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*Supplementary Materials*

# Effect of Ni-Mo carbide catalyst formation on furfural hydrogenation

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## 1. Mass Transfer Calculations

Weisz-Prater Criterion for Internal Diffusion (Fogler, p839):

If $C_{WP} = \frac{r_{(obs)}\rho_c {R_p}^2}{D_{eff} C_{As}} < 1$ , then internal mass transfer effects can be neglected.

Mears Criterion for External Diffusion (Fogler, p841; Mears, 1971):

If $C_M = \frac{r_{(obs)}\rho_b R_p n}{k_c C_{Ab}} < 0.15$ , then external mass transfer effects can be neglected.

Where:

$r_{obs}$= observed reaction rate, mol/$kg_{cat}$·s

n= reaction order

$R_p$= catalyst particle radius, m

$\varrho_c$ = bulk density of catalyst bed, kg/$m^3$

$\varrho_b$ = bulk density of catalyst bed, kg/$m^3$

$\varrho_b$ = (1-Φ)·$\varrho_c$ (Φ=porosity)

$D_{eff}$ = effective diffusivity, $m^2$/s $D_{eff}$=0.1$D_{AB}$

For the estimation of $D_{AB}$ the Wilke-Chang equation was used.

$D_{AB} = \frac{7.4\times10^{-8}(\Phi\times M)^{1/2}T}{\eta V^{0.6}} \times 10^{-4}$ , $m^2$/s (where Φ – dimensionless association factor; M – the molecular weight of the solvent, g/mol; T – temperature of reaction, K; η – the solvent viscosity, cPs; V – the liquid molar volume at the solute's normal boiling point, $cm^3$/mol.)

$C_{As}$ = gas concentration of A at the external surface of the catalyst, mol/$m^3$.

$C_{Ab}$ = bulk gas concentration of A, mol/$m^3$.

$k_c$ = external mass transfer coefficient, m/s

## 1. Mass Transfer Calculations for furfural hydrogenation

In the current work, a 300 mL autoclave with 60 mL of 5 wt% of furfural in isopropyl alcohol was used and the initial hydrogen pressure was 6.0 MPa at T = 423 K. A catalyst particle size of 0.071 mm was employed for the kinetic study.

For the furfural hydrogenation, the obtained highest reaction rate was $3.93\times10^{-2}$ mol $kg_{cat}^{-1}$ $s^{-1}$.

$r_{obs}$=$3.93\times10^{-2}$ mol·$kg_{cat}^{-1}$·$s^{-1}$

n=1

$R_p$= $3.55\times10^{-5}$ m

$\varrho_c \approx \varrho_b \approx \varrho_{cat}$ = 1370 kg/$m^3$

$C_{As} \approx C_{Ab}$= 1730 mol /$m^3$

$D_{eff} = \frac{7.4\times10^{-8}(\Phi\times M)^{1/2}T}{\eta V^{0.6}} \times 10^{-5} = \frac{7.4\times10^{-8}\sqrt{1\times60.09}\times423}{0.011\times82.8^{0.6}} \times 10^{-5} = 1.56\times10^{-8}$ $m^2/s$

The parameter $k_c \approx 1.3 \times10^{-4}$ m/s was calculated according data presented in study Hajek, J., & Murzin, D. Y. (2004). Liquid-Phase Hydrogenation of Cinnamaldehyde over a Ru− Sn Sol−Gel

Catalyst. 1. Evaluation of Mass Transfer via a Combined Experimental/Theoretical Approach. *Industrial & engineering chemistry research*, *43*(9), 2030-2038.

$$C_{WP} = \frac{r_{(obs)}\rho_c {R_p}^2}{D_{eff}C_{As}} = \frac{3.93\times10^{-2}\text{-}1370\cdot(3.55\times10^{-5})^2}{1.56\times10^{-8}\cdot1730} = 0.0025 < 1$$

$$C_M = \frac{r_{(obs)}\rho_b R_p n}{k_c C_{Ab}} = \frac{3.93\times10^{-2}\text{-}1370\cdot3.55\times10^{-5}\cdot1}{1.3\times10^{-4}\cdot1730} = 0.00085 < 0.15$$

Therefore, internal and external diffusion effects could be neglected during the kinetic experiments.

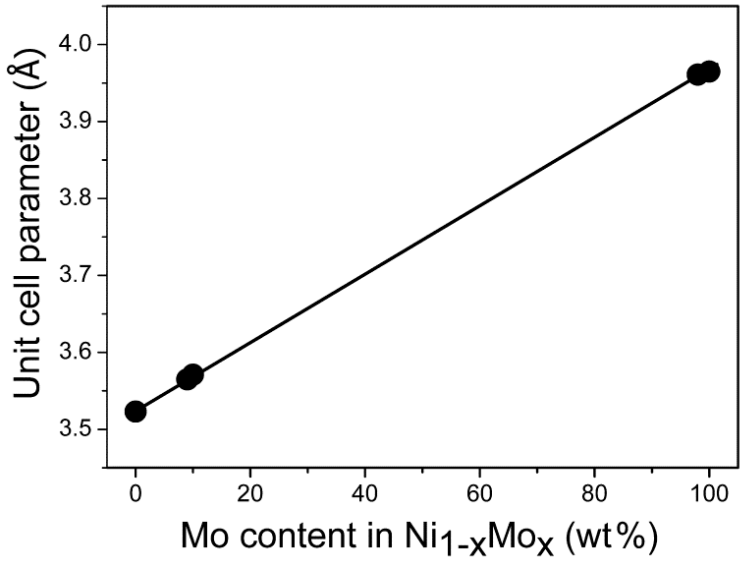


**Figure S1.** The dependence of the lattice parameter on the parameter $x$ in $Ni_{1-x}Mo_x$. Mo (JCPDS card No. 421120); Ni (JCPDS card No. 40850); $Mo_{0.09}Ni_{0.91}$ (JCPDS card No. 105048); $Mo_{0.36}Ni_{0.64}$ (JCPDS card No. 105045); $Mo_{0.984}Ni_{0.016}$ (JCPDS card No. 105049).