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APPENDICES

APPENDIX A

Calculation of sample

M.W. of Si	= 28.0855
M.W. of SiO ₂	= 60.0845
Weight percent of SiO ₂ in Sodium Silicate	= 28.5
M.W. of Al	= 26.9815
M.W. of AlCl ₃	= 133.3405
Weight percent of purity of AlCl ₃	
M.W. of Cu	= 63.54
M.W. of Cu(CH ₃ COO) ₂ H ₂ O	= 99

A-1 Calculation of Si/Al ratio for MFI type zeolite.

The calculation is based on weight of Sodium Silicate (Na₂OsiO₂H₂O) in B1 and B2 solutions.

$$\begin{aligned}\text{Mole of Si used} &= \frac{\text{wt.(\%purity)} * (\text{M.W. of Si})}{100 (\text{M.W. of SiO}_2)} \quad (\text{A-1.1}) \\ &= 69 * (28.5/100) * (28/60) \\ &= 0.3273\end{aligned}$$

$$\text{Si/Al atomic ratio} = 50$$

$$\text{Mole of Al required} = 0.3272/50 = 6.5458 * 10^{-3} \text{ mole}$$

$$\begin{aligned}\text{Amount of AlCl}_3 &= 6.5458 * 10^{-3} * 133 * (100/97) \\ &= 0.8998 \text{ g}\end{aligned}$$

This is the amount of AlCl₃ used in A1 and A2 solutions

A-2 Calculation of reaction flow rate.

This study uses flow rate of stream gas by using the formula of GHSV (gas hourly space velocity) as follows:

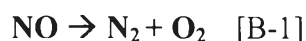
$$\begin{aligned}\text{GHSV} &= \frac{\text{Volumetric flow rate}}{\text{Volume of Catalyst}} \\ \text{Volumetric flow rate} &= 30,000 * \text{Volume of catalyst.} \\ \text{at STP: Volumetric flow rate} &= \frac{\text{Volumetric flow rate} * (273.15+t)}{273.15}\end{aligned}$$

where t = room temperature, °C

APPENDIX B

Thermodynamic stability of nitrogen oxide.

Even though NO is an endothermic compound, no decomposition is observed at 825 K. The thermodynamic parameters (S° , H_f° and G_f°) corresponding to NO and the Gibbs free energy of the reaction are given in Table B-1:



for a relatively broad range of temperature [139].

From a thermodynamic point of view, as can be seen from Table B-1, the NO molecule is unstable even at 298 K and 1 atm. This is due to the electronic structure of the bond in NO. The reaction is spin-forbidden, and NO is kinetically stable. Thus, the high energy of dissociation ($153.3 \text{ kcal mol}^{-1}$) and to corresponding extremely low decomposition rates.

In the presence of a reductant, reactions lead to a strong decrease in the Gibbs free energy values. This explains that such reactions are used in practical applications. The introduction of oxygen here leads to an additional reduction in the free energy.

Table B-1 Evolution of the thermodynamic parameters: entropy (S°), enthalpy (H_f°), Gibbs free energy of NO (G_f°), and Gibbs free energy of the NO decomposition (Stull et al. 1969 [139]).

T(K)	NO	H_{fs}° (kcal mol ⁻¹)	NO reaction	
	S° (cal mol K)		G_f° (kcal mol ⁻¹)	$(G_f^\circ)_f$ (kcal mol ⁻¹)
298	50.35	21.60	20.72	-2 20.72
300	50.40	21.60	20.71	-2 20.71
400	52.45	21.61	20.41	-2 20.41
500	54.06	21.62	21.62	-2 20.11
600	55.41	21.62	19.81	-2 19.81
700	56.57	21.62	19.51	-2 19.51
800	57.61	21.63	19.21	-2 19.21
900	58.54	21.63	18.91	-2 18.91
1000	59.39	21.69	18.60	-2 18.60

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VITA

Miss Tapanee Dangsawai was born in Bangkok, Thailand, on August, 1974. She received a second class honours of Bachelor degree of Science from Chulalongkorn University in March 1995. Then, she has continued studying in Doctoral degree of Engineering from the department of Chemical Engineering, Chulalongkorn University since May, 1995.

