

Fig. 15. Comparison of observed pressure drops of gas-liquid-solid three-phase horizontal flow with calculated values from Eq. (5).

tubes.<sup>3)</sup> Gas-liquid-solid three-phase flow might have lower pressure drops than liquid-solid two-phase flow at the same fluids velocities when gas blowing has a diminishing effect on stagnant solid particles.

A proposed empirical correlation containing hydrodynamic parameters used for liquid-solid two phase flow is applicable to the estimation of pressure drop of horizontal gas-liquid-fine solid particles three-phase flow.

#### Nomenclature

$C_d$	= $(4/3)gd_p(\rho_p - \rho_{\text{water}})/(\rho_{\text{water}} v_t)$ , drag coefficient of a particle	[—]
$C_s$	= solid weight percent in slurry	[wt%]
$C_v$	= solid volume fraction in slurry	[—]
$D_T$	= tube diameter	[cm]
$d_p$	= average particle size	[ $\mu\text{m}$ ]
$g$	= acceleration of gravity	[ $\text{m/s}^2$ ]
$\Delta P_{GL}$	= calculated pressure drop from Lockhart-Martinelli correlation	[—]

$\Delta P_L$	= $4fu_L^2\rho_L/(2D_T)$ , calculated pressure drop from Fanning equation with linear velocity	[Pa]
$\Delta P/L$	= pressure drop per unit tube length	[kPa/m]
$s$	= density ratio of solid particle to liquid	[—]
$U_G$	= superficial gas velocity	[cm/s]
$U_L$	= superficial liquid or slurry velocity	[cm/s]
$U_{s0}$	= superficial slurry velocity of liquid-solid flow	[cm/s]
$u_L$	= $U_L/(1 - \epsilon_G)$ , linear velocity of liquid or slurry	[cm/s]
$v_t$	= terminal velocity of a particle	[cm/s]
$\epsilon_G$	= gas holdup	[—]
$\epsilon_{G0}$	= gas holdup of two-phase flow ( $= 0.90\epsilon_{G,Y}$ )	[—]
$\epsilon_{G,Y}$	= estimated gas holdup from Yokota's correlation using slurry density and viscosity	[—]
$\rho_L$	= liquid or solid density	[ $\text{kg/m}^3$ ]

#### Acknowledgment

This work was supported in part by a Grant-in-Aid by the Japan Securities Scholarship Foundation.

#### Literature Cited

- 1) Chisholm, D. and A. D. K. Laird: *Trans. ASME*, **80**, 276 (1958).
- 2) Hatate, Y., C. J. Louh and C. Y. Wen: *AIChE Symp. Ser.*, **77**(202), 11 (1981).
- 3) Hatate, Y., H. Nomura, T. Fujita, S. Tajiri, N. Hidaka and A. Ikari: *J. Chem. Eng. Japan*, **19**, 56 (1986).
- 4) Lockhart, R. W. and R. C. Martinelli: *Chem. Eng. Prog.*, **45**, 39 (1949).
- 5) Scott, D. S. and P. K. Rao: *Can. J. Chem. Eng.*, **49**, 302 (1971).
- 6) Toda, M., K. Shimazaki and S. Maeda: *Kagaku Kogaku Ronbunshu*, **4**, 56 (1978).
- 7) Yokota, T.: *Kagaku Kōgaku*, **29**, 687 (1965).
- 8) Zandi, I. and G. Govatos: *Proc. Am. Soc. Civ. Engr.*, **93** (HY3), 145 (1967).

## CRITERIA FOR THERMAL EFFECTIVENESS FACTORS

CHUNG-SUNG TAN

Department of Chemical Engineering, National Tsing Hua University, Hsinchu, Taiwan 300, R.O.C.

**Key Words:** Endothermic Reaction, Effectiveness Factor, Thiele Modulus, Nusselt Numbers, Criterion

The conventional approach to evaluation of the effectiveness factor for exothermic reactions assumes catalyst particles to be isothermal.<sup>2,7)</sup> However, this approach may not be valid for endothermic reactions, as has been pointed out by Maymo *et al.*<sup>3)</sup> and Tan

and Smith.<sup>6)</sup> This is because of the relatively low temperature and reaction rates in catalyst particles for endothermic reactions, which make mass transport less important. Under these circumstances the energy balance rather than the mass balance should be considered. Tan and Smith<sup>6)</sup> calculated and compared effectiveness factors and axial concentration and tem-

Received November 11, 1985. Correspondence concerning this article should be addressed to C. S. Tan.

perature profiles in a fixed-bed reactor by three models: I) an exact solution accounting for both intraparticle concentration and temperature gradients; II) a thermal effectiveness model neglecting intraparticle concentration gradient; III) an isothermal model neglecting intraparticle temperature gradient. They observed that model II gives results much closer to those of the exact model than model III for endothermic reactions in a wide range of parameters. The equations used in these three models are written as follows.

Model I)

$$\frac{d^2 C^*}{dx^2} + \frac{2}{x} \frac{dC^*}{dx} - \Phi^2 C^* \times \exp \left\{ \gamma \left[ 1 - \frac{1}{\beta(C_s^* - C^*) + 1 - \beta \frac{(Nu)_m}{(Nu)_h} (C_s^* - 1)} \right] \right\} = 0 \quad (1)$$

$$\eta_{\text{exact}} = \frac{3(Nu)_m(1 - C_s^*)}{\Phi^2} \quad (2)$$

Model II)

$$\frac{d^2 T^*}{dx^2} + \frac{2}{x} \frac{dT^*}{dx} + \Phi^2 \beta C^* \exp \left[ \gamma \left( 1 - \frac{1}{T^*} \right) \right] = 0 \quad (3)$$

$$\eta_{\text{therm}} = \frac{3(Nu)_m}{\Phi^2} (1 - C_s^*) \quad (4)$$

Model III)

$$\eta_{\text{isoth}} = \frac{3(Nu)_m}{\Phi^2} \left[ \frac{\Phi^* \cosh \Phi^* - \sinh \Phi^*}{\Phi^* \cosh \Phi^* + [(Nu)_m - 1] \sinh \Phi^*} \right] \quad (5)$$

where

$$\Phi^* = \Phi \exp \left[ \frac{\gamma}{2} \left( 1 - \frac{1}{T_s^*} \right) \right] \quad (6)$$

Details for obtaining the solutions of three models are given by Tan and Smith.<sup>6)</sup> But it can be imagined that when the parameter  $\beta$  approaches zero the isothermal assumption (i.e. model III) should be more suitable than the assumption of neglecting the concentration gradient (model II). Also, it can be seen from Table 1 that for some sets of parameters model III gives better results than model II for endothermic reactions. Hence the objective of this communication is to find a criterion for the use of the model II to calculate the effectiveness factors for endothermic reactions.

Tan and Smith<sup>6)</sup> observed that a maximum of error of  $\eta_{\text{therm}}$  exists somewhere in the range of  $\Phi$  in all combinations of  $\gamma$ ,  $\beta$ ,  $(Nu)_m$  and  $(Nu)_h$ . The exact location of the maximum depends on all the other parameters. By Figs. 1 and 2 it can be found that the error of  $\eta_{\text{therm}}$  increases with the mass Nusselt number  $(Nu)_m$ . However, such increases are not distinguished in the range of small Thiele modulus  $\Phi$ . The effect of

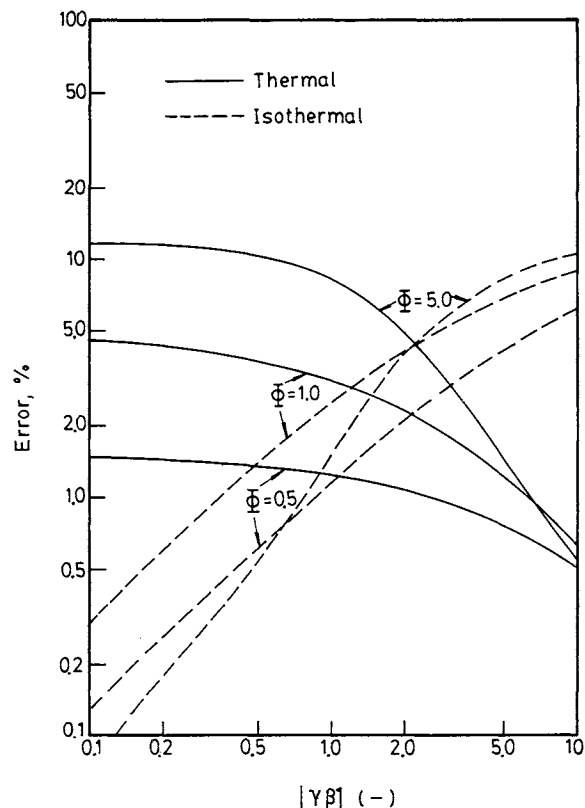


Fig. 1. Errors in effectiveness factors calculated by Models II and III for  $(Nu)_m = 1.0$  and  $(Nu)_h = 1.0$ .

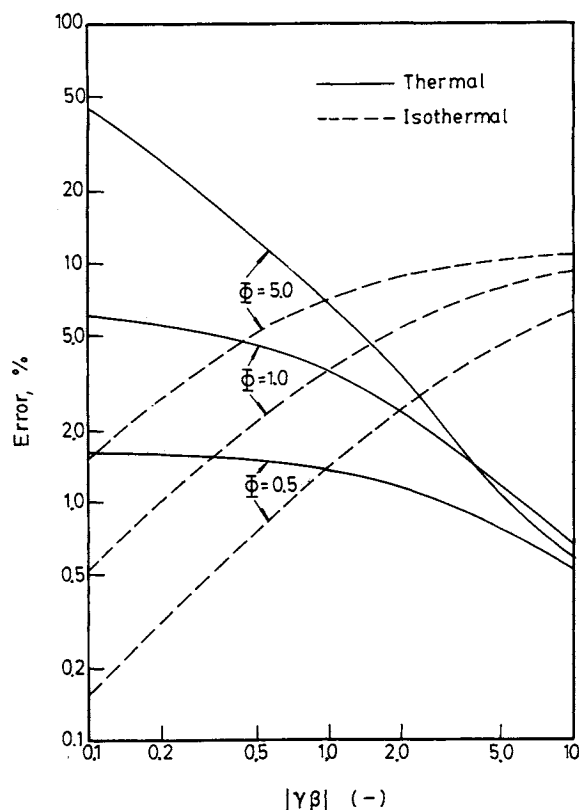


Fig. 2. Errors in effectiveness factors calculated by Models II and III for  $(Nu)_m = 10^3$  and  $(Nu)_h = 1.0$ .

**Table 1.** Comparison of effectiveness factors calculated by exact (I), thermal (II) and isothermal (III) Models

$\gamma$	$\beta$	$ \gamma\beta $	$(Nu)_m$	$(Nu)_h$	$\Phi$	$\eta_{\text{exact.}}$	$\eta_{\text{therm.}}$	$\eta_{\text{isoth.}}$	% Error*	
									Therm.	Isoth.
10	-0.01	0.1	1.0	1.0	0.1	0.996	0.996	0.996	0.0	0.0
10	-0.01	0.1	1.0	1.0	1.0	0.701	0.734	0.703	4.63	0.31
10	-0.01	0.1	1.0	1.0	5.0	0.0950	0.106	0.0950	11.49	0.08
10	-0.01	0.1	1.0	1.0	10	$2.69 \times 10^{-2}$	$2.90 \times 10^{-2}$	$2.69 \times 10^{-2}$	8.06	0.02
10	-0.01	0.1	1.0	1.0	50	$1.18 \times 10^{-2}$	$1.20 \times 10^{-2}$	$1.18 \times 10^{-2}$	1.99	0.05
10	-0.1	1.0	1.0	1.0	0.1	0.992	0.993	0.993	0.07	0.07
10	-0.1	1.0	1.0	1.0	1.0	0.598	0.617	0.613	3.20	2.53
10	-0.1	1.0	1.0	1.0	5.0	$8.37 \times 10^{-2}$	$9.09 \times 10^{-2}$	$8.50 \times 10^{-2}$	8.56	1.48
10	-0.1	1.0	1.0	1.0	10	$2.51 \times 10^{-2}$	$2.73 \times 10^{-2}$	$2.53 \times 10^{-2}$	8.59	0.49
10	-0.1	1.0	1.0	1.0	50	$2.95 \times 10^{-4}$	$3.00 \times 10^{-4}$	$2.94 \times 10^{-4}$	1.51	-0.26
10	-0.2	2.0	1.0	1.0	0.1	0.988	0.989	0.989	0.06	0.13
10	-0.2	2.0	1.0	1.0	1.0	0.518	0.530	0.540	2.33	4.21
10	-0.2	2.0	1.0	1.0	5.0	$6.99 \times 10^{-2}$	$7.34 \times 10^{-2}$	$7.28 \times 10^{-2}$	4.89	4.06
10	-0.2	2.0	1.0	1.0	10	$2.22 \times 10^{-2}$	$2.35 \times 10^{-2}$	$2.27 \times 10^{-2}$	5.88	2.21
10	-0.2	2.0	1.0	1.0	50	$1.12 \times 10^{-3}$	$1.17 \times 10^{-3}$	$1.12 \times 10^{-3}$	4.68	0.15
20	-0.1	2.0	1.0	1.0	1.0	0.521	0.533	0.542	2.37	4.09
20	-0.1	2.0	1.0	1.0	10	$2.27 \times 10^{-2}$	$2.42 \times 10^{-2}$	$2.31 \times 10^{-2}$	6.71	1.76
10	-0.3	3.0	1.0	1.0	0.1	0.984	0.985	0.986	0.06	0.19
10	-0.3	3.0	1.0	1.0	1.0	0.460	0.468	0.485	1.81	5.40
10	-0.3	3.0	1.0	1.0	5	$5.84 \times 10^{-2}$	$6.01 \times 10^{-2}$	$6.21 \times 10^{-2}$	2.94	6.23
10	-0.3	3.0	1.0	1.0	10	$1.89 \times 10^{-2}$	$1.95 \times 10^{-2}$	$1.98 \times 10^{-2}$	3.28	4.75
10	-0.3	3.0	1.0	1.0	50	$1.04 \times 10^{-3}$	$1.09 \times 10^{-3}$	$1.06 \times 10^{-3}$	4.31	1.09
30	-0.1	3.0	1.0	1.0	1.0	0.465	0.474	0.489	1.88	5.16
30	-0.1	3.0	1.0	1.0	5.0	$6.17 \times 10^{-2}$	$6.40 \times 10^{-2}$	$6.50 \times 10^{-2}$	3.73	5.36
10	-1.0	10	1.0	1.0	0.1	0.959	0.959	0.965	0.06	0.62
10	-1.0	10	1.0	1.0	1.0	0.272	0.273	0.300	0.65	8.84
10	-1.0	10	1.0	1.0	0.5	$2.64 \times 10^{-2}$	$2.65 \times 10^{-2}$	$2.91 \times 10^{-2}$	0.53	10.1
10	-1.0	10	1.0	1.0	5.0	$8.19 \times 10^{-3}$	$8.23 \times 10^{-3}$	$8.98 \times 10^{-3}$	0.44	9.64
10	-1.0	10	1.0	1.0	10	$4.56 \times 10^{-4}$	$4.57 \times 10^{-4}$	$4.92 \times 10^{-4}$	0.28	7.99
10	-0.01	0.1	1.0	1.0	0.1	0.996	0.996	0.996	0.007	0.007
10	-0.01	0.1	50	1.0	0.1	0.999	0.995	0.999	0.07	0.007
10	-0.01	0.1	$10^3$	1.0	0.1	0.999	0.9996	0.999	0.07	0.007
10	-0.01	0.1	1.0	1.0	1.0	0.701	0.734	0.703	4.63	0.31
10	-0.01	0.1	50	1.0	1.0	0.903	0.956	0.907	5.95	0.51
10	-0.01	0.1	$10^3$	1.0	1.0	0.908	0.962	0.912	5.98	0.51
10	-0.01	0.1	1.0	1.0	5.0	0.095	0.106	0.095	11.49	0.08
10	-0.01	0.1	50	1.0	5.0	0.363	0.526	0.368	44.85	1.37
10	-0.01	0.1	$10^3$	1.0	5.0	0.381	0.556	0.387	45.85	1.52
10	-0.1	1.0	50	1.0	1.0	0.711	0.736	0.736	3.49	3.57
10	-0.1	1.0	$10^3$	1.0	1.0	0.714	0.739	0.739	3.50	3.58
10	-0.1	1.0	50	1.0	5.0	0.149	0.158	0.160	6.24	7.20
10	-0.1	1.0	$10^3$	1.0	5.0	0.150	0.160	0.161	6.13	7.35
10	-0.01	0.1	$10^3$	10	0.1	0.999	0.999	0.999	0.07	0.007
10	-0.01	0.1	$10^3$	10	1.0	0.931	0.990	0.936	6.31	0.54
10	-0.01	0.1	$10^3$	10	5.0	0.459	0.815	0.467	77.7	1.72
10	-0.1	1.0	$10^3$	10	1.0	0.869	0.914	0.912	5.10	4.95
10	-0.1	1.0	$10^3$	10	5.0	0.337	0.407	0.387	20.78	14.83
10	-0.2	2.0	$10^3$	10	1.0	0.813	0.848	0.888	4.20	9.12
10	-0.2	2.0	$10^3$	10	5.0	0.263	0.291	0.327	10.4	24.9
10	-0.1	1.0	$10^3$	$10^2$	1.0	0.890	0.938	0.936	5.36	5.15
10	-0.1	1.0	$10^3$	$10^2$	5.0	0.398	0.513	0.467	28.7	17.1
10	-0.2	2.0	$10^3$	$10^2$	1.0	0.850	0.888	0.933	4.57	9.86
10	-0.2	2.0	$10^3$	$10^2$	5.0	0.344	0.398	0.456	15.9	32.6

\* Calculation based on five digits.

the heat Nusselt number  $(Nu)_h$  on the error can be found in Fig. 2 and Fig. 3. Also, the error of  $\eta_{\text{therm}}$  increases with  $(Nu)_h$  but is not significant when  $\Phi$  is small. From the above observation and Eqs. (1) to (6) it is hard to develop a criterion, involving all the parameters such as  $\gamma$ ,  $\beta$ ,  $(Nu)_m$ ,  $(Nu)_h$  and  $\Phi$ , for the

use of model II (thermal effectiveness model) to calculate the effectiveness factor for endothermic reactions. However, very simple criteria that are relatively independent of  $(Nu)_m$ ,  $(Nu)_h$  and  $\Phi$  can be found by looking at Figs. 1 to 3 and extensive calculations (not given in this note), and may be written as

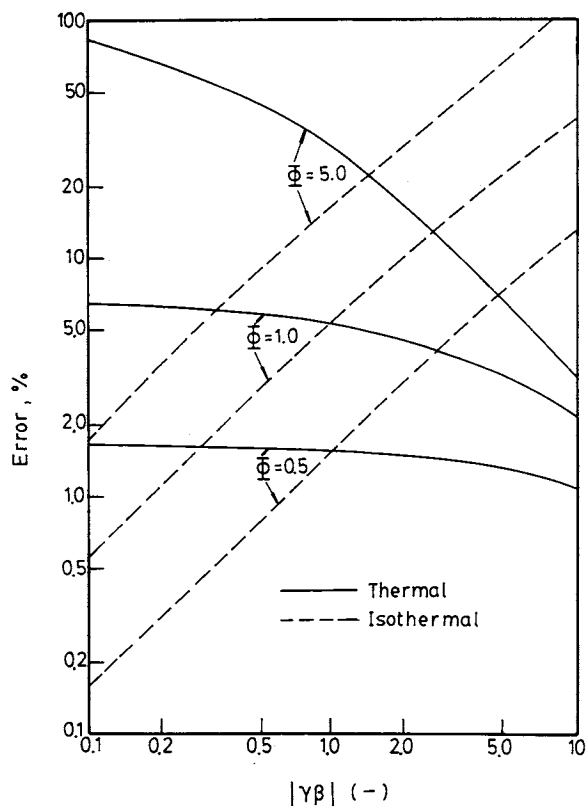


Fig. 3. Errors in effectiveness factors calculated by Models II and III for  $(Nu)_m = 10^3$  and  $(Nu)_h = 100$ .

follows:

for  $|\gamma\beta| > 2.0$  thermal effectiveness model  
(model II) is valid (7)

for  $|\gamma\beta| < 1.0$  isothermal model (model III)  
is valid (8)

for  $1 < |\gamma\beta| < 2.0$  exact model is better (9)

The deviations of effectiveness factors from exact ones using criteria (7) and (8) are normally less than ten percent and become smaller as  $\Phi$  decreases. The practical Thiele modulus is seldom larger than 2.0, hence criterion (7) is not a very severe one for the use of model II to calculate effectiveness factors for endothermic reactions.

Satterfield and Sherwood,<sup>5)</sup> using the data of Prater,<sup>4)</sup> estimated the parameters  $\gamma$  and  $\beta$  as 40 and  $-0.18$ , respectively for the dehydrogenation of cyclohexane at 25 atm and 450°C. The absolute value of  $\gamma\beta$  is 7.2, which satisfies criterion (7) and suggests that model II should be used. From Table I in the notes of Maymo *et al.*<sup>3)</sup> it can be observed that model II gives effectiveness factors almost identical to the exact ones

(the worst case less than 10% different at  $\Phi = 50$ ), but model III gives results about 80% to 98% higher than the exact ones. Another example involves the dehydrogenation of butene to butadiene studied by Dumez and Froment<sup>1)</sup> at 0.25 atm and 600°C. The parameters estimated based on the information provided by these two authors are  $\gamma \approx 18$  and  $\beta \approx -0.03$ . The absolute value of  $\gamma\beta$  is 0.54, which is less than 1.0 and satisfies criterion (8). Hence the isothermal approach should be the correct one as is identified in the paper of Dumez and Froment,<sup>1)</sup> in which the predicted results obtained by neglecting the temperature gradient in catalyst particles agree well with the experimental ones.

#### Nomenclature

$C$	= concentration of catalyst particles	[mol/m <sup>3</sup> ]
$C_b$	= local bulk-phase concentration	[mol/m <sup>3</sup> ]
$C_s$	= surface concentration	[mol/m <sup>3</sup> ]
$C^*$	= dimensionless concentration, $C/C_b$	[-]
$C_s^*$	= dimensionless surface concentration, $C_s/C_b$	[-]
$D_e$	= effective diffusivity	[m <sup>2</sup> /s]
$E$	= activation energy	[kJ/mol]
$h$	= heat transfer coefficient	[kJ/s · m <sup>2</sup> · K]
$k$	= reaction rate constant	[l/s]
$k_e$	= effective thermal conductivity	[kJ/s · m · K]
$k_f$	= mass transfer coefficient	[m/s]
$R$	= particle radius	[m]
$R_g$	= gas constant	[kJ/mol · K]
$T$	= temperature in catalyst particle	[K]
$T_b$	= bulk-phase temperature	[K]
$T^*$	= dimensionless temperature, $T/T_b$	[-]
$\beta$	= $(-\Delta H)C_b D_e / k_e T_b$	[-]
$\gamma$	= $E/R_g T$	[-]
$\eta_{\text{exact}}$	= effectiveness factor calculated by exact model (model I)	[-]
$\eta_{\text{isoth}}$	= effectiveness factor calculated by isothermal model (model III)	[-]
$\eta_{\text{therm}}$	= effectiveness factor calculated by thermal model (model II)	[-]
$\Phi$	= Thiele modulus based on $T_b$ , $R(k/D_e)^{1/2}$	[-]

#### Literature Cited

- 1) Dumez, F. J. and G. F. Froment: *Ind. Eng. Chem. Proc. Des. Dev.*, **15**, 291 (1965).
- 2) Froment, G. F. and K. B. Bischoff: "Chemical Reactor Analysis and Design," Wiley, New York (1979).
- 3) Maymo, J. A., R. E. Cunningham and J. M. Smith: *Ind. Eng. Chem. Fundam.*, **5**, 280 (1966).
- 4) Prater, C. D.: *Chem. Eng. Sci.*, **8**, 284 (1958).
- 5) Satterfield, C. N. and T. K. Sherwood: "The Role of Diffusion in Catalysis," Addison-Wesley Publishing Co., Reading, Mass. (1963).
- 6) Tan, C. S. and J. M. Smith: *Chem. Eng. Sci.*, **13**, 1329 (1984).
- 7) Weisz, P. B. and J. S. Hicks: *Chem. Eng. Sci.*, **53**, 663 (1961).