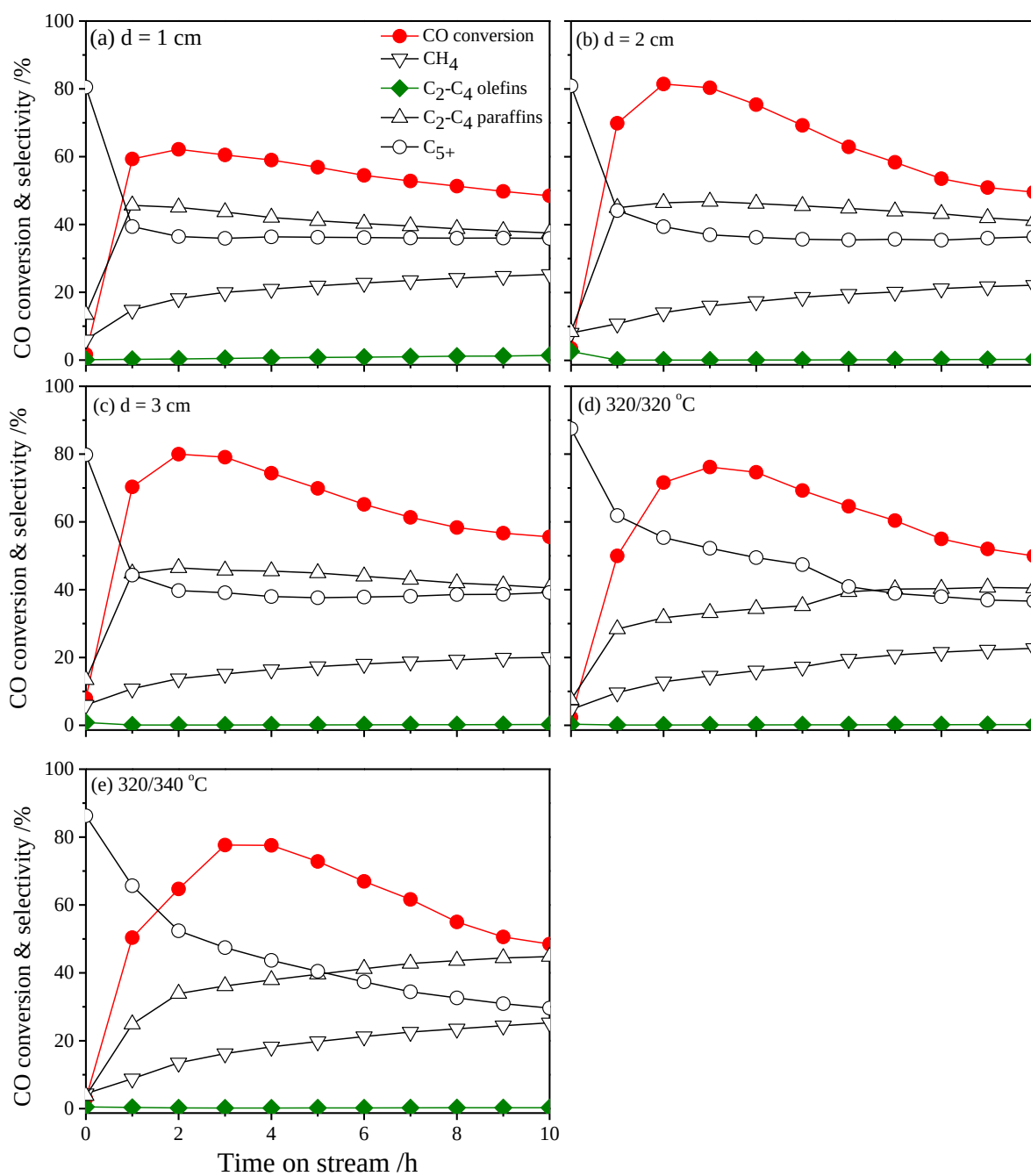


Fig. S7. Time-dependences of CO conversion and the selectivities to hydrocarbons over FeMn-HZSM-5 catalyst system layering in one reactor and two tandem reactors.

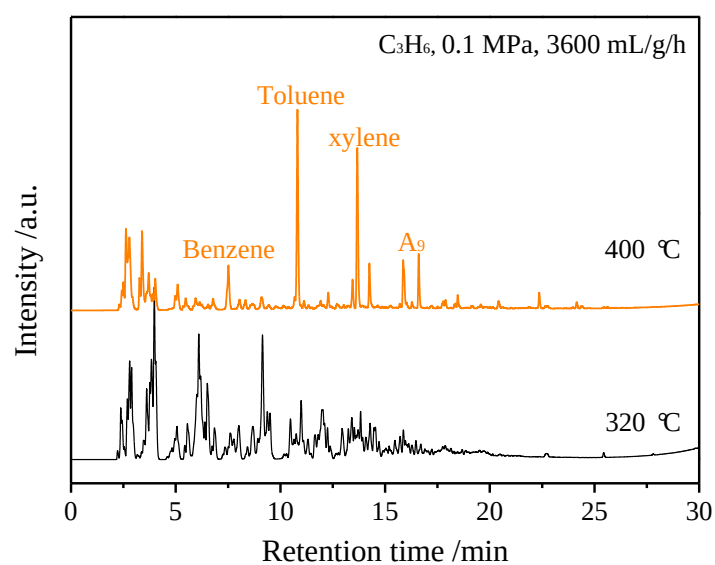


Fig. S8. GC spectra of the liquid products obtained from model reaction with propylene in N₂ over HZSM-5 at 320 °C and 400 °C.

Table S1. Conversion and selectivity to hydrocarbons in the model reactions over HZSM-5 (Si/Al = 12.5) zeolite.

Feed	Temp.	P	Conv.	Selectivity /%											
	/°C	/MPa	/%	CH ₄	C ₂ ⁼	C ₂ ^o	C ₃ ⁼	C ₃ ^o	C ₄ ⁼	<i>n</i> -C ₄ ^o	<i>i</i> -C ₄ ^o	C ₅₋₆ ⁼	<i>n</i> -C ₅₋₆ ^o	<i>i</i> -C ₅₋₆ ^o	Liquids
20%C ₂ H ₄ in CO/H ₂ ^{a)}	320	1.0	84.4	0.7	–	44.1	2.6	4.0	3.9	3.2	3.3	1.4	3.7	2.2	30.9
20%C ₂ H ₄ in N ₂	320	1.0	55.1	0.2	–	1.2	6.3	4.0	10.0	5.8	5.3	3.6	8.7	3.1	51.8
20%C ₂ H ₄ in CO/H ₂	450	1.0	99.8	10.2	–	55.5	0.2	20.0	0	1.2	1.2	0	0.1	0.1	11.5
20%C ₂ H ₄ in N ₂	450	1.0	81.7	3.6	–	10.7	5.7	39.9	3.4	5.8	6.8	0.9	1.9	1.7	19.6

^{a)} CO/H₂ = 1:1 in molar ratio.