

# GEOMETRIC FACTOR FOR DIFFUSION IN POROUS MEDIA

MASASHI MITANI

Department of General Education, Dohto University, Monbetsu 094

**Key Words:** Pore Diffusion, Porous Media, Porous Solid, Pore Tortuosity Factor, Diffusibility

Whenever the effective diffusion coefficient in porous media is theoretically predicted, it is necessary to evaluate the geometric factor in the media, for example, diffusibility or tortuosity. Despite years of study,<sup>4,20,27)</sup> no reliable expression of the factor has been obtained. In this communication, the general character of the factor which covers various types of the porous media, from packed beds of solid particles to consolidated porous media, will be confirmed from the analysis of a number of literature data concerning pore diffusion.

## 1. Diffusibility

Diffusibility  $\delta$  is defined as follows.<sup>20)</sup>

$$\delta = D_e/D_T \quad (1)$$

Generally,  $\delta$  is expressed in terms of porosity  $\varepsilon$  and tortuosity  $\tau$ , so that

$$\delta = \varepsilon/\tau \quad (2)$$

Diffusibility or tortuosity has been correlated with porosity by many investigators. For packed beds of various solids, Currie<sup>6)</sup> extensively tested the following formula, which was originally derived by Bruggeman.<sup>4)</sup>

$$\delta = \varepsilon^m \quad (3)$$

While Bruggeman<sup>4)</sup> has shown theoretically that  $m$  is 3/2 for spherical particle, Currie<sup>6)</sup> introduced one more correction factor into Eq. (3) to modify the equation. Similar types of formula have also been used by other investigators<sup>38,43)</sup> to evaluate the geometric factor.

## 2. Analysis of Data and Discussion

Figure 1 shows the relation between  $\delta$  and  $\varepsilon$  based on the literature data<sup>6-8,14,16,26,34)</sup> of tortuosity or diffusibility in packed beds or unconsolidated porous media. The curves of Eq. (3) for appropriate values of  $m$  are superimposed on this figure. The data for each bed reasonably coincide with Eq. (3) for each  $m$  value depending on the shape of the particles in the bed.

From the figure, it is found that  $m$  value changes from 1.5 or 2.0 for spherical or granular materials to about 10 for materials with plate-like structure.

The relation between  $\varepsilon$  and  $\delta$  for consolidated particles which have only macropores, such as various catalyst supports,<sup>33,35)</sup> tableted metal oxide catalysts,<sup>3,13,40)</sup> carbonyl iron tablets,<sup>20)</sup> silica gel,<sup>13)</sup> porcelain<sup>35)</sup> and others,<sup>24,28,32)</sup> is illustrated in Fig. 2, provided that the mean radius of the pore is greater than about 200 Å. The data for the bidispersed porous media<sup>5,15,17,18,21,25,31,39,41)</sup> having micropores and macropores are also included in this figure, taking into account only macropore porosity, but these are limited to the media in which macropore diffusion is inferred to dominate overall diffusion flux. These data are also expressed by Eq. (3) with  $m$  of 1.5 to 3.0.

For the case of media having only micropores, such as porous glasses,<sup>2,3,9-11,18,19,23,30,42)</sup> alumina<sup>3,12,28,29,43)</sup> and silica-alumina<sup>3,12,25,37)</sup> catalysts and other catalysts,<sup>1,13,22,34,36,40)</sup> Eq. (3) is also usable as shown in Fig. 3, though the data disperse more than in the previous cases.

For bidispersed porous media in which the diffusion flux in micropores is comparable with that in macropores, effective diffusion coefficients predicted by a simplified parallel-pore model with the geometric factor of Eq. (5) were compared with the experimental diffusion coefficients reported by several investigators. The parallel-pore model is expressed by

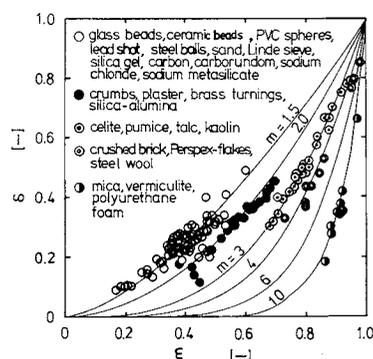
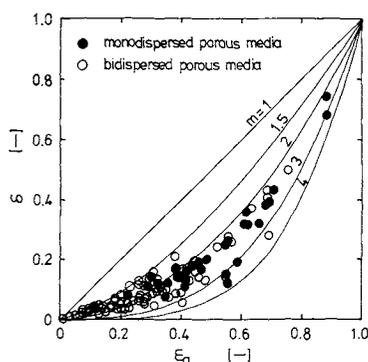


Fig. 1. Relation between  $\delta$  and  $\varepsilon$  for gaseous diffusion in packed beds or unconsolidated porous media.

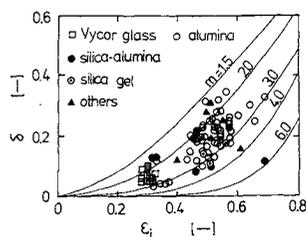
Received October 21, 1983. Correspondence concerning this article should be addressed to M. Mitani.

**Table 1.** Effective diffusion coefficients in bidispersed porous media

Porous media	Gas systems	Effective diffusion coefficients calculated				Observed $D_e$ [cm <sup>2</sup> /s]
		By Eq. (4)		By random pore model [cm <sup>2</sup> /s]	By parallel pore model [cm <sup>2</sup> /s]	
		$m_{a,i}=2.0$ [cm <sup>2</sup> /s]	$m_{a,i}=2.5$ [cm <sup>2</sup> /s]			
Alumina No. 2 <sup>5)</sup>	N <sub>2</sub> -He	0.0022	0.0013	0.00313	—	0.00147
Alumina <sup>17)</sup>	H <sub>2</sub> -N <sub>2</sub>	1.19	0.750	1.29	—	0.850
Graphite <sup>44)</sup>	CH <sub>4</sub> -N <sub>2</sub>	0.00196	0.00072	0.00265	0.00828	0.00169



**Fig. 2.** Relation between  $\delta$  and  $\epsilon_a$  for macropore diffusion.



**Fig. 3.** Relation between  $\delta$  and  $\epsilon_i$  for micropore diffusion.

$$D_e = \epsilon_a^{m_a} D_{T_a} + \epsilon_i^{m_i} D_{T_i} \quad (4)$$

Where  $D_{T_a}$  and  $D_{T_i}$  are diffusion coefficients in the straight round macropore and micropore, respectively.  $m_a$  and  $m_i$  refer to the shape factors for these pores.  $D_e$  obtained by Eq. (4) for appropriate values of the shape factor are summarized in **Table 1**, being compared with the effective diffusion coefficients<sup>5,17,44)</sup> observed experimentally and calculated by other pore models.

### Summary

Diffusibility is well expressed by Eq. (3) over a wide range of porosity and for various types of media. The shape factor in the equation varies widely for unconsolidated packed beds and narrowly for consolidated porous media.

The geometric factor predicted by Eq. (3) may be reasonably introduced into the parallel pore model to evaluate the effective diffusion coefficient for porous media.

### Nomenclature

$D_e$	= effective diffusion coefficient	[cm <sup>2</sup> /s]
$D_T$	= diffusion coefficient in a straight round pore	[cm <sup>2</sup> /s]
$m$	= shape factor	[—]
$\delta$	= diffusibility	[—]
$\epsilon$	= porosity	[—]
$\tau$	= tortuosity	[—]

### <Subscripts>

$a$	= macropore
$i$	= micropore

### Literature Cited

- 1) Ash, R., R. M. Barrer and R. T. Lowson: *Surface Sci.*, **21**, 265 (1970).
- 2) Barrer, R. M. and J. A. Barrie: *Proc. Roy. Soc.*, **A213**, 250 (1952).
- 3) Brown, L. F., H. W. Haynes and W. H. Manogue: *J. Catalysis*, **14**, 220 (1969).
- 4) Bruggeman, D. A. G.: *Ann. Phys.*, **24**, 636 (1935).
- 5) Cunningham, R. S. and C. J. Geankoplis: *Ind. Eng. Chem. Fundam.*, **7**, 535 (1968).
- 6) Currie, J. A.: *Brit. J. Appl. Phys.*, **11**, 318 (1960).
- 7) Edwards, M. F. and C. N. Kenney: *Trans. Inst. Chem. Engrs. (London)*, **44**, T189 (1966).
- 8) Evans, E. V. and C. N. Kenney: *Trans. Inst. Chem. Engrs. (London)*, **44**, T189 (1966).
- 9) Gilliland, E. R., R. F. Baddour and J. L. Russell: *AIChE J.*, **4**, 90 (1958).
- 10) Gilliland, E. R., R. F. Baddour and H. H. Engel: *AIChE J.*, **8**, 530 (1962).
- 11) Gilliland, E. R., R. F. Baddour, G. P. Perkinson and K. J. Sladek: *Ind. Eng. Chem. Fundam.*, **13**, 95 (1974).
- 12) Gorring, R. L. and A. J. de Rosset: *J. Catalysis*, **3**, 341 (1964).
- 13) Grachev, G. A. and K. G. Ione: *Kinetica i Kataliz*, **11**, 765 (1970).
- 14) Gunn, D. J.: *Trans. Inst. Chem. Engrs. (London)*, **47**, T351 (1969).
- 15) Hamai, S. and M. Mitani: *Kagaku Kōgaku*, **34**, 170 (1970).
- 16) Hamai, S. and M. Mitani: *Kagaku Kōgaku*, **34**, 1086 (1970).
- 17) Hashimoto, K., K. Sakashita, F. Arai and H. Kobayashi: Preprint of the 5th Reaction Engineering Symposium of The Soc. of Chem. Engrs., Japan, p. 49 (1965).
- 18) Henry, J. P., R. S. Cunningham and C. J. Geankoplis: *Chem. Eng. Sci.*, **22**, 11 (1967).
- 19) Higashi, K., H. Ito and J. Oishi: *J. Atomic Energy Soc. Japan*, **5**, 846 (1963).
- 20) Hoogschagen, J.: *Ind. Eng. Chem.*, **47**, 906 (1955).
- 21) Horak, Z. and P. Schneider: *Chem. Eng. J.*, **2**, 26 (1971).

- 22) Horiguchi, Y., R. R. Hudgins and P. L. Silveston: *Can. J. Chem. Eng.*, **49**, 76 (1971).
- 23) Hwang, S.-T. and K. Kammermeyer: *Can. J. Chem. Eng.*, **44**, 82 (1966).
- 24) Katsumata, K., K. Yamada and K. Mukaida: Preprint of the Hokkaido Meeting of The Soc. of Chem. Engrs., Japan, p. 12 (1979).
- 25) Kawazoe, K. and I. Sugiyama: *Kagaku Kōgaku*, **30**, 1007 (1966).
- 26) Knox, J. H. and L. McLaren: *Anal. Chem.*, **36**, 1477 (1964).
- 27) Masamune, S. and J. M. Smith: *AIChE J.*, **8**, 217 (1962).
- 28) Omata, H. and L. F. Brown: *AIChE J.*, **18**, 967 (1972).
- 29) Raghavan, N. S. and L. K. Doraiswamy: *Ind. Eng. Chem. Process Des. Dev.*, **16**, 519 (1977).
- 30) Rao, M. R. and J. M. Smith: *AIChE J.*, **10**, 293 (1964).
- 31) Rothfeld, L. B.: *AIChE J.*, **9**, 19 (1963).
- 32) Sakashita, K., F. Arai and H. Kobayashi: *Kagaku Kōgaku*, **31**, 920 (1967).
- 33) Satterfield, C. N. and P. J. Cadle: *Ind. Eng. Chem. Process Des. Dev.*, **7**, 256 (1968).
- 34) Schneider, P. and J. M. Smith: *AIChE J.*, **14**, 886 (1968).
- 35) Scott, D. S. and F. A. L. Dullien: *AIChE J.*, **8**, 113 (1962).
- 36) Sladek, K. J., E. R. Gilliland and R. F. Baddour: *Ind. Eng. Chem. Fundam.*, **13**, 100 (1974).
- 37) Villet, R. H. and R. H. Wilhelm: *Ind. Eng. Chem.*, **53**, 837 (1961).
- 38) Wakao, N. and J. M. Smith: *Chem. Eng. Sci.*, **17**, 825 (1962).
- 39) Wakao, N. and T. Funaki: *Kagaku Kōgaku*, **31**, 485 (1967).
- 40) Wakao, N. and K. Tachibana: Preprint of the 33rd Annual Meeting of The Soc. of Chem. Engrs., Japan, No. 1, p. 124 (1968).
- 41) Wang, C.-T. and J. M. Smith: *AIChE J.*, **29**, 132 (1983).
- 42) Weaver, J. A. and A. B. Metzner: *AIChE J.*, **12**, 655 (1966).
- 43) Weisz, P. B. and A. B. Schwartz: *J. Catalysis*, **1**, 399 (1962).
- 44) Yang, R. T. and R.-T. Liu: *Ind. Eng. Chem. Process Des. Dev.*, **18**, 245 (1979).

## PRESSURE CONTROL BY MICROCOMPUTER (APPLICATION OF NONMINIMAL PROTOTYPE DDC ALGORITHM)

MASAO IMAEDA

*Department of Precision Mechanics, Tokushima University, Tokushima 770*

**Key Words:** Process Control, Microcomputer, Direct Digital Control, Pseudo Random Binary Signal, Least-Square Method

### Introduction

Since the microcomputer began to be used as a controller, developments in the DDC system have been actively studied. In this regard the author developed the Nonminimal Prototype DDC Algorithm, which offers better control performance than either the conventional analog PID or the discrete PID control, and its performance with digital simulation was discussed.<sup>1)</sup>

In this paper, control of a pressure tank is chosen as an example to illustrate the application of a Nonminimal Prototype DDC Algorithm using a personal microcomputer. This system is used to supply water at a constant flow rate to the adjoining plant. From experimental results, the Nonminimal Prototype DDC gives better control, as expected. However, a saturation problem in the control valve appears.

### 1. Experimental Control System

A schematic diagram of the experimental control

system is shown in **Fig. 1**. The function of this system is to supply water at a constant flow rate to the adjoining plant by keeping the pressure in the tank constant. Water entering the tank is controlled with a diaphragm valve. The tank is 0.55 m i.d. and has a volume of 0.309 m<sup>3</sup>. The pressure in the tank is measured by a diaphragm manometer. The signal is transferred to a PANAFACOM C-15 microcomputer via DC-amplifier and A/D converter. The A/D and the D/A converters are 12 and 8 bites respectively. Samplings of tank pressure are taken at intervals controlled by the microcomputer. The system is operated with the following conditions:

tank pressure:  $1.47 \times 10^5$  Pa  
water flow rate: 64.2 kg/min

A block diagram of this control system is illustrated in **Fig. 2**.

### 2. System Responses

To apply the Nonminimal Prototype DDC Algorithm, the process dynamics must be expressed in the 2nd order with a time delay. In this paper a PRBS (Pseudo Random Binary Signal), generated in the

Received June 2, 1983. Correspondence concerning this article should be addressed to M. Imaeda.