

$E$  = activity (amount) of immobilized enzyme, g  
 $E_r$  = activation energy for reaction, k cal/g mole  
 $E_m$  = activation energy for Michaelis-Menten constant, k cal/g mole  
 $E_d$  = activation energy for deactivation, k cal/g mole  
 $F$  = generalized form of the immobilized enzyme catalyzed reaction expression  
 $g_1, g_2$  = deactivation functions  
 $i$  = constant  
 $I$  = inhibitor concentration, g/l  
 $k$  = reaction velocity constant,  $(s)^{-1}$  (other units dependent on step)  
 $k_d$  = deactivation rate constant,  $(s)^{-1}$  (other units dependent on step)  
 $K_I$  = equilibrium rate constant for inhibitor reaction  
 $K_m'$  = normalized Michaelis-Menten constant,  $K_m/S_{A0}$   
 $p, q$  = constants  
 $R$  = gas constant, cal  $(g \text{ mole}^{-1} \text{ } ^\circ K)^{-1}$   
 $S_A$  = substrate concentration, g/l  
 $S_{A0}$  = substrate concentration at  $t = 0$ , g/l  
 $t$  = time, s  
 $T$  = temperature,  $^\circ K$   
 $X_A$  = fractional conversion of substrate A  
 $Y_A$  = fraction of unconverted substrate A,  $S_A/S_{A0}$

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Manuscript received February 20, 1978; revision received August 25, and accepted September 7, 1978.

## Effectiveness Factors in Trickle-Bed Reactors

P. A. RAMACHANDRAN and J. M. SMITH

University of California  
 Davis, California 95616

Downflow of gas and liquid over a bed of catalyst particles can result in partial coverage, or wetting, of the particles with flowing liquid at low liquid rates (Satterfield, 1975). When this occurs, the concentration around the outer surface of a spherical particle is not uniform, nor is the concentration field within the particle symmetrical with respect to radial position. In this situation, the usual expressions for the effectiveness factor are not applicable. What is needed for design is an overall effectiveness factor  $\eta_o$  based upon bulk stream concentrations, which accounts for the partial liquid coverage. Two approximate solutions are presented in this note; one is an explicit equation for  $\eta_o$ , and the other is a two-

dimensional representation of the catalyst particle requiring numerical solution.

The overall effectiveness factor will include interphase transport effects, and these depend upon the type of reaction. When the limiting reactant is in the gas, but at least slightly soluble in the liquid, mass transfer from gas to liquid and liquid to particle must occur in order for reactant to reach the catalyst from the liquid covered surface. Only mass transfer from gas to particle is necessary for reactant to reach the catalyst on the gas covered part of the particle. An example is the removal of a pollutant from a liquid by catalytic oxidation with air in a trickle-bed reactor. Another possibility is that the limiting reactant is in the liquid phase. Now, reactant reaches the catalyst only through the liquid covered part of the particle, and only liquid to particle mass transfer

affects  $\eta_o$ . Under some conditions, hydrodesulfurization in a trickle bed would correspond to this case. These two types of reactions are considered here. In both cases, it is assumed that the pores of the catalyst particles are completely filled with liquid owing to capillary forces.

## TWO-DIMENSIONAL MODEL

The porous particle is represented by an infinitely long rectangular slab with three sides ( $x = L$ ,  $y = 0$ ,  $y = W$ ) impermeable to reactants and the fourth side ( $x = 0$ ) covered for a distance  $WF$  with liquid and a distance  $(1 - F)W$  with gas (Figure 1).

The system is isothermal and the reaction assumed to be first order and irreversible in limiting reactant A. Then a steady state conservation equation for A, in terms of its intraparticle concentration  $\bar{C}_A$  in the liquid filled pores, is

$$D_A \left( \frac{\partial^2 \bar{C}_A}{\partial x^2} + \frac{\partial^2 \bar{C}_A}{\partial y^2} \right) = k \bar{C}_A \quad (1)$$

The boundary conditions on the three impermeable sides are

$$\frac{\partial \bar{C}_A}{\partial x} = 0 \quad \text{at } x = L \quad (2)$$

$$\frac{\partial \bar{C}_A}{\partial y} = 0 \quad \text{at } y = 0 \quad \text{and } y = W \quad (3)$$

In this two-dimensional model,  $\bar{C}_A$  varies in both the  $y$  and  $x$  directions.

### Limiting Reactant in the Gas

The boundary conditions at  $x = 0$  depend upon the type of reaction. For a gas phase reactant

$$K_{gLs}(C^*_A - C_{A,s}) = -D_A \left( \frac{\partial \bar{C}_A}{\partial x} \right)_{x=0}; \quad \text{for } 0 < y < WF \quad (4)$$

$$K_{gs}(C^*_A - C_{A,s}) = -D_A \left( \frac{\partial \bar{C}_A}{\partial x} \right)_{x=0}; \quad \text{for } WF < y < W \quad (5)$$

The mass transfer coefficients, like  $D_A$ , are based upon the void plus nonvoid outer surfaces of the porous particle. The surface concentrations  $C_{A,s}$  are different in the two equations since the first is for the liquid covered part of the particle surface and the second for the gas covered part. Mass transfer coefficient  $K_{gs}$  will be of the order of a gas to particle mass transfer coefficient and larger than the composite coefficient  $K_{gLs}$  from gas to liquid to particle. It is assumed, in using the composite mass transfer coefficient in Equation (4), that the mass transfer rate from gas to liquid is equal to that from liquid to particle. This will be a reasonable assumption at locations in the reactor where the concentration  $C_{A,L}$  in the bulk liquid is not changing rapidly with axial position. The liquid-phase concentration  $C^*_A$  is that in equilibrium with A in the gas. When Henry's law is valid for A,  $C^*_A = C_{\text{gas}}/H_A$ . If  $K_{gL}$  represents the overall coefficient from gas to liquid, and  $K_{Ls}$  that from liquid to particle, the composite coefficient is given by

$$\frac{1}{K_{gLs}} = \frac{1}{K_{gL}} + \frac{1}{k_{Ls}} \quad (6)$$

### Limiting Reactant in the Liquid

For  $x = 0$ , the boundary conditions are

$$k_{Ls}(C_{A,L} - C_{A,s}) = -D_A \left( \frac{\partial \bar{C}_A}{\partial x} \right)_{x=0}; \quad \text{for } 0 < y < WF \quad (7)$$

$$\left( \frac{\partial \bar{C}_A}{\partial x} \right)_{x=0} = 0; \quad \text{for } WF < y < W \quad (8)$$

The problem formulated by Equations (1) to (5) or by (1) to (3) and (7) and (8) can be solved numerically by a finite-difference method to establish  $\bar{C}_A(x, y)$ . Then, the overall effectiveness factor is obtained by integrating the rate of reaction over the volume (per unit length in the  $z$  direction) determined by the rectangle  $x = L$   $y = W$ . Since  $\eta_o$  is defined by the expression

$$\eta_o = \frac{\text{total rate}}{k C^*_A L W} \quad (9)$$

the equation for the effectiveness factor is

$$\eta_o = \frac{\int_0^L \int_0^W \bar{C}_A dx dy}{C^*_A L W} \quad (10)$$

For a gaseous reactant, the overall effectiveness factor can be expressed as a function of  $K_{gLs}$ ,  $K_{gs}$ ,  $F$  and the Thiele modulus defined as

$$\phi = \frac{V}{S_{\text{ext}}} \sqrt{k/D_A} \quad (11)$$

or

$$\phi = L \sqrt{k/D_A} \quad (12)$$

for the rectangular slab. For a liquid phase reactant,  $\eta_o$  depends upon  $k_{Ls}$ ,  $F$ , and  $\phi$ .

## APPROXIMATE EXPLICIT SOLUTION

### Limiting Reactant in the Gas

Suppose that the slab is divided into two separate parts by a plane at  $y = WF$  (Figure 1). If the additional exposed sides formed by this division are impermeable to reactant, the intraparticle concentration is independent of  $y$  so that the conventional expression for effectiveness factor can be used. Thus, for the liquid covered part of the face, the rate of reaction is given by

$$(\text{Rate})_L = K_{gLs}(C^*_A - C_{A,s})(FW) = k\eta C_{A,s}(FW)L \quad (13)$$

where the particle effectiveness given by the usual expression is

$$\eta = \frac{\tanh \phi}{\phi} \quad (14)$$

Equation (13) may be used to express  $C_{A,s}$  in terms of  $C^*_A$ . Then, Equation (14), with the following definition for the effectiveness factor for the wetted part

$$\eta_L = \frac{(\text{Rate})_L}{k C^*_A W F L}$$

leads to

$$\eta_L = \frac{(1/\phi) \tanh \phi}{1 + (\phi/Sh_{gLs}) \tanh \phi} \quad (15)$$

where

$$Sh_{gLs} = K_{gLs} L/D_A \quad (16)$$

A similar development for the part of the face covered by gas leads to

$$\eta_g = \frac{(1/\phi) \tanh \phi}{1 + (\phi/Sh_{gs}) \tanh \phi} \quad (17)$$

where

$$Sh_{gs} = K_{gs}L/D_A \quad (18)$$

Finally, assume that the overall effectiveness factor is given by the weighted average of the wetted and gas covered parts. Then

$$\eta_o = \frac{(F/\phi) \tanh \phi}{1 + \frac{\phi}{Sh_{gLs}} \tanh \phi} + \frac{[(1-F)/\phi] \tanh \phi}{1 + \frac{\phi}{Sh_{gs}} \tanh \phi} \quad (19)$$

Figure 2 shows  $\eta_o$  as a function of the mass transfer coefficients and the Thiele modulus for  $F = 0.75$ . The solid curve represents the explicit solution of Equation (19), while the dotted line corresponds to the numerical solution given by Equation (10) and Equations (1) to (5). The explicit and numerical solutions differ by no more than 13% for these particular values of  $F$ ,  $Sh_{gLs}$ , and  $Sh_{gs}$ .

Figure 2 demonstrates that as the ratio  $Sh_{gs}/Sh_{gLs}$  increases,  $\eta_o$  increases. This is due to the increased rate of direct mass transfer on the gas covered part of the particle surface. Because of the same mass transfer effects, it is expected that the effectiveness factor would decrease as the fraction of surface wetted by liquid increases. Figure 3 shows this decrease for two values of  $\phi$  and a specific set of Sherwood numbers. Such a decrease has been noted earlier (Colombo et al, 1976; Satterfield, 1975; Sedricks and Kenney, 1973).

#### Limiting Reactant in the Liquid

For a liquid phase reactant, a similar, explicit expression can be postulated. In this case it is instructive to use the modified Thiele modulus proposed by Dudukovic (1977). This modulus is based upon the wetted, external area

$$\phi' = \frac{V}{S_{L,ext}} \left( \frac{k}{D_A} \right)^{1/2}$$

For our rectangular slab approximation

$$\phi' = \frac{LW}{WF} \left( \frac{k}{D_A} \right)^{1/2} = \phi/F \quad (20)$$

Then, the usual expression for  $\eta$  is

$$\eta = \frac{F \tanh (\phi/F)}{\phi} \quad (21)$$

With these definitions, the equation for  $\eta_o$  is

$$\eta_o = \frac{\frac{F}{\phi} \tanh (\phi/F)}{1 + (\phi/Sh_{Ls}) \tanh (\phi/F)} \quad (22)$$

where

$$Sh_{Ls} = k_{Ls} L/D_A \quad (23)$$

Here, the overall effectiveness factor is based upon the bulk concentration in the liquid  $C_{A,L}$ . When the mass transfer resistance from liquid to particle is negligible,  $Sh_{Ls} \rightarrow \infty$ , and Equation (22) reduces to the expression proposed by Dudukovic (1977) for a particle with pores completely filled with liquid.

For a liquid phase reactant, comparison of the explicit solution given by Equation (22) with the numerical solution shows somewhat larger deviations than for the gaseous reactant case. For the liquid phase reactant case, steep gradients would occur within the slab in the  $y$  direction. These gradients are not accounted for in the

explicit solution while they are considered in the numerical approximation.

#### APPLICATION OF APPROXIMATION METHODS

Herskowitz et al. (1978) has measured rates for the hydrogenation of  $\alpha$ -methyl styrene in a trickle-bed reactor operated at 40.6°C and 1 atm. The catalyst bed (palladium/aluminum oxide particles) was short so that the

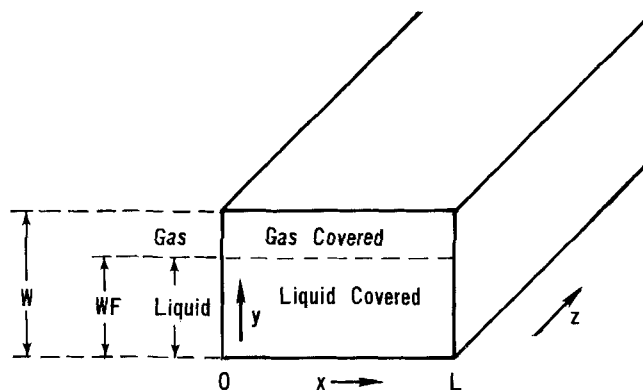


Fig. 1. Rectangular slab catalyst particle (face at  $x = 0$  exposed to reactant; five other faces impermeable).

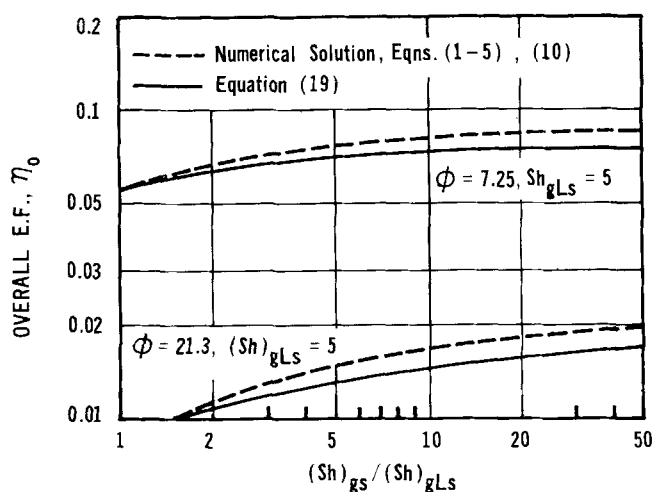


Fig. 2. Effectiveness factors for a gas-phase limiting reactant for  $F = 0.75$ .

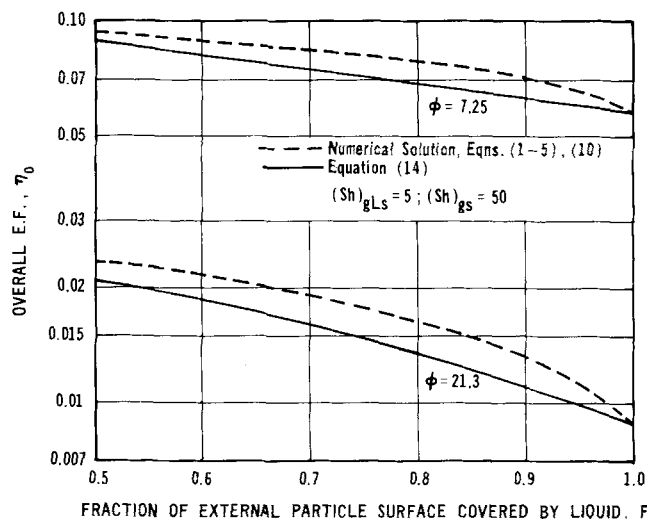


Fig. 3. Effectiveness factors as a function of fraction wetted for a gas-phase limiting reactant.

TABLE 1. DATA FOR HYDROGENATION OF  $\alpha$ -METHYL STYRENE  
[HERSKOWITZ ET AL., 1978]

Reactor ID = 2.54 cm  
Mass of catalyst particles = 1.0g  
Catalyst particle density = 1.53 g/cm<sup>3</sup>  
Catalyst particles (spherical) radius,  $r_s$  = 0.081 cm  
Bed void fraction = 0.48  
Porosity of catalyst particles = 0.50

Experimental, overall effectiveness factors  $\eta_o$

Liquid flow rate 10 <sup>2</sup> , cm/s	Ext. surface covered by liquid, $F$	Mass transfer coefficient $K_{gLs} \times$ cm <sup>3</sup> /s	0.75% Pd catalyst $\eta_o$	2.50% Pd catalyst $\eta_o$
0.25	0.72	0.55	0.056	0.018
0.50	0.79	1.15	0.061	0.016
0.75	0.82	1.79	0.065	0.015
1.00	0.84	1.98	0.066	0.015
1.60	0.90	3.02	0.072	0.015
2.0	0.93	3.30	0.073	0.014
3.0	0.96	3.85	0.075	0.014
5.0	0.95	3.85	0.076	0.014
7.0	0.95	4.40	0.080	0.015
10	1.0	5.50	0.086	0.015

conversion was low (differential reactor conditions). The gas phase entering the bed was pure hydrogen, and the liquid was  $\alpha$ -methyl styrene saturated with hydrogen. This is an example of the limiting reactant being in the gas phase so that hydrogen was supplied from both gas and liquid covered parts of the external surface of the particles.

Reaction rates were measured over a wide range of liquid flow rates and for two catalyst activities (corresponding to 0.75 and 2.50% palladium on aluminum oxide). Experimental values of  $\eta_o$  were evaluated from the data from an expression similar to Equation (9). These overall effectiveness factors and other information about the reactor system are given in Table 1 for the two catalyst activities.

Since the gas was pure hydrogen, the resistance to mass transfer on the gas covered surface of the particles could be neglected ( $K_{gs} \rightarrow \infty$ ). The observation that the rate did not vary with gas flow rate provided addi-

tional evidence for this assumption of equilibrium between the gas and the liquid filled pores. Using a three-dimensional simulation of the catalyst particles and the data for the two catalyst activities, Herskowitz et al. (1978) were able to evaluate  $F$  and  $K_{gLs}$  for each liquid flow rate. These results are also given in Table 1. The values of  $F$ , increasing to unity with increasing flow rate, are typical of information available in the literature (Satterfield, 1975). Also, the results for  $K_{gLs}$  are in reasonable agreement with composite mass transfer coefficients evaluated from available correlations for trickle-bed reactors (Goto and Smith, 1975).

To predict  $\eta_o$  by the explicit method, Equation (19) with  $Sh_{gs} = \infty$  is applicable. To use this expression, the Thiele modulus and  $(Sh)_{gLs}$  are required. From experiments independent of the trickle-bed data, it was found that  $D_A = 0.90 \times 10^{-4}$  cm<sup>2</sup>/s, and  $k = 6.58$  s<sup>-1</sup> (0.75% palladium catalyst) and 56.1 s<sup>-1</sup> (2.5% palladium). Since the modulus for spherical particles is  $(r_s/3)\sqrt{k/D_A}$ , comparison with Equation (12) shows that  $L$  equal to  $r_s/3$  should be used in calculating the modulus for use in the approximate solutions. Then,  $\phi = 7.25$  (0.75% palladium) and  $\phi = 21.3$  for the 2.5% palladium particles. In evaluating  $(Sh)_{gLs}$ , this same characteristic length, along with the values for  $D_A$  and  $K_{gLs}$ , was employed. In Figure 4 are shown the experimental  $\eta_o$  and values (solid curve) calculated from Equation (19) for both catalyst activities. To see the effect of incomplete wetting,  $\eta_o$  was also calculated from Equation (19) for  $F = 1$  for the 0.75% palladium catalyst. The effectiveness factors are now reduced significantly, as indicated by the dashed line. Equation (19) includes the effect of gas to liquid to particle mass transport, and this was important in this example. This is evident by comparison with the upper, dot-dash curve which was prepared by neglecting the mass transfer resistance, that is, by taking  $F = 1$  and  $(Sh)_{gLs} = \infty$ . The much larger effectiveness factor is independent of liquid flow rate. This application, at least, suggests that the simple approximation given by Equation (19) may be useful for obtaining a reasonable estimate of  $\eta_o$ .

#### ACKNOWLEDGMENT

This work was supported financially by NSF Grant ENG-76-01153.

#### NOTATION

- $\bar{C}_A$  = concentration of reactant A in the liquid filled pores within the rectangular catalyst slab;  $C_A^*$  is the concentration in the liquid in equilibrium with  $C_g$  in gas phase;  $C_{A,L}$  is the concentration in the bulk liquid;  $C_{A,s}$  is the concentration in the liquid at the surface of the particle, moles/cm<sup>3</sup>
- $D_A$  = effective diffusivity of A (based upon void plus nonvoid area) within the pores of the catalyst, cm<sup>2</sup>/s
- $F$  = fraction of the external particle surface covered by liquid
- $H_A$  = Henry's law constant for A,  $C_g/C_A^*$
- $K_{gs}$  = mass transfer coefficient, gas to particle, based upon void plus nonvoid surface covered by gas, cm/s
- $K_{gLs}$  = composite mass transfer coefficient from gas to particle based upon void plus nonvoid surface covered by liquid, cm/s
- $K_{gL}$  = overall mass transfer coefficient from gas to liquid, based upon void plus nonvoid surface cov-

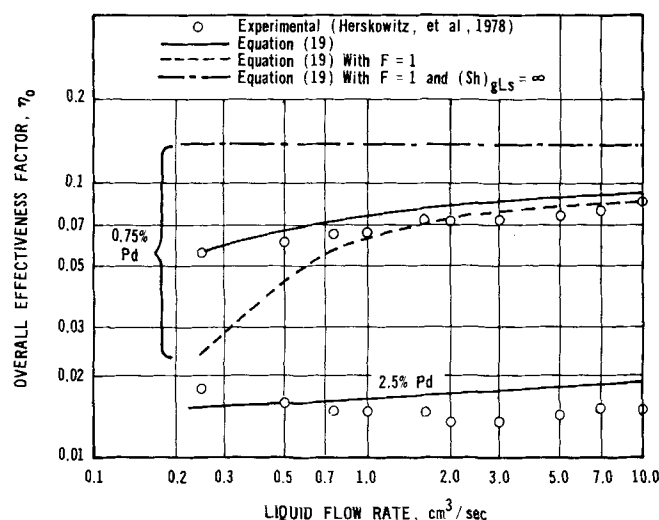


Fig. 4. Overall effectiveness factors for hydrogenation of  $\alpha$ -methyl styrene.

$k_{Ls}$  = 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

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

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

$\eta_o$  = overall catalyst effectiveness factor  
 $\eta_L$  = overall effectiveness factor for the liquid covered surface of the catalyst slab [Equation (15)]  
 $\eta_g$  = overall effectiveness factor for the gas covered surface of the catalyst slab [Equation (17)]

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Manuscript received June 2, 1978; revision received September 1, and accepted September 7, 1978.

## Convective Mixing in Tube Networks

PETER W. SCHERER

and

FREDERICK R. HASELTON

Department of Bioengineering  
 College of Engineering and Applied Science  
 University of Pennsylvania  
 Philadelphia, Pennsylvania 19104

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 SF<sub>6</sub> 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

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

Correspondence concerning this note should be addressed to Peter W. Scherer.

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