Korean J. Chem. Eng., **22**(2), 184-189 (2005)

Taylor Dispersion Coefficients for Longitudinal Laminar Flow in Shell-and-tube Exchangers

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(*Received 20 October 2004 • accepted 15 January 2005*)

Abstract−The problem of determining the shell-side Taylor dispersion coefficient for a shell-and-tube configuration is examined in detail for square and hexagonal arrays of tubes for the case when the shell side flow is laminar and parallel to the tubes. A multipole expansion method is employed to determine fluid velocity and concentration field for the fluid on the shell side. The numerical results for the shell side Taylor dispersion coefficient are compared with those by a cell theory. The cell theory agrees well with the numerical results at small area fractions and gives better estimates for hexagonal arrays. Finally, we present formulas for determining Taylor dispersion coefficient for the periodic arrays.

Key words: Taylor Dispersion Coefficient, Shell-and-tube Exchanger, Multipole Expansion Method, Square and Hexagonal Array, Cell Theory

INTRODUCTION

One of the mass transport phenomena encountered in many chemical processes is dispersion of a chemical solute due to a combination of molecular diffusion and variation in the velocity of the fluid flowing in the processes. The axial dispersion for longitudinal laminar flow in a tube, referred to in the literature as Taylor dispersion, has long been an important research topic for its widespread use since it was first analyzed by Taylor [1953]. This axial dispersion problem with no chemical reaction at the tube wall was also examined by Aris [1956]. Many studies have been performed to extend the work of Taylor and Aris to various systems with chemical reactions [Dill and Brenner, 1982; Shapiro and Brenner, 1986; Balakotaiah and Chang, 1995; Balakotaiah, 2004].

This paper is concerned with axial dispersion on the shell-side laminar flow parallel to tubes in periodic arrangements. Heat (or mass) transfer problems for shell-side longitudinal laminar flow was first examined by Sparrow et al. [1961] who dealt with the problem of determining heat transfer coefficients for laminar longitudinal flow on the shell-side when the tubes are placed in a periodic arrangement. Koo and Sangani [2003] investigated the case of random arrays of tubes using a multipole expansion method to calculate velocity and solute concentration of the shell-side fluid and thus determine Sherwood numbers for the shell-side flow. A similar approach is employed in the present study to obtain Taylor dispersion coefficients for longitudinal laminar flow on the shell side, which may be important in transport processes using a shell-and-tube configuration such as hollow fiber contactors and heat exchangers. We calculated velocity and concentration fields using an exact numerical scheme to determine the Taylor dispersion coefficient and made a comparison with cell theory approximations.

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FORMULATION OF THE PROBLEM AND THE METHOD

In the shell-and-tube configuration shown in Fig. 1, we consider the problem of determining the shell-side axial dispersion coefficient resulting from the combination of molecular diffusion of a solute in the plane normal to the tubes and the variations in the axial velocity of the fluid. The solute concentration *c* satisfies the usual convection-diffusion equation,

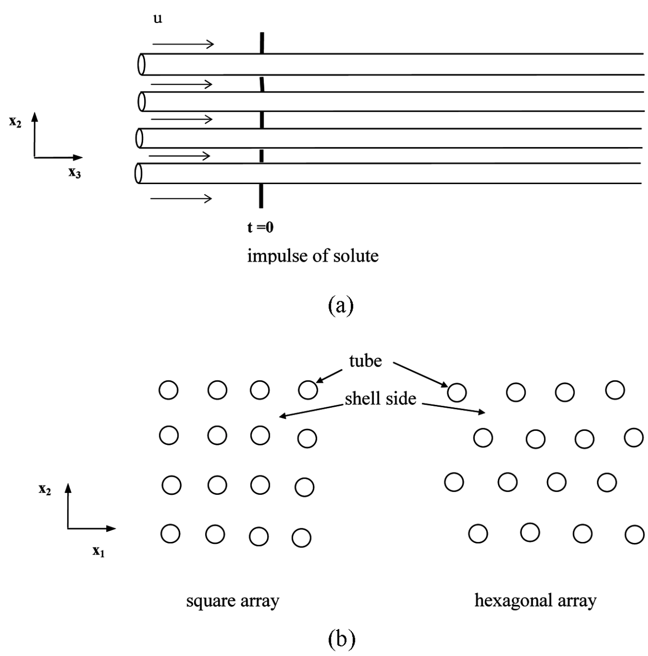

Fig. 1. (a) Shell-and-tube configuration with an impulse of solute. (b) Schematic diagram for periodic arrays of tubes.

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x_3}=D_M\nabla^2 c, \tag{1}$$

where D_M is the molecular diffusivity of the solute in the shell side fluid. We take the x_3-axis to be along the axes of the tubes and (x_1, x_2) to be the coordinates of a point in the plane normal to the tubes. The distances are non-dimensionalized by a, the radius of the tubes. And the axial velocity of fluid on the shell side is denoted by u. The average concentration of the solute $\langle c\rangle_s$ defined by

$$\langle c\rangle_s=\frac{1}{(1-\phi)\tau}\int_{A_s} c\,dA \tag{2}$$

satisfying a similar equation

$$\frac{\partial\langle c\rangle_s}{\partial t}+\langle u\rangle_s\frac{\partial\langle c\rangle_s}{\partial x_3}=D_T\frac{\partial^2\langle c\rangle_s}{\partial x_3^2} \tag{3}$$

with D_T being the Taylor dispersion coefficient. Here, τ is the area of the unit cell non-dimensionalized by a^2, ϕ is the area fraction of the tubes, and A_s is the area occupied by the shell side fluid. The spatial average over the shell side area is denoted by a subscript s outside the angular brackets. The average velocity of the fluid on the shell side is $\langle u\rangle_s=U/(1-\phi)$, U being the superficial velocity. Since the above equations are linear we may choose a relatively simple form of $\langle c\rangle_s$ to evaluate the Taylor dispersion coefficient. We follow Koch and Brady [1985] and take

$$\langle c\rangle_s=(x_3-\langle u\rangle_s t)/U \tag{4}$$

which clearly satisfies Eq. (3). Now substituting

$$c=\langle c\rangle_s+a^2 f(x_1, x_2)/D_M \tag{5}$$

into Eq. (1) we obtain

$$\frac{u}{U}-\frac{1}{1-\phi}=a^2\nabla^2 f. \tag{6}$$

Note that the Laplacian operator is taken in the x_1-x_2 plane.

We shall restrict our analysis to the case of non-adsorbing, non-reacting tube walls. The boundary conditions for the concentration are therefore spatial periodicity and the vanishing normal component of ∇f at the surface of the tubes: The positions of the center of N tubes will be denoted by $\mathbf{x}^\alpha$, α=1, 2, ..., N. These centers lie within a unit cell of a periodic array. Note that N=1 for the case of periodic arrays.

$$\mathbf{n}\cdot\nabla f=0 \quad \text{at } |\mathbf{x}-\mathbf{x}^\alpha|=1. \tag{7}$$

Averaging Eq. (1) over the shell side after substituting for c from Eq. (5) and recasting the resulting expression in the form given by Eq. (3) we obtain the following expression for the Taylor dispersion coefficient

$$\frac{D_T}{D_M}=1+\lambda Pe^2,\quad \lambda=\frac{1}{1-\phi}\left[\langle f\rangle_s-\frac{\langle uf\rangle_s}{U}\right], \tag{8}$$

where $Pe=aU/D_M$ is the Peclet number. And $\langle f\rangle_s$ and $\langle uf\rangle_s$ are defined by

$$\langle f\rangle_s=\frac{1}{(1-\phi)\tau}\int_{A_s} f\,dA, \tag{9}$$

$$\langle uf\rangle_s=\frac{1}{\tau}\int_{A_s} uf\,dA. \tag{10}$$

We shall use the method of multipole expansion for determining the velocity and concentration fields. The method uses periodic fundamental singular solutions of Laplace and biharmonic equations and their derivatives to construct velocity and concentration fields. We shall describe here in more detail the procedure for determining the velocity field that follows the analysis presented in Sangani and Yao [1988]. The shell side fluid velocity satisfies

$$\nabla^2 u=G, \tag{11}$$

where G is the pressure gradient non-dimensionalized by $\mu U/a^2$. A multipole expansion expression for the velocity field is given by [Sangani and Yao, 1988]

$$u=U_0+\sum_{\alpha=1}^{N}\sum_{n=0}^{\infty}[A_n^\alpha\partial_1^n+\tilde{A}_n^\alpha\partial_1^{n-1}\partial_2]S_1(\mathbf{x}-\mathbf{x}^\alpha), \tag{12}$$

where A_n^α and $\tilde{A}_n^\alpha$ are the 2^n-multipoles induced by the presence of tube α, $\tilde{A}_0\equiv 0$, and $\partial_k^n=(\partial^n/\partial x_k^n)$ (k=1, 2) is a short-hand notation for the *n*-th order partial derivative with respect to x_k. The function S_1 is a spatially periodic function satisfying [Hasimoto, 1959]

$$\nabla S_1(\mathbf{x})=4\pi\left[\frac{1}{\tau}-\sum_{x_L}\delta(\mathbf{x}-\mathbf{x}_L)\right]. \tag{13}$$

In the above expression, $\mathbf{x}_L$ are the coordinates of the lattice points of the array and δ is the Dirac delta function. In addition to the above differential equation we require that the integral of S_1 over the unit cell be zero. A Fourier series representation of S_1 and an efficient technique based on Ewald summation for evaluating S_1 are described by Hasimoto [1959]. Substituting Eq. (12) into Eq. (11), and making use of Eq. (13), we find that the non-dimensional pressure gradient is related to the sum of monopoles:

$$G=\frac{4\pi}{\tau}\sum_{\alpha=1}^{N}A_0^\alpha=4\phi\langle A_0\rangle, \tag{14}$$

where $\langle A_0\rangle$ is the average monopole. The multipoles A_n^α and $\tilde{A}_n^\alpha$ and the constant U_0 in Eq. (12) are to be determined from the no-slip boundary condition u=0 on the surface of the tubes and Eq. (11), which states that the non-dimensional superficial velocity is unity. For this purpose it is convenient to re-expand u around the center of each tube. For example, u is expanded near tube α as

$$u=\sum_{n=0}^{\infty}[u_n^\alpha(r)\cos n\theta+u_n^\alpha(r)\sin n\theta] \tag{15}$$

with

$$u_n^\alpha(r)=a_n^\alpha r^{-n}+e_n^\alpha r^n \text{ for } n\ge 1,\quad u_0^\alpha(r)=a_0^\alpha\log r+e_0^\alpha+Gr^2/4, \tag{16}$$

where $r=|\mathbf{x}-\mathbf{x}^\alpha|$. The terms singular at r=0 in the above expression arise from the singular part of S_1 at r=0. Noting that S_1 behaves as $-2\log r$ as $r\to 0$ [Hasimoto, 1959], and using the formulas for the derivatives of logr given in Appendix, we obtain

$$a_0^\alpha=-2A_0^\alpha,\quad a_n^\alpha=2(-1)^n(n-1)!A_n^\alpha \quad \text{for } n\ge 1. \tag{17}$$

The coefficients $\tilde{A}_n^\alpha$ are similarly related to $\tilde{a}_n^\alpha$. The coefficients of the regular terms, such as e_n^α, are related to the derivatives of the regular part of u at $\mathbf{x}=\mathbf{x}^\alpha$ [Sangani and Yao, 1988]. For example,

$$e_n^\alpha=\frac{1}{n!}[\partial_1^n-\xi_n\partial_1^{n-2}\nabla^2]u^r(\mathbf{x}^\alpha), \tag{18}$$

$$\tilde{e}_n^\alpha = \frac{1}{n!}[\partial_1^{n-1}\partial_2 - \tilde{\xi}_n\partial_1^{n-3}\partial_2\nabla^2]u^r(\mathbf{x}^\alpha), \tag{19}$$

where ξ_n=n/4 for n≥2, $\tilde{\xi}_n$=(n−2)/4 for n≥3, and $\xi_0=\xi_1=\tilde{\xi}_1=\tilde{\xi}_2=0$. In Eqs. (18)-(19), u^r denotes the regular part u obtained by removing the singular part, −2logr, from S1($\mathbf{x}-\mathbf{x}^\alpha$).

To determine the relation between U_0 in Eq. (12) and the superficial velocity we must integrate u over the area A_s occupied by the shell side fluid. Since the integrals of S_1 and its derivatives over the unit cell vanish, it is easier to evaluate the integral of u over A_s by integrating Eq. (12) over the unit cell and subtracting from it the integral of u inside the tubes. With the non-dimensional superficial velocity taken as unity, the above procedure yields

$$1 = U_0 - \frac{1}{\tau}\sum_{\alpha=1}^{N}\int_{r=0}^{1}\int_{\theta=0}^{2\pi} u^\alpha(r,\theta)\, r\,dr\,d\theta. \tag{20}$$

Care must be taken in carrying out the above integration to account for the singular nature of u^α at $\mathbf{x}=\mathbf{x}^\alpha$. Upon integrating, we obtain

$$U_0 = 1+\phi(1-\phi/2)\langle A_0\rangle + 2\phi\langle A_2\rangle. \tag{21}$$

The no-slip boundary condition on the surface of the tube, together with the orthogonality of trigonometric functions, requires that

$$u_n^\alpha(1) = \tilde{u}_n^\alpha(1) = 0. \tag{22}$$

Substituting for a_n^α and e_n^α from Eq. (17) and Eq. (18) into expressions for u_n^α and applying Eq. (22) we obtain a set of linear equations in the multipole coefficients A_n^α. This set is truncated by retaining only the terms with n≤N_s to yield a total of $2N_s+1$ equations in the same number of unknowns, solving which yields the velocity of the fluid on the shell side.

The concentration of the fluid on the shell side is determined in a similar manner. A formal solution of Eq. (3) that is spatially periodic is given by

$$\begin{aligned} f(\mathbf{x}) = \sum_{\alpha=1}^{N}\sum_{n=0}^{\infty} & [B_n^\alpha\partial_1^n + \tilde{B}_n^\alpha\partial_1^{n-1}\partial_2]S_1(\mathbf{x}-\mathbf{x}^\alpha) \\ & + [A_n^\alpha\partial_1^n + \tilde{A}_n^\alpha\partial_1^{n-1}\partial_2]S_1(\mathbf{x}-\mathbf{x}^\alpha) \end{aligned} \tag{23}$$

where the spatially periodic function S_2 satisfies

$$\nabla^2 S_2 = S_1 \tag{24}$$

As shown by Hasimoto [1959]

$$S_m(\mathbf{x}) = \frac{1}{\pi\tau(-4\pi^2)^{m-1}}\sum_{k\neq 0} k^{-2m}\exp(2\pi i\mathbf{k}\cdot\mathbf{x}), \tag{25}$$

where the summation is over all reciprocal lattice vectors except $\mathbf{k}=\mathbf{0}$. As mentioned earlier, Hasimoto [1959] has described a method for evaluating these functions using the Ewald summation technique.

Substituting for f and u_s from Eq. (23) and Eq. (12) into Eq. (6) and using Eq. (13) and Eq. (24), we find that, in order for Eq. (23) to be the solution for f, we must have

$$\frac{4\pi}{\tau}\sum_{\alpha=1}^{N} B_0^\alpha = U_0 - \frac{1}{1-\phi}. \tag{26}$$

To determine the multipoles B_n, we expand f near the center of each tube. Near tube α

$$f(\mathbf{x}) = \sum_{n=0}^{\infty} f_n^\alpha(r)\cos n\theta + \tilde{f}_n^\alpha(r)\sin n\theta, \tag{27}$$

with

$$f_0^\alpha = -\frac{1}{4}r^2(1-\log r)a_0^\alpha + \frac{r^2}{4}e_0^\alpha + b_0^\alpha\log r + g_0 + \frac{r^4}{64}G - \frac{1}{1-\phi}\frac{r^2}{4}, \tag{28}$$

$$f_1^\alpha = \frac{1}{2}r\left(\log r - \frac{1}{2}\right)a_1^\alpha + \frac{r^3}{8}e_1^\alpha + b_1^\alpha r^{-1} + g_1^\alpha r, \tag{29}$$

$$f_n^\alpha = \frac{r^{2-n}}{4(1-n)}a_n^\alpha + \frac{r^{n+1}}{4(n+1)}e_n^\alpha + b_n^\alpha r^{-n} + g_n^\alpha r^n \quad \text{for } n\geq 2, \tag{30}$$

and similar expressions for $\tilde{f}_n^\alpha$. Once again, the coefficients of the singular terms, e.g., b_n^α, can be related to the multipoles induced by tube *a* (i.e., A_n^α and B_n^α) and the coefficients of regular terms, g_n^α can be related to the derivatives of the regular part of f at $\mathbf{x}=\mathbf{x}^\alpha$. The results are given in the Appendix. The condition of vanishing flux integrated over the surface of the tube yields

$$B_0^\alpha = \frac{1}{4}A_0^\alpha - \frac{1}{32}G + \frac{1}{4\phi} - \frac{1}{2}A_2^\alpha - \frac{1}{4(1-\phi)}. \tag{31}$$

Thus, we see the monopole induced is not an unknown. On noting that U_0 is given by Eq. (21), we see that the condition Eq. (26) is automatically satisfied.

The average concentration of the shell side fluid is determined by integrating f given by Eq. (23) over the entire unit cell and subtracting from it the integrals over the area occupied by the tubes. The latter are evaluated using the local expansion near each tube (cf. Eq. (27)). The resulting expression is

$$\begin{aligned} \langle f\rangle_s = & \frac{3\phi}{8(1-\phi)} - \frac{\phi\langle g_0\rangle}{1-\phi} + \frac{\phi}{96}\frac{(27-11\phi)}{1-\phi}\langle a_0\rangle \\ & + \frac{\phi}{1-\phi}\langle b_2\rangle - \frac{\phi}{24(1-\phi)}\langle a_4\rangle. \end{aligned} \tag{32}$$

Here, $\langle g_0\rangle$, $\langle a_0\rangle$, $\langle b_2\rangle$, and $\langle a_4\rangle$ are averages of each coefficient defined in the same manner as $\langle A_0\rangle$ in Eq. (14).

For determining $\langle uf\rangle_s$, we need to integrate the product uf over the area occupied by the shell side fluid. This is difficult because it would require evaluating S_1, S_2, and their derivatives at many points outside the tubes. It is more efficient instead to solve for an auxiliary function ψ defined by

$$\nabla^2\psi = f, \quad \psi = 0 \quad \text{at } |\mathbf{x}-\mathbf{x}^\alpha| = 1. \tag{33}$$

Substituting for f from Eq. (33) into Eq. (10) and using Green's theorem we obtain

$$\begin{aligned} \tau\langle uf\rangle_s = \int_{A_s} uf\,dA = \int_{A_s} u\nabla^2\psi\,dA = \int_{A_s}\psi\nabla^2 u\,dA \\ + \int_{\partial A_s}(u\nabla\psi - \psi\nabla u)\cdot n\,dl. \end{aligned} \tag{34}$$

The integral over ∂A_s, which consists of the unit cell boundary and the surface of the tubes, vanishes owing to the boundary condition u=ψ=0 on the tube surface and the spatial periodicity of ψ and u. On using Eq. (11) we obtain

$$\langle uf\rangle_s = \frac{G}{\tau}\int_{A_s}\psi\,dA. \tag{35}$$

A formal expression for ψ can be written in the same way as for u and f:

$$\psi(\mathbf{x})=\psi_0+\sum_{\alpha=1}^{N}\sum_{n=0}^{\infty}[C_n^{\alpha}\partial_1^n+\tilde{C}_n^{\alpha}\partial_1^{n-1}\partial_2]S_1$$
$$+[B_n^{\alpha}\partial_1^n+\tilde{B}_n^{\alpha}\partial_1^{n-1}\partial_2]S_2+[A_n^{\alpha}\partial_1^n+\tilde{A}_n^{\alpha}\partial_1^{n-1}\partial_2]S_3 \tag{36}$$

where S_1, S_2 and S_3, and their derivatives, are to be evaluated at $\mathbf{x}-\mathbf{x}^{\alpha}$, and $\nabla^2 S_3=S_2$. Eq. (25) with m=3 can be used to evaluate S_3. The coefficients ψ_0, C_n and $\tilde{C}_n$ are to be evaluated from the boundary condition $\psi=0$ on the surface of the tubes. Finally, since $\nabla^2 S_1=4\pi/\tau$ at all points outside the tubes, we require that

$$\sum_{\alpha=1}^{N}C_0^{\alpha}=0. \tag{37}$$

To determine the coefficients $\tilde{C}_n^{\alpha}$, we expand ψ near the surface of each tube as

$$\psi=\sum_{n=0}^{\infty}\psi_n(r)\cos n\theta+\psi_n(r)\sin n\theta \tag{38}$$

with

$$\psi_n=\psi_n^r+\psi_n^s, \tag{39}$$

$$\psi_n^r=h_n r^n+\frac{g_n}{4(1+n)}r^{n+2}+\frac{e_n}{32(n+1)(n+2)}r^{n+4}$$
$$+\frac{G}{32\cdot 12\cdot 6}r^6\delta_{n0}-\frac{\delta_{n0}}{64(1-\phi)}r^4 \quad \text{for } n\geq 0. \tag{40}$$

For the purpose of applying boundary condition at r=1, we evaluate ψ_n^s at r=1 using

$$\psi_n^s=\beta_1 A_n+\beta_2 A_{n+2}+\beta_3 A_{n+4}+\beta_4 B_n+\beta_5 B_{n+2}+\beta_6 C_n, \tag{41}$$

where

$$\beta_1=\frac{(-1)^n(n-3)!}{16},\qquad \beta_2=\frac{(-1)^{n+1}(n-2)!(n+2)}{8},$$
$$\beta_3=\frac{(-1)^n n!(n+3)(n+4)}{16n},\qquad \beta_4=\frac{(-1)^{n+1}(n-2)!}{8},$$
$$\beta_5=\frac{(-1)^{n+1}n!(n+2)}{2n},\qquad \beta_6=2(-1)^n(n-1)!$$
$$\beta_1=3/64,\quad \beta_2=1/4,\quad \beta_4=1/2,\quad \beta_3=\beta_5=\beta_6=0 \qquad \text{for } n=0,$$
$$\beta_1=5/32,\quad \beta_2=3/8,\quad \beta_4=12 \qquad \text{for } n=1,$$
$$\beta_1=3/32 \qquad \text{for } n=2. \tag{42}$$

Now the integral of ψ over the area occupied by the shell side fluid can be determined by integrating ψ given by Eq. (36) over the unit cell first and then subtracting from it the integrals inside the tubes using the Eq. (38) for ψ near each tube. The final result for the mixing-cup based concentration difference is

$$\langle uf\rangle_s=-G\phi\Big[\frac{5}{32\cdot 9}\langle A_0\rangle+\frac{5}{32}\langle A_2\rangle+\frac{3}{8}\langle A_4\rangle+\frac{5}{4}\langle A_6\rangle$$
$$+\frac{5}{16}\langle B_0\rangle+\frac{\langle B_2\rangle}{2}-\frac{3}{2}\langle B_4\rangle+\langle C_0\rangle-2\langle C_2\rangle+\langle h_0\rangle$$
$$+\frac{\langle g_0\rangle}{8}+\frac{1}{32\cdot 6}\left(\langle e_0\rangle-\frac{1}{1-\phi}\right)+\frac{G}{32\cdot 12\cdot 8\cdot 6}-\frac{\psi_0}{\phi}\Big]. \tag{43}$$

Here, the averages of multipoles and coefficients are also defined in the same manner as $\langle A_0\rangle$ in Eq. (14).

RESULTS AND DISCUSSION

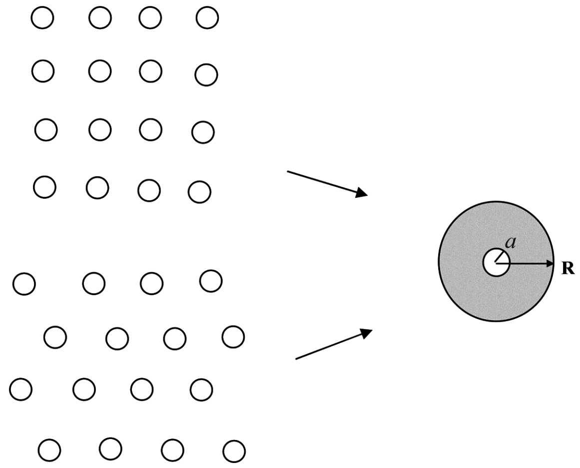

Fig. 2. Cell model.

The results of exact calculations are compared with the predictions obtained by using a cell theory [Happel, 1959] which is more appropriate for periodic arrays than effective-medium theory. In this theory, the periodic unit cell is replaced by a fluid cell of outer radius $R=\phi^{-1/2}$ and inner radius unity, as shown in Fig. 2. The fluid velocity is given by

$$u=-2A_0\log r+\frac{G}{4}r^2+e_0. \tag{44}$$

The constants are determined by using Eq. (14) and the boundary conditions u=0 at r=1 and $\partial u/\partial r=0$ at r=R, and the condition that the average velocity of the fluid in the cell equals $1/(1-\phi)$. This yields

$$-\frac{1}{A_0}=\log R^2-\frac{3}{2}+\frac{2}{R^2}-\frac{1}{2R^4}. \tag{45}$$

Similarly, from Eq. (6) the concentration for the shell side fluid is given by

$$f=A_0\left[\frac{1}{2}r^2(1-\log r)+\frac{1}{R^2}\left(\frac{r^4}{16}-\frac{r^2}{4}\right)\right]$$
$$-2B_0\log r-\frac{r^2}{4(1-\phi)} \quad \text{for } r>1. \tag{46}$$

The constant B_0 is determined by using the conditions of no flux at r=1 and at r=R. The average concentrations of the fluids, and hence the Taylor dispersion coefficients, can be determined once this constant is determined. The results are given below.

$$\langle f\rangle_s=\frac{2}{R^2-1}\Big\{A_0\left(\frac{R^4}{6}-\frac{R^4\log R}{8}-\frac{R^2}{16}-\frac{5}{48}\right)$$
$$+B_0\left(-R^2\log R+\frac{R^2-1}{2}\right)-\frac{R^4-1}{16(1-\phi)}\Big\}, \tag{47}$$

$$\langle uf\rangle_s=\frac{2}{R^2}\Big[A_0^2\Big\{\left(-\frac{R^4\log R}{4}+\frac{1}{16}(R^4-1)\right)\left(1-\frac{1}{R^2}\right)$$
$$+\frac{5}{48}\left(-R^2\log R+\frac{1}{6}\left(R^4-\frac{1}{R^2}\right)\right)+\frac{R^4}{8}\log R(2\log R-1)$$
$$+\frac{1}{32}(R^4-1)+\frac{1}{2R^2}\left(\frac{R^6}{6}-\frac{R^4}{4}+\frac{1}{12}\right)$$

$$+\frac{1}{R^4}\left(\frac{R^8}{128}-\frac{5R^6}{96}+\frac{R^4}{16}-\frac{7}{384}\right)\Bigg\}$$

$$+A_0B_0\Bigg\{2R^2\left((\log R)^2-\log R+\frac{1}{2}\right)-1$$

$$-\frac{2}{R^2}\left(\frac{R^4}{4}\log R-\frac{R^4-1}{16}-\frac{R^2}{2}\log R+\frac{R^2-1}{4}\right)\Bigg\}$$

$$-\frac{A_0}{4(1-\phi)}\left\{-\frac{1}{2}R^4\log R+\frac{1}{8}(R^4-1)+\frac{1}{R^2}\left(\frac{R^6}{6}-\frac{R^4}{4}+\frac{1}{12}\right)\right\}\Bigg] \quad (48)$$

The results for the coefficient λ as a function of area fractions of tubes for square and hexagonal arrays are given in Table 1. We find that the coefficient l by the exact calculations shows minimum value around the area fractions of 0.2 and 0.4 for square and hexagonal array, respectively. This interesting behavior is due to difference in dependency of $\langle f\rangle_s$ and $\langle uf\rangle_s/U$ on the area fractions. The difference between the two terms by the exact calculations for hexagonal array is plotted as a function of area fraction in Fig. 3. The difference $\langle f\rangle_s-\langle uf\rangle_s/U$ decreases with f rapidly at low area fractions before reaching the minimum around ϕ=0.4 and 0.5 beyond which the difference slightly increases with ϕ. Both the velocity and concentration fields are disturbed due to the presence of a tube and the magnitude of the disturbance increases with ϕ. Therefore, it is expected that $\langle uf\rangle_s$ is more affected by the disturbance than $\langle f\rangle_s$ at high ϕ where the disturbance becomes quite significant, and thus the difference between the two terms gets large at high ϕ.

Table 1. λ for square and hexagonal arrays

ϕ	Simulation		Cell theory
	Square array	Hexagonal array	
0.01	0.275	0.241	0.238
0.05	0.101	0.083	0.081
0.1	0.067	0.049	0.048
0.15	0.054	0.036	0.034
0.2	0.050	0.028	0.027
0.25	0.050	0.024	0.022
0.3	0.054	0.021	0.018
0.35	0.062	0.019	0.016
0.4	0.075	0.017	0.014
0.45	0.094	0.018	0.012
0.5	0.122	0.020	0.011
0.55	0.160	0.024	0.010
0.6	0.209	0.033	0.009
0.65	0.268	0.053	0.008
0.7	0.326	0.209	0.007

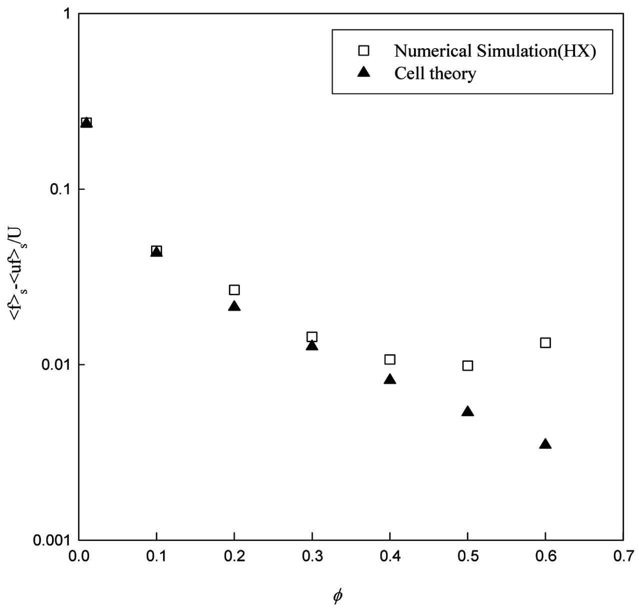

Fig. 3. $\langle f\rangle_s-\langle uf\rangle_s/U$ versus ϕ.

Table 1 also shows the predictions obtained by using the cell theory. The coefficient λ by the cell theory decreases monotonically with ϕ even at high ϕ, unlike the exact calculation results. It seems that the accuracy of cell theory approximation is reduced at high ϕ. However, it is seen that the cell theory is somewhat more accurate for hexagonal arrays, as might be expected based on the observation that a hexagonal cell is closer to the circular cell used in the theory than a square cell, as shown in Fig. 2 representing that a tube at origin is surrounded by six adjacent tubes with equal distance from the tube in hexagonal arrays while eight tubes are placed near a tube at origin with two different distances from the tube in square arrays. Thus the predictions of the coefficient λ by the cell theory are in better agreement with those obtained by exact calculations for the hexagonal arrays than those for square arrays. We see that the agreement between the two is good for area fractions of tubes less than about 0.3.

Lastly, we note that the dispersion in square array is greater than in hexagonal array. It is easily expected that variance of fluid velocity resulting from disturbance by neighboring tubes is larger in square arrays since the neighboring tubes are placed in unequal distance from a tube at origin than that in hexagonal arrays, and thus the dispersion is affected by the velocity variance.

CONCLUSION

We determined Taylor dispersion coefficients for shell-side longitudinal flow along the axes of tubes in square and hexagonal arrays for the case of non-absorbing, non-reacting tube walls. The results for Taylor dispersion coefficients for square and hexagonal arrays are compared with a cell theory approximation for wide range of area fractions of tubes. Agreement between the cell theory and numerical results is excellent at small area fractions. At larger area fractions, the cell theory gives better estimates for hexagonal arrays.

ACKNOWLEDGMENTS

This research was supported by a Korea University grant.

APPENDIX

Formulas for determining the coefficients of regular terms

$$g_n^\alpha=\frac{1}{n!}\partial_1^n T_s^r(\mathbf{x}^\alpha)-\frac{e_{n-2}^\alpha}{4(n-1)}-\frac{G}{64}\delta_{n4} \quad (A1)$$

$$\tilde{g}_n^\alpha=\frac{1}{n!}\partial_1^{n-1}\partial_2 T_s^r(\mathbf{x}^\alpha)-\frac{\tilde{e}_{n-2}^\alpha}{4(n-1)}\frac{n-2}{n} \quad (A2)$$

$$h_n^{\alpha}=\frac{1}{n!}\partial_1^n\psi^r(\mathbf{x}^{\alpha})-\frac{g_{n-2}^{\alpha}}{4(n-1)}-\frac{e_{n-4}^{\alpha}}{32(n-2)(n-3)}+\frac{\delta_{n4}}{64(1-\phi)}-\frac{G}{32\cdot 12\cdot 6}\delta_{n6} \tag{A3}$$

$$\tilde{h}_n^{\alpha}=\frac{1}{n!}\partial_1^{n-1}\partial_2\psi^r(\mathbf{x}^{\alpha})-\frac{n-2}{n}\frac{\tilde{g}_{n-2}^{\alpha}}{4(n-1)}-\frac{n-4}{n}\frac{\tilde{e}_{n-4}^{\alpha}}{32(n-2)(n-3)} \tag{A4}$$

NOMENCLATURE

A_s : area occupied by the shell side fluid
a : radius of tubes
c : concentration of solute on shell side
D_M : molecular diffusivity
D_T : Taylor dispersion coefficient
G : pressure gradient non-dimensionalized by $\mu U/a^2$ in axial direction of tubes
Pe : Peclet number based on shell-side flow
r : radial distance from the center of the tube at origin
U : superficial velocity of the fluid on the shell side
u : fluid velocity on the shell side
$\mathbf{x}^{\alpha}$: position vector of the center of tube a
$\mathbf{x}_L$: coordinates (position vector) of the lattice points of the array
δ : Dirac's delta function
ϕ : area fraction of the tubes
ρ : density of the shell fluid
τ : unit cell area non-dimensionalized by a^2
μ : viscosity of fluid
$\langle c\rangle_s$, $\langle u\rangle_s$: spatial average of c and u over shell side
$\langle a_n\rangle$, $\langle b_n\rangle$, $\langle e_n\rangle$, $\langle g_n\rangle$, $\langle h_n\rangle$: averages of coefficients over N tubes in a unit cell
$\langle A_n\rangle$, $\langle B_n\rangle$, $\langle C_n\rangle$: averages of multipoles over N tubes in a unit cell

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