Title: PHENOL PRODUCTION KINETIC MODEL IN THE CYCLOHEXANOL DEHYDROGENATION PROCESS

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Supporting Information

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1 Table SI-1. Physico-chemical properties of reduced catalyst.

Catalyst	Composition, wt.%	Cu, wt. %	Physical and Chemical Properties											
			d_p mm	ρ_p g cm^{-3}	ρ_L g cm^{-3}	S_{BET}, m^2 g^{-1}	V_P, cm^3 g^{-1}	Acidity, μmolNH$_3$ g^{-1}				Phases XRD	Cu crystallite size, nm
								Weak	Moderate	Strong	Total	Reduced	Reduced
T-2130 SüdChemie	CuO,33 ZnO,66 C graphite,1	26	3	2.30	1.76	43.4	0.223	3	27	0	30	Cu ZnO C graphite	9

Table SI-2. Experimental runs carried out for cyclohexanol dehydrogenation in FBR (W=10 g). Initial molar fraction at the reactor entrance: y_{OLo} = 0.95, y_{ONEo} = 0.05, y_{H2o} = 0.

Runs	T, K	Q_L, kg/ h	W/Q_L, g_{cat}·h/kg
1	563	0	0
		0.100	102
		0.056	177
		0.028	355
		0.020	496
		0.016	633
		0.010	1013
		0.007	1364
		0.006	1773
2	523	0	0
		0.100	102
		0.056	177
		0.028	355
		0.020	496
		0.016	633
		0.013	771
		0.010	1013
		0.007	1364
		0.006	1773
3	493	0	0
		0.100	102
		0.056	177
		0.028	355
		0.020	496
		0.013	771
		0.010	1013
		0.007	1364
		0.006	1773

Table SI-3. Reactants and phenol.

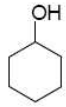
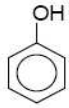
Compound	Acronym	Formula	MW	CAS#	Molecular Structure
Cyclohexanol	*OL*	$C_6H_{12}O$	100	108-93-0	
Cyclohexanone	*ONE*	$C_6H_{10}O$	98	108-94-1	
Hydrogen	*H2*	H_2	2	1333-74-0	
Phenol	*PhOH*	C_6H_6O	94	108-95-2	

Table SI-4. Kinetic parameters, residual sum of squares and standard deviation values obtained by fitting cyclohexanone data obtained in runs 1-3 to models in Table 2.

Parameters	Values		
	M1	M2	M3
E_1/R , K	6896	6867	6900
$Ln\ (k_{01})$	16.96	17.03	
k_{01}, $mmol/atm \cdot g_{cat} \cdot h$	23208	24890	17.13
K_{OL}, atm	0.846	0.464	0.453
K_{ONE}, atm	1.610	0.754	0.765
K_{H2}, atm	-	0.080	-
K'_{H2} , $atm^{1/2}$	-	-	0.099
SQR^*	$8.11\ 10^9$	$8.10\ 10^9$	$8.12\ 10^9$
R^2	99.38	99.38	99.38
σ_{st}^2	$1.88\ 10^4$	$2.01\ 10^4$	$2.12\ 10^4$

* for cyclohexanone concentration.

Table SI-5. Kinetic parameters, residual sum of squares and standard deviation values obtained by fitting phenol data obtained in runs 1-3 to kinetic expressions in Table 3.

Parameters	Values	
	S1	S2
E_2/R , K	13661	-
$Ln\ (k_{02})$	23.95	-
k_{02}, $mmol/atm \cdot g_{cat} \cdot h$	$2.52\ 10^{10}$	-
E_3/R , K	-	15634
$Ln\ (k_{03})$	-	34.95
k_{03}, $mmol/atm \cdot g_{cat} \cdot h$	-	$1.51\ 10^{15}$
SQR^*	$2.61\ 10^{6}$	$1.48\ 10^{8}$
R^2	99.72	84.45
σ_{st}^2	$3.37\ 10^{2}$	$2.54\ 10^{3}$

* for phenol concentration.