

# Hydrodeoxygenation of gamma-valerolactone on transition metal phosphide catalysts

Gwang-Nam Yun, Atsushi Takagaki, Ryuji Kikuchi, S. Ted Oyama

## Supplemental Information

$$\frac{-r'_a \rho_b R n}{k_c C_{Ab}}$$

If  $\frac{-r'_a \rho_b R n}{k_c C_{Ab}} < 0.15$ , then external mass transfer effects can be neglected.

**Table S1-1.** Parameters in the Mears criterion

R	Catalyst particle radius / cm	0.09
n	reaction order	1
$\rho_b$ (Ni <sub>2</sub> P, CoP, Pd)	bulk density of catalyst bed, g/cm <sup>3</sup>	6.E-03
$\rho_b$ (MoP, WP)	bulk density of catalyst bed, g/cm <sup>3</sup>	8.E-03
$C_{Ab}$	bulk gas concentration of A at 300 °C, mol/cm <sup>3</sup>	4.2E-07
$k_c$	mass transfer coefficient, cm/s	102

**Table S1-2.** Observed reaction rates and calculated Mears criterion

	Ni <sub>2</sub> P	CoP	MoP	WP	Pd
Temperature /°C	Observed reaction rate /mol g <sup>-1</sup> s <sup>-1</sup>				
250	2.06E-06	3.98E-07	3.43E-07	3.15E-08	4.72E-07
275	4.58E-06	9.13E-07	4.60E-07	7.02E-08	7.04E-07
300	8.80E-06	2.08E-06	8.40E-07	1.53E-07	1.14E-06
325	1.12E-05	3.92E-06	1.44E-06	3.00E-07	1.99E-06
350	1.14E-05	6.73E-06	2.58E-06	5.64E-07	3.07E-06
Temperature /°C	Mears criterion				
250	2.37E-05	4.58E-06	5.26E-06	4.83E-07	5.43E-06
275	5.52E-05	1.10E-05	7.40E-06	1.13E-06	8.49E-06
300	1.11E-04	2.63E-05	1.41E-05	2.58E-06	1.44E-05
325	1.47E-04	5.16E-05	2.53E-05	5.26E-06	2.62E-05
350	1.57E-04	9.23E-05	4.72E-05	1.03E-05	4.20E-05

