

k_{Ls} = mass transfer coefficient from liquid to particle, based upon void plus nonvoid surface covered by liquid, cm/s
 k = reaction rate constant, s^{-1}
 L = thickness of rectangular slab of catalyst (dimension perpendicular to face exposed to reactant)
 r_s = radius of spherical catalyst particle, cm
 S_{ext} = external surface of the catalyst particle, cm^2
 Sh_{gLs} = Sherwood number, $K_{Ls}L/D_A$
 Sh_{gs} = Sherwood number, $K_{gs}L/D_A$
 Sh_{Ls} = Sherwood number, $k_{Ls}L/D_A$
 V = volume of catalyst particle (or slab), cm^3
 W = width of the rectangular catalyst slab (dimension of the face of the slab exposed to reactant), cm
 x = coordinate perpendicular to face of slab exposed to reactant, cm
 y = coordinate in the direction of the exposed face of the slab, cm

Greek Letters

ϕ = Thiele modulus of slab equivalent to catalyst particle [Equation (12)]
 ϕ' = modified Thiele modulus, ϕ/F
 η = catalyst effectiveness factor for uniform concentration over the external particle surface (neglect-

ing external mass transfer resistances) [Equation (14)]

η_o = overall catalyst effectiveness factor
 η_L = overall effectiveness factor for the liquid covered surface of the catalyst slab [Equation (15)]
 η_g = overall effectiveness factor for the gas covered surface of the catalyst slab [Equation (17)]

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Convective Mixing in Tube Networks

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Ultman and Blatman (1977a) have recently published a compartmental dispersion model for the analysis of mixing in tube networks based on the solution of the convective diffusion equation presented by Gill and Sankarasubramanian (1970) for the mixing of a gas tracer in fully developed parabolic flow. In their model, Ultman and Blatman ignore the effect of axial velocity profile distortion and consider the velocity to be parabolic in each branch of their tube networks. We present below an analysis of gas dispersion in networks which neglects molecular diffusion but accounts for the effect on gas mixing of pure axial streaming through axial velocity profile distortion.

Comparison of the predictions of this theory with SF₆ data of Ultman and Blatman and with benzene vapor data previously collected by one of the authors suggests that for high Peclet numbers and short residence times, the axial streaming theory is superior to the compartmental dispersion model.

Furthermore, the convective mixing theory may be able to explain the difference in tracer dispersion observed between inspiratory and expiratory flow through a five-generation model of the bronchial airway (Scherer

et al., 1975) on the basis of differences in the longitudinal velocity profiles, although further expiratory velocity profile measurements are necessary before any firm conclusions can be reached.

THEORETICAL ANALYSIS

Consider the three-dimensional laminar stream tube flowing steadily through the symmetric tube network shown in Figure 1. Axial distance x is measured along the tube centers, where x_o represents the point of injection of a gas tracer pulse at time $t = 0$, and x_1 represents a fixed point downstream where the average tracer concentration across the tube is monitored.

If we neglect the bending of the stream tube and the secondary motions induced by the bending, and if we assume the Peclet number au/D is high, the tracer gas concentration in the stream tube is described to a good approximation by the convective transport equation in cylindrical coordinates:

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = 0 \quad (1)$$

If the x dependence of the axial velocity u is neglected, the solution of Equation (1) is

$$c = c_o(x - u(r, \theta)t) \quad (2)$$

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The convective solution [Equation (2)] for the tracer concentration distribution does not apply in regions close to the tube walls where molecular diffusion must be included in order to satisfy the no flux through the wall boundary condition $\partial c / \partial r_{r=a} = 0$. The solution should be a good approximation, however, in regions of the stream tube where the local Peclet number $\gg 1$.

We now define the mean residence time \bar{t} and time variance σ_t^2 observed downstream at point x_1 as

$$\bar{t} = \int_0^\infty t \left\{ \frac{1}{A} \int_A u A c dA \right\} dt \quad (3)$$

and

$$\sigma_t^2 = \int_0^\infty (t - \bar{t})^2 \left\{ \frac{1}{A} \int_A u A c dA \right\} dt \quad (4)$$

where c is given by Equation (2), and the integral $1/A \int_A u A c dA$ represents the fractional tracer concentration per unit time averaged across the stream tube of cross-sectional area A .

Since the integrands of (3) and (4) are continuous in x , r , θ , and t , the order of integration can be interchanged to give

$$\bar{t} = \frac{1}{A} \int_A \left\{ \int_0^\infty t u A c dt \right\} dA \quad (5)$$

and

$$\sigma_t^2 = \frac{1}{A} \int_A \left\{ \int_0^\infty (t - \bar{t})^2 u A c dt \right\} dA \quad (6)$$

Introducing the transformation from t to η , defined by $\eta = x_1 - ut$, noting $\bar{\eta}(x_1, t = 0) = 0$, writing $u = \bar{u} + u'$ where $\bar{u} = 1/A \int_A u dA$, expanding $1/(\bar{u} + u')$ as the series $1/\bar{u}(1 - u'/\bar{u} + (u'/\bar{u})^2 - \dots)$ and keeping only leading terms, we get

$$\bar{t} = \frac{x_1}{\bar{u}} \quad (7)$$

and

$$\sigma_t^2 = \frac{1}{A} \int_A \frac{\sigma_x^2}{u^2} dA + \left(\frac{u'}{\bar{u}} \right)^2 \bar{t}^2 \quad (8)$$

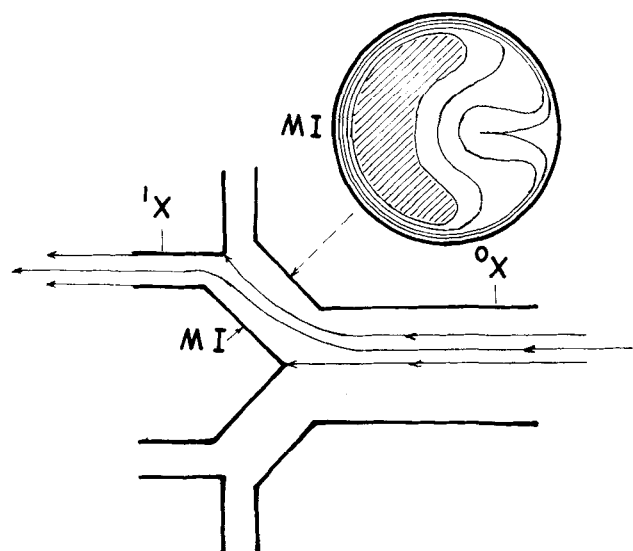


Fig. 1. A stream tube for steady laminar inspiratory flow through a two-generation symmetric branched network. Inset shows isovelocity contours in the tube cross section downstream from the first bifurcation. Shaded region is high speed core against inside wall (I.W.).

where, in doing the integrations, it has been noted that

$$\int_{-\infty}^{+\infty} A c(\eta) d\eta = 1, \bar{\eta}(x_1, t = 0) = 0 \\ = \int_{-\infty}^{+\infty} \eta A c(\eta) d\eta$$

and

$$\sigma_x^2 = \int_{-\infty}^{+\infty} \eta^2 A c(\eta) d\eta$$

The difference in variance $\Delta(\sigma_t^2)$ between that observed at $\bar{t} = 0$ and that observed downstream at $\bar{t} = x_1/\bar{u}$ is, then, from (8)

$$\Delta(\sigma_t^2) = \left(\frac{u'}{\bar{u}} \right)^2 \bar{t}^2 \quad (9)$$

where

$$\left(\frac{u'}{\bar{u}} \right)^2 = \frac{1}{A} \int_A \left(\frac{u'}{\bar{u}} \right)^2 dA \quad (10)$$

The integral appearing in (9) and (10) cannot be evaluated without knowing the lateral boundary of the average stream tube within the model. In order to compare the theory with experimental data, we take an average by integrating over the cross sections of several stream tubes contained within the central physical tube of the model in question. In doing the integrations over the central tube cross section, representative velocity profiles reported in the literature were used (Schreck and Mockros, 1970; Schroter and Sudlow, 1969).

Introduction of the nondimensionalizations

$$\tau = \frac{D}{a^2} \bar{t} \quad \text{and} \quad \tilde{\sigma}^2 = \frac{D^2}{8a^4} \Delta(\sigma_t^2)$$

where a is the physical model central tube radius, allows comparison of the predictions of the above theory with Ultman and Blatman's experimental data for a two-generation network of tubes of constant diameter and with benzene vapor data previously collected by the author (Scherer, 1975). Using the above nondimensionalizations in Equation (9), we finally get

$$\ln(\tilde{\sigma}^2) = 2 \ln \tau + \ln \left[\frac{1}{8} \left(\frac{u'}{\bar{u}} \right)^2 \right] \quad (11)$$

DISCUSSION AND COMPARISON WITH EXPERIMENTS

Equations (9) and (11) show that if mixing by convection alone is considered, the change in the time variance of an injected tracer peak between two points along a stream tube is, to a good approximation, determined by the positive dimensionless velocity profile parameter $(u'/\bar{u})^2$ defined by Equation (10). In Equation (10), the region of integration must extend over only that part of the stream tube cross sections where the convective solution (2) applies. For Poiseuille flow in a straight tube, the approximate boundary of this region r' can be estimated from

$$N_{Pe} = \frac{u(a - r')}{D} \geq 1$$

For the range of air-SF₆ flow rates used by Ultman and Blatman, the tube cross section covered by $0 \leq r' \leq 0.95a$ is appropriate.

Figure 2 shows a comparison of Equation (11) with experimental SF₆ dispersion data collected by Ultman and Blatman (1977a) and with experimental benzene disper-

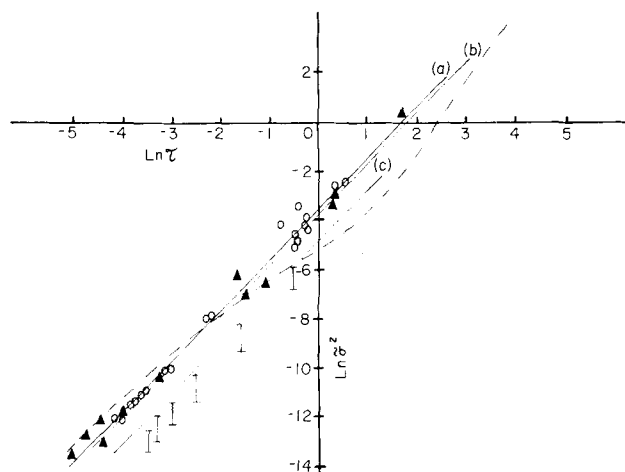


Fig. 2. Comparison of experimental tracer impulse-response data (Δ , \circ , $|$) with the theory of Ultman and Blatman for parabolic flow in a straight tube (dashed curve) and with the straight lines predicted by Equation (11). $\Delta = U, B$ SF₆ data for Poiseuille flow in a straight tube; $\circ = U, B$ SF₆ data for inspiratory flow through a two-generation symmetric network; $|$ = Scherer et al. data for expiratory flow in a five-generation symmetric network. Straight line intercepts are (a) = -3.43, (b) = -3.64, and (c) = -4.78.

sion data (Scherer, 1975) obtained in a five-generation model of the bronchial tree. Also shown for comparison is the prediction of the Ultman and Blatman compartmental mixing model. In Figure 2, line (a) represents the prediction of Equation (11) for Poiseuille flow, line (b) for inspiratory flow in a two-generation network, and line (c) for expiratory flow in a two-generation network.

The first important point of agreement between the convective theory and the experiments is that when experimental values of $\ln \tilde{\sigma}^2$ are plotted against values of $\ln \tau$, the curves are very nearly straight lines, with slopes equal to 2.0, as predicted by Equation (11).

The theoretical intercepts are given by the values of $\ln [1/8 (u'/\bar{u})^2]$ for the various flows. For the case of Poiseuille flow (a) in a straight tube, $(u'/\bar{u})^2$ can be evaluated exactly by integration between the limits $0 \leq r' \leq 0.95a$ to give $\ln [1/8 (u'/\bar{u})^2] = -3.43$, in good agreement with experiment. For the gas dispersions studied in two- and five-generation networks, the values of $(u'/\bar{u})^2$ for forward and reverse flow were calculated by numerical integration of representative velocity profiles (see Figure 1) reported in the literature (Schreck and Mockros, 1970; Schroter and Sudlow, 1969).

The comparison of the convective theory and experiment shown in Figure 2 suggests that for expiratory flow in the five-generation network, the average value of $(u'/\bar{u})^2$ is less than for expiratory flow in a two-generation network (c); that is, the average velocity profile is probably flatter in the five-generation than in the two-generation network. The shift in the theoretical lines (b) and (c) for a two-generation network shows qualitatively the slight decrease in mixing due to the flattening of the velocity profiles in expiratory flow, which has been reported in the literature (Schroter and Sudlow, 1969; Pedley, 1977). It should be noted, however, that Ultman and Blatman (1977a) found no experimental difference in $\tilde{\sigma}^2$ for inspiratory and expiratory flow in their two-generation symmetric tube model. It may be that several generations in series are required to obtain a flat enough velocity profile to influence tracer dispersion.

CONCLUSION

The theory of convective mixing in tube networks presented above is approximate in that axial variation in longitudinal velocity is neglected and only average representative values of the axial velocity profiles within the tube networks are used. Even with these approximations, however, agreement with available experimental data is good. In particular, the SF₆ data reported by Ultman and Blatman (1977a) agree with the theory over a wide range of residence times.

The agreement obtained between the experiments and theory presented here suggests that in regions of tube networks where the Peclet number is greater than about 50, as often occurs in flows of aerosols, liquid dyes, and heavier gases, and for residence times less than about 2 s, $\tau < 1.0$, the major mode of mixing is by convection, and dispersion depends mostly on axial velocity profile distortion.

NOTATION

- A = average cross-sectional area of the stream tube passing through the tube network, cm²
- a = radius of central tube in physical model, cm
- c = fractional tracer concentration normalized by the total tracer mass injected, cm⁻³
- c_0 = fractional tracer concentration injected at $t = 0$, which is uniformly distributed across the tube and a function of x only, cm⁻³
- D = molecular diffusion coefficient, cm²/s
- r = radial cylindrical coordinate, cm
- t = time, s
- \bar{t} = tracer residence time, s
- $u(r, \theta)$ = average value of axial velocity in the stream tube, cm/s
- \bar{u} = mean velocity averaged over stream tube cross-section, cm/s
- x = axial distance along tube centers, cm

Greek Letters

- η = transformation variable, cm
- θ = angular cylindrical coordinate, rad
- σ_t^2 = time variance, s
- $\tilde{\sigma}^2$ = dimensionless time variance
- τ = dimensionless residence time

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