Supplementary Information

Kinetics and reactor modeling of the conversion of n-pentane using HZSM-5 catalysts with different Si/Al ratio

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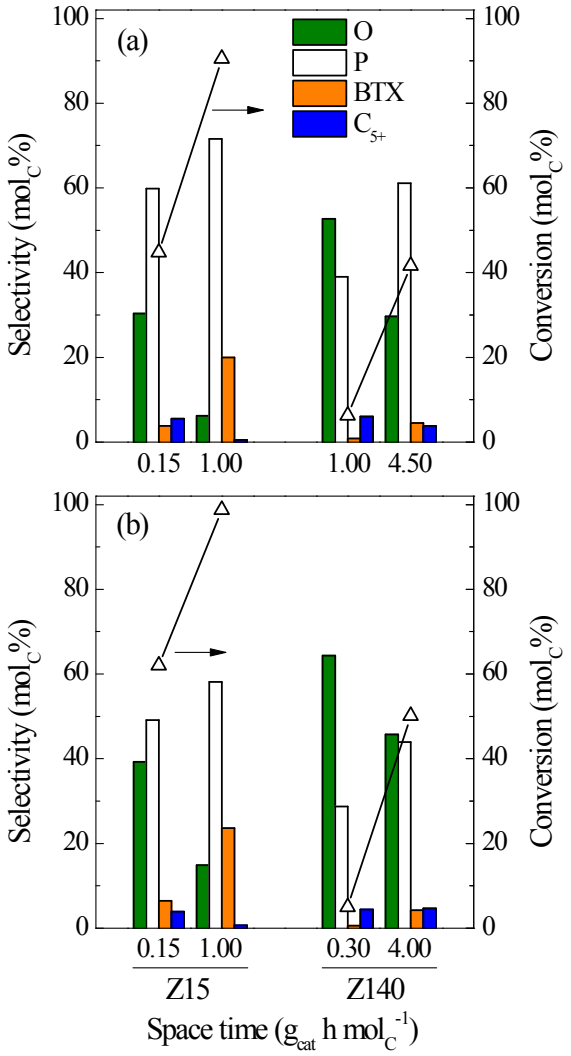

Fig. S1. Conversion and selectivity with Z15 and Z140 catalysts using different values of space time at (a) 500 ºC and (b) 550 ºC.

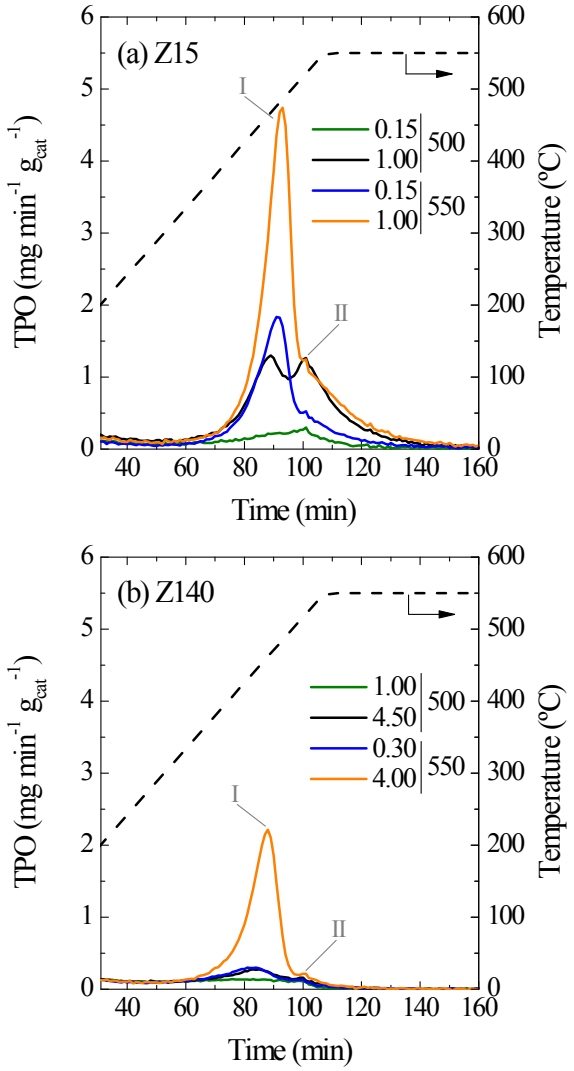

Fig. S2. TPO profile of (a) Z15 and (b) Z140 catalysts used at 500 and 550 ºC

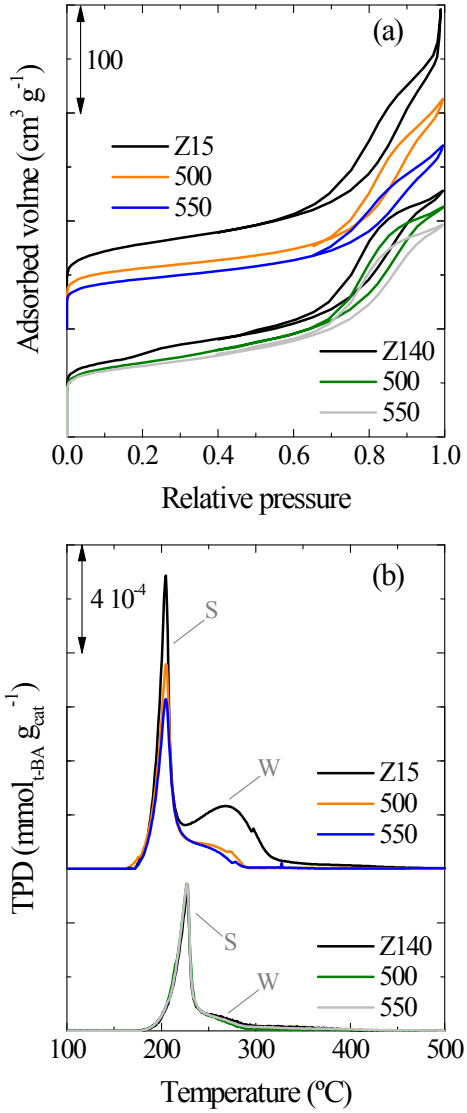

Fig. S3. (a) N_2 adsorption-desorption isotherms and (b) t-BA TPD of the fresh and used Z15 and Z140 catalysts at 500 and 550 ºC (Space time, 1.00 g_{cat} h mol_C^{-1})

Table S1. Kinetic constant at 500 ºC and activation energy values for the catalytic cracking of n-pentane over Z15 and Z140 catalysts

	Z15		Z140	
	k*	**E (kJ mol^{-1})**	**k***	**E (kJ mol^{-1})**
Kinetic rates				
k_1 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(8.54 ± 0.07) 10^{-1}	(6.15 ± 0.15) 10^{1}	(2.50 ± 1.66) 10^{-2}	(6.74 ± 1.89) 10^{1}
k_2 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(8.57 ± 0.27) 10^{-1}	(3.84 ± 1.13) 10^{1}	(6.46 ± 4.15) 10^{-2}	(3.91 ± 1.66) 10^{1}
k_3 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(2.45 ± 0.89) 10^{-1}	(7.07 ± 1.65) 10^{1}	(1.42 ± 0.81) 10^{-2}	(7.24 ± 0.45) 10^{1}
k_4 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-2})**	(4.13 ± 1.15) 10^{0}	(3.77 ± 1.11) 10^{1}	(2.45 ± 0.12) 10^{-1}	(3.76 ± 0.69) 10^{1}
k_5 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-2})**	(4.14 ± 1.29) 10^{0}	(3.74 ± 1.15) 10^{1}	(4.19 ± 1.52) 10^{-1}	(3.81 ± 1.51) 10^{1}
k_6 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-2})**	(1.34 ± 0.47) 10^{0}	(2.62 ± 0.48) 10^{1}	(1.27 ± 0.13) 10^{-1}	(2.72 ± 0.54) 10^{1}
k_7 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(6.56 ± 0.62) 10^{-1}	(2.66 ± 0.12) 10^{1}	(2.63 ± 0.16) 10^{-2}	(2.78 ± 0.92) 10^{1}
k_8 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(3.40 ± 0.08) 10^{0}	(1.01 ± 0.10) 10^{1}	(1.64 ± 0.86) 10^{-1}	(1.04 ± 0.15) 10^{1}
k_9 **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(5.72 ± 0.13) 10^{-1}	(1.54 ± 0.26) 10^{1}	(1.77 ± 0.22) 10^{-2}	(1.59 ± 0.75) 10^{1}
k_{10} **(mol$_C$ g$_{cat}^{-1}$ h^{-1} atm^{-1})**	(1.05 ± 0.41) 10^{-3}	(2.36 ± 0.31) 10^{1}	(1.07 ± 0.95) 10^{-3}	(2.29 ± 1.07) 10^{1}
Deactivation rate				
k_d **(atm^{-1} h^{-1})**	(3.14 ± 0.06) 10^{-1}	(3.00 ± 0.15) 10^{1}	(1.05 ± 0.29) 10^{-1}	(3.21 ± 0.78) 10^{1}
d	(1.01 ± 0.12) 10^{0}		(1.13 ± 0.20) 10^{0}	

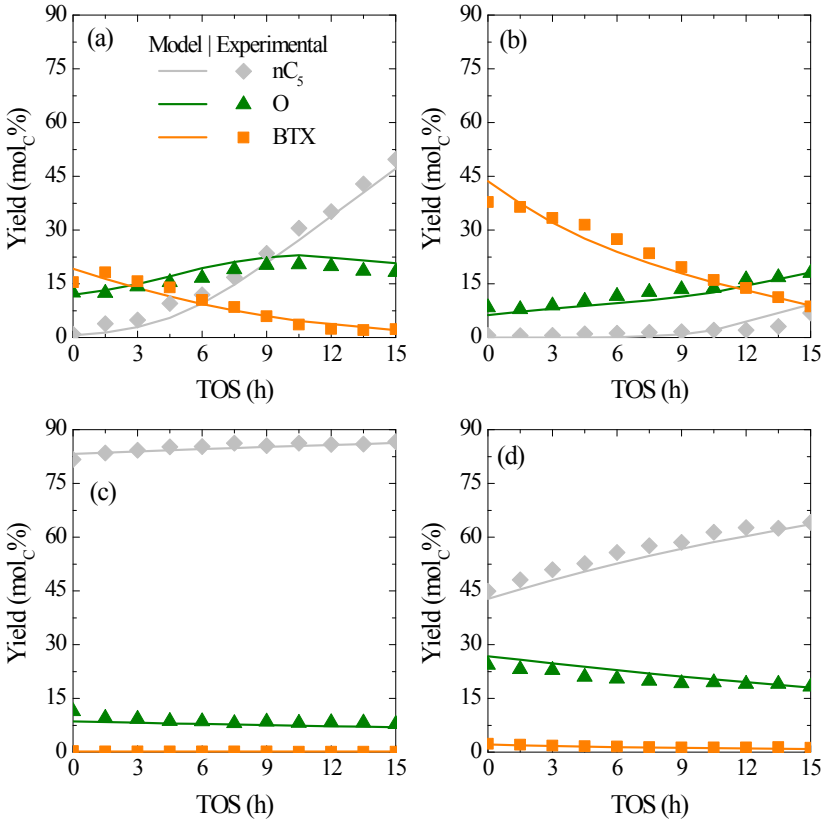

Fig. S5. Comparison of the predicted results with the model (lines) and additional experimental runs (dots) for the evolution with time on stream of yields using the Z15 catalyst and space time values of (a) 1.0 and (b) 3.5 g_{cat} h mol_C^{-1} and using Z140 catalyst and space time values of (c) 1.0 and (d) 3.5 g_{cat} h mol_C^{-1}, at 550 ºC.

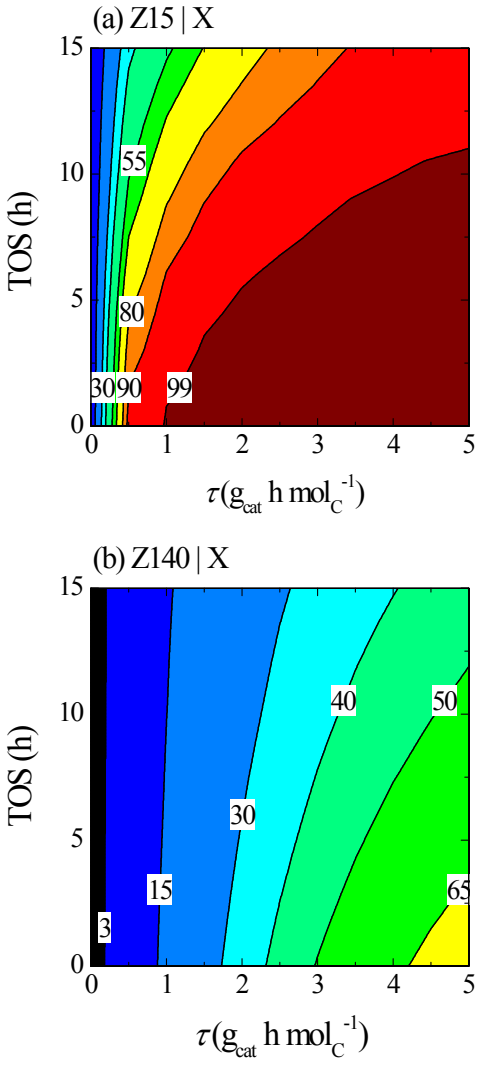

Fig. S6. Simulated contour maps for (a) Z15 and (b) Z140 catalysts of the evolution with the time on stream and space time of the n-pentane conversion at 550 ºC