# PHYSICAL MODEL FOR MASS TRANSFER IN A PACKED BED

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This is to certify that the

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### ABSTRACT

## PHYSICAL MODEL FOR MASS TRANSFER IN A PACKED BED

By

#### Raymond Leon Porter

A new method for calculating mass, heat and momentum transfer between particles of a fixed bed and the fluid flowing through it is shown. Overall mass and heat transfer coefficients and pressure loss per unit length of bed are computed from fluid properties--viscosity, heat capacity, superficial velocity, thermal conductivity, density, diffusion coefficient of active component through the fluid; and the bed characteristics--porosity, particle size, specific surface per unit volume and an index defining the distribution of passage cross sections within the bed. Values calculated for gases in the Reynolds number range from 5 to 33,000 show an average deviation of 3% from literature correlations [5, 8, 15, 31, 40, 54, 58]. Values for liquids in the Reynolds number range from 0.003 to 33,000 and for Schmidt numbers up to 70,600 deviate an average of 5% from literature results [15, 27, 54, 59, 60]. These figures are for fixed beds with voids fractions ranging from 0.38 to 0.70.

It is believed that the values calculated in ranges not corroborated by experimental investigators are of equivalent accuracy. This is because the method developed in this thesis is not a simple correlation of experimental data, but is based on a theoretical treatment of a reasonable physical model for a packed bed using principles of fluid dynamics and transport phenomena.

The physical model consists of a network of passages arranged in parallel and series with complete mixing assumed at the passage junctions. The passages are assumed to have a distribution of cross sections as described by the index mentioned above. This distribution of cross sections has an effect on coefficients computed for the complete Reynolds number range. Its effect is greatest at extremely low Reynolds numbers where it gives Nusselt and Sherwood numbers which are considerably lower for the bed than for the limiting values of the individual passages.

In the region of fully developed velocity profiles through the passages, treatment of the passages as cylinders with lengths equal to packing size proved to be satisfactory and convenient. In the region of developing boundary layers the length was taken to be half the packing size to allow for boundary layer separation over surfaces curved in the direction of flow. Typically it occurs at about 90 degrees around the curve for surfaces such as cylinders or spheres.

The method presented here is in the form of a computer program due to the complexity of handling different cross sections in parallel with different flow patterns in the various cross sections. PHYSICAL MODEL FOR MASS TRANSFER IN A PACKED BED

By

Raymond Leon Porter

# A THESIS

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## INTRODUCTION

A large number of chemical processes, especially catalytic processes, are carried out in packed bed reactors. With improvements in catalytic reactors, ion exchange columns, leaching beds, chromatographic columns and gas adsorbers, it has become increasingly important to predict accurately the performance of packed beds. Proper design involves a knowledge of heat, mass and momentum transport between fluid and solid surfaces.

Mass transfer between the packing and the flowing fluid can occur in either direction depending upon the process. In either case the physical phenomena is similar. There is a transfer of some chemical specie to and from the phase boundary through a series of resistances. Resistances may be due to diffusion in either phase, laminar or turbulent convection in the fluid, or due to slow chemical formation or reaction of the active chemical substance.

In some processes the controlling resistance is in the flowing fluid, such as in a catalytic reactor where there is a slow flow rate and a fast chemical reaction rate. In such a case the size of the equipment is determined by the mass transfer rate between the fluid and solid particles. When the fluid flow rate is rapid and the reaction rate is slow, chemical kinetics dictates the design. Knowledge of the mass transfer rate for a particular process is essential for design and it is dependent upon the type of heterogeneous system.

Mechanism of mass transfer has been explained by several theories. The film concept assumes that most of the resistance to mass transfer occurs in a stagnant layer next to the solid surface. Mass transfer through the film is by diffusion. Boundary layer studies show that there is also considerable resistance in the bulk flow stream and in the buffer region next to the film adhering to the solid surface. Another completely different explanation called the 'penetration theory' holds that the flowing fluid is a mass of eddies which continually expose fresh surfaces of fluid to the solid. No matter which theory is followed mass transfer rates are generally expressed in terms of a mass transfer coefficient,  $k_c$ , just as heat transfer rates are given in terms of a heat transfer film coefficient, h.

Variables influencing mass transfer coefficients in packed beds are size and shape of the voids, viscosity and density of the flowing fluid, and the diffusivity of the active substance in the fluid. As with many other chemical engineering processes, correlations are effected using dimensionless groups. The common ones for mass transfer are Reynolds number, Schmidt number and Sherwood number. Reynolds number is a measure of fluid flow rate. Schmidt number contains only the physical properties of the fluid and its active component which makes it similar to the Prandtl number of heat transfer. Sherwood number contains the mass transfer coefficient and the diffusivity and is analogous to the Nusselt number of heat transfer. For packed beds particle diameter is commonly used in place of effective diameter of voids and fluid velocity based on empty cross sectional area is used in place of interstitial velocity.

For flow through pipes the analogy between heat and mass transfer exists because they both occur due to molecular diffusion and

convective mixing. Thus heat transfer correlations can be used to calculate numerical values for mass transfer rates to or from pipe walls. There is, however, less literature data concerning heat transfer in packed beds than there is for mass transfer.

Momentum transfer, in terms of pressure drop, in a packed bed can easily be determined from existing equations. However, attempts to show the analogy between momentum and mass transfer have not been successful.

Most of the correlations for mass transfer in packed beds are given in the literature by a relationship between Reynolds number and Sherwood number divided by Schmidt number to the one-third power. Recent correlations give mass transfer rates which are in reasonable agreement with reliable reported data. The best correlations are for liquids flowing at high Reynolds numbers. For gases at lower Reynolds number flow rates, correlations are more difficult because diffusion coefficients are so much higher for gases than for liquids. Equations necessarily have to be more complicated.

Keeping in mind all of the complexities of packed beds it was decided to formulate a physical model for a packed bed which would take into account factors such as fluid properties, packing arrangements, nature of flow and the inter-relationships among these factors. Due to the ready availability of digital computers it was thought that a fairly sophisticated model could be devised which could be readily solved by the computer for desired results.

For simplicity reasons it was decided to derive the model on the basis of heat transfer and then make the necessary analogies for application to mass transfer. It was also thought that some

correlation could be obtained between mass and momentum transfer in packed beds, namely an equation in which mass transfer coefficient is a function of pressure loss per unit length of bed.

#### LITERATURE SURVEY

#### PACKED BEDS

The scientific means by which mass transfer occurs in packed beds has been investigated by many persons. One of the first investigations was by Colburn [9] in 1933 who wrote an analogy between frictional resistance to fluid flow, heat transfer and mass transfer which was based on flow through tubes and across tube banks. He reported the equation:

$$Nu = 0.33 \text{ Re}^{-6} \text{ Pr}^{1/3}$$

for heat transfer across tube banks. Using the same analysis Chilton and Colburn [7] later suggested as a basis for correlation of heat transfer data the following equation:

 $h/CG Pr^{2/3} = J_h = f(Re_p)$ 

and for mass transfer a similar equation:

$$k_{c}$$
 **Q**/G Sc<sup>2/3</sup> = J<sub>d</sub> = f(Re<sub>p</sub>)

Graphs of J versus Reynolds number were presented for turbulent flow inside tubes, across tube banks and parallel to flat plates. They reported that the mass transfer equation disregarded free convection at low Reynolds numbers and any liquid film resistance at the gasliquid interface on the tubes. Mass velocity was for the relative motion between the two phases. By using water evaporation data from a through circulation dryer experiment Gamson, Thodos and Hougen [19] reported values of  $J_d$  averaged about 8% lower than  $J_h$  values. They assumed in the calculations that the surface temperature of the particles was equal to the adiabatic saturation temperature. One of their recommended equations was:

$$J_d = 16.8 (Re_p)^{-1}$$
 for  $Re_p < 40$ 

Sherwood [50] pointed out that if the surface temperature were not at the adiabatic saturation temperature the  $J_d$  values could vary widely whereas the  $J_h$  values would vary little.

Wilke and Hougen [57] used the same type of experiment as Gamson et. al. and by controlling heating conditions and changing the method of wetting the packing arrived at a different equation.

$$J_d = 1.82 (Re_p)^{-.51}$$
 for  $Re_p < 100$ 

They also assumed the surface temperature to be equal to the adiabatic saturation temperature.

Hurt [25] used different sizes and shapes of packing and measured the height of a transfer unit for gas controlled systems. He showed good agreement between heat and mass transfer factors when employing cylindrical particles. The relationship between height of a transfer unit and  $J_d$  is:

$$J_{d} = Sc^{2/3}/(H_{t})a$$

where a is the specific surface area per unit volume. The agreement was poor for other packing shapes. Hurt did not, however, report the surface area or the voids fraction of his packed beds. Resnick and White [45] ran experiments with fixed and fluidized beds of naphthalene particles. Results showed J values lower than those of Gamson et. al. which was attributed to the use of smaller particles.

McCune and Wilhelm [36] obtained data for the mass transfer in both fixed and fluidized bed between flakes of P-naphthol and flowing water. Gamson [18] collected data for water evaporation from porous particles into a flowing air stream. Hobson and Thodos [24] observed data during mass transfer to water or methyl ethyl ketone adsorbed on fixed bed particles. Brötz [6] analyzed these authors' data and came up with the equations:

$$J_{d} = 1.46 (Re_{p})^{-.41} (1 - \epsilon)^{.61} \qquad \text{for } Re_{p} / (1 - \epsilon) > 100$$
$$J_{d} = 17 (Re_{p})^{-1} (1 - \epsilon)^{1.2} \qquad \text{for } Re_{p} / (1 - \epsilon) < 100$$

using an equivalent diameter for particle diameter.

By changing temperature and pressure, the effect of gas properties on the mass transfer coefficient was studied by Shulman and Margolis [51]. They reported that  $J_d$  was independent of pressure in their equation:

$$J_{d} = 1.195 \left[ \frac{Re}{p} / (1 - \epsilon) \right]^{-.36}$$

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Hobson and Thodos [24] measured evaporation rates of water and organic compounds from spherical packing into air, carbon dioxide, ammonia and nitrogen. It was found that the temperature of the bed decreased linearly in the direction of flow but the Schmidt number remained practically constant, so the temperature effect was disregarded. Ergun [12] correlated a mass of experimental data and arrived at an equation for pressure drop in packed beds in terms of dimensionless groups.

$$(-\Delta P)g_{c}^{D}p\varepsilon^{3}/[\rho u^{2}L(1-\varepsilon)] = 150(1-\varepsilon)/Re_{p} + 1.75$$

At low Reynolds numbers the 1.75 is negligible and at high Reynolds numbers it is dominant.

Chu, Kalil and Wetteroth [8] correlated data on heat and mass transfer in liquid-solid and gas-solid systems and arrived at the equation:

$$J_d = 1.77 [(Re_p/(1 - \epsilon)]^{-.44}$$
 for 30 <  $Re_p/(1 - \epsilon)$  < 5000

**Epstein** [11] determined an axial mixing factor to correct heat and mass transfer coefficients to account for non-plug flow in packed beds. The fixed bed is treated as a series of perfect mixers in his mathematical treatment.

Thoenes and Kramers [54] determined mass transfer coefficients for fluids flowing around single active spheres surrounded by similar inactive spheres using eight different packing arrangements. The acive spheres were either soluble in the flowing fluid or were porous and soaked with liquid which evaporated into a gas stream. Graphs of  $[Sh_p/Sc^{1/3}][\epsilon/(1 - \epsilon)]$  (which is equivalent to  $\epsilon J_d Re_p/[1 - \epsilon]$ ) versus  $Re_p/(1 - \epsilon)$  were presented. A review of 438

mass transfer measurements was expressed by the equation:

$$Sh_{p}[\epsilon/(1-\epsilon)] = 1.0 Sc^{1/3} [Re_{p}/(1-\epsilon)]^{1/2}$$

which was said to be good for a  $\text{Re}_{\text{D}}$  /(1 -  $\epsilon$ ) range between 40 and 4000,

a voids fraction range between 0.25 and 0.50 and a Schmidt number range between 1 and 4000. It was said to have a mean deviation of  $\pm$  10%. An even better correlation was obtained by assuming that the total mass transfer was due to three contributions: laminar convective transfer, turbulent convective transfer and one for diffusion in stagnant areas. The latter is important for gas flows at Reynolds numbers less than 500. For gases the stagnant regions near the contact points of adjacent spheres are important because diffusion coefficients for gases are so much larger than for liquids. The following equation was correlated:

$$Sh_{p}[\epsilon/(1-\epsilon)] = 1.26 Sc^{1/3}[Re_{p}/(1-\epsilon)]^{1/3} + 0.054 Sc^{4}[Re_{p}/(1-\epsilon)]^{.8}$$
$$+ 0.8 [Re_{p}/(1-\epsilon)]^{.2}$$

in which the first term is for laminar convection, the second for turbulent convection and the last for diffusion.

Al-Khudayri [1] made a correlation for predicting the mass transfer coefficient in packed beds. The correlation is a plot of  $[Sh_p/Sc^{1/3}][\epsilon/(1 - \epsilon)]$  versus  $Re_p/(1 - \epsilon)$ . For liquid-solid systems the deviation of experimental data of other investigators was 30% and was higher for gas-solid systems. His experimental work consisted of the absorption of ammonia from a helium-ammonia flow stream onto the surface of 0.726 cm. diameter alundum spheres coated with copper II chloride. Laminar flowswere used and mass transfer coefficients were calculated from the data. His results checked closely with those of other investigators for gases at low flow rates. Al Khudayri pointed out that void volume and void surface area are more valid to use than packing diameter when expressing the mass

transfer characteristics of the bed. If packing diameter is used, a correction needs to be made to compensate for variations in voids fraction.

DeAcetis and Thodos [10] made careful temperature measurements of air and packing surface during the evaporation of water from the surface of porous ceramic spheres into an air stream. They found that contrary to usual assumptions, temperature of the packing surface is not the same as the wet-bulb temperature of the entering air, unless high air flow rates are used. They summarized their date and that of other investigators up to 1960 in graphs of  $J_h$  and  $J_d$  versus  $Re_p$ . The ratio of  $J_h$  to  $J_d$  reported was 1.51 compared to the value of 1.08 given by Gamson, Thodos and Hougen which was obtained on the assumption that the temperature of the air entering the bed.

Bradshaw and Bennett [5] measured mass transfer coefficients for air flowing through short beds of naphthalene spheres and cylinders. They reported the equation:

$$J_d = 2.0/\text{Re}_p \text{Sc}^{1/3} + 1.97/\text{Re}_p^{1/2}$$

which was said to cover the Reynolds number range from 40 to 10,000.

Sen Gupta and Thodos [22] analyzed the data of other workers and found  $J_d$  to be inversely proportional to voids fraction for mass transfer to flowing gases in packed beds.

Kusik and Happel [31] made a theoretical study of gas diffusion rates in packed beds using a free-surface model (spherical particle surrounded by a spherical envelope) with boundary layer theory. The Reynolds number  $(\text{Re }/\epsilon)$  range covered was from 100 to 1000 with p voids fractions of 0.3 to 1.0. Simplified forms of momentum and diffusion equations were solved to predict dissolution rates in a particle bed and to analyze the effects of molar velocity perpendicular to the spherical catalytic surface. Boundary layer equations were solved by using Pohlhausen's method of introducing polynomials describing velocity and density distributions. One equation arrived at was:

$$\frac{1}{3} = 0.93[\varepsilon - 0.75(1 - \varepsilon)(\varepsilon - 0.2)]^{-1/2} \operatorname{Re}_{p}^{1/2}$$

The authors confirm that the change in boundary layer thickness due to normal convective velocity was the same for boundary layers on spheres as for flat plate geometry. The results of the study showed that the assumption in film theory that the film thickness does not change with mass transfer rate is correct. This means that film theory can be used for the bulk of chemical engineering problems involving heterogeneous catalysis.

Williamson, Bazaire and Geankoplis [59] obtained liquid phase mass transfer coefficients for packed beds of benzoic acid spheres with water passing through. The recommended equations were:

St Sc.<sup>58</sup> = 2.40 
$$(\text{Re}_{p}/\epsilon)^{-.66}$$
  
for Re<sub>p</sub>/ $\epsilon$  from 0.08 to 125 and:  
St Sc.<sup>58</sup> = 0.442  $(\text{Re}_{p}/\epsilon)^{-.31}$   
for Re<sub>p</sub>/ $\epsilon$  from 125 to 5000.

Galloway and Sage [16] developed analytical expressions for heat and mass transport from spheres to a turbulent air stream taking into account Reynolds number, sphere diameter, and level of turbulence. Sphere size ranged from droplets to 1 ft. in diameter and superficial Reynolds number values ranged from 2 to  $1.33 \times 10^6$ . By analyzing the works of other investigators it was shown by graphical means that the assumption of Nusselt number to be a single valued function of the square root of Reynolds number leads to an average deviation of 60%. Their analysis begins with the Frossling [14] equation for macroscopic transfer from spheres with zero turbulence:

Nu = 2.00 + 0.552 Re 
$$\frac{1/2}{p^{\infty}}$$
 Pr.

Relationships derived for predicting convective thermal and material transport were:

$$[(Nu - 2.00)]/Re_{p^{\infty}}^{1/2} Pr_{\infty}^{1/3} = 0.538 + 0.1807 d^{1/2} + 0.328$$
$$a_{t} (a_{t} + 0.0405)Re_{p}^{1/2}$$
$$[(Sh - 2.00)]/Re_{p^{\infty}}^{1/2} Sc_{\infty}^{1/3} = 0.439 + 0.1807 d^{1/2} + 0.234$$
$$a_{t} (a_{t} + 0.0500)Re_{p}^{1/2}$$

where d is sphere diameter and a is the longitudinal level of turbulence.

Mickley, Smith, Korchak [37] measured velocity profiles and turbulence parameters in the voids of a 1 ft. square bed of rhombohedrally arranged 1.5 in. diameter table tennis balls. A hot wire anemometer was used and the superficial Reynolds number range covered was from 4780 to 7010. Turbulence energy spectra showed that eddy shedding behind the particles did not occur in the wolds between spheres. Since high heat transfer coefficients are known to be caused by eddy shedding and high turbulence level, the high local heat transfer coefficients in the volds characteristic of rhombohedral packing must be explained by a high level of turbulence intensity. The mean void velocity showed a maximum within 1.5 particle diameters from the wall. There was a 10% difference in the mean velocity at the center of the bed compared with the maximum region.

Rhodes and Peebles [46] determined local mass transfer rates at room temperature by measuring radius changes in 1.5 in. diameter benzoic acid spheres by passing water around them at various flow rates using simple cubic and rhombohedral packing arrays. The Reynolds number range covered was from 166 to 3410 based on superficial velocity. Mass transfer tests were carried out by placing the test sphere in an assembled array of inert, insoluble spheres. Analysis of results for the cubic array (voids fraction ~= 0.4764), in terms of Sherwood number versus degrees from the front stagnation point, suggested that the flow pattern around the test sphere had the following characteristics: (a) The region around the forward contact point (0 to 10 deg.) showed the minimum mass transfer rate. (b) The over-all maximum mass transfer rate occurs between 50 to 80 degrees forward from the front stagnation point. It was suggested that this is the ring of attachment of the boundary layer of the sphere above. In this region mass transfer rates are 2.2 to 3 times the over-all

average. A streamline arriving at this location splits into two streamlines: one circling upward forming the principle eddy of the wake of the preceding sphere and the other streamline attaching itself as a boundary layer that follows along the sphere surface until it reaches a ring of separation between 103 and 122 degrees depending upon the Reynolds number. (c) A region of essentially zero mass transfer occurs where there is a point of contact between spheres. (d) The region to the rear of the separation ring is a wake region where the local mass transfer rates are less than the average over the entire sphere. In the rhombohedral array (voids fraction = 0.2595) the orientation of packing was such that each sphere was entirely behind another sphere in the flowing stream. thus giving the limiting case for investigating extremes of local mass transfer rates. Considerably higher maximum Sherwood numbers were reported between 30 and 50 degrees from the front stagnation point than for the cubic array.

Wilson and Geankoplis [60] reported studies of mass transfer and reviewed earlier works. They used a bed of randomly packed benzoic acid spheres with an average diameter of 0.251 in. Water or propylene glycol were allowed to flow down through the bed. For superficial Reynolds numbers between 55 and 1500 and voids fractions between 0.35 and 0.75 they recommend:

$$eJ_{d} = 0.250/Re_{p}^{0.31}$$

Between superficial Reynolds numbers of 0.0016 and 55 the equation given was:

$$eJ_{d} = 1.09/Re_{p}^{2/3}$$

This equation was shown to correlate data over a Schmidt number range of 165 to 70,600.

Petrovic and Thodos [40] determined mass transfer factors in a packed bed by vaporizing water and heavy hydrocarbons from the surface of 0.0721 to 0.370 in. diameter random packed spheres into air. Using this data and recalculating various other studies by Thodos and coworkers to correct the data for axial mixing, their recommended equation is:

$$eJ_{d} = 0.357/Re_{p}^{0.359}$$

The results of this study covered the superficial Reynolds number range between 3 and 230 for voids fractions between 0.416 and 0.778 and were said to hold for solid-gas systems subjected to either upward or downward flow.

Satterfield [48] compared the equations of Wilson and Geankoplis and Petrovic and Thodos and found that they only differ 15% or less over a range of superficial Reynolds numbers between 55 and 1500.

Gillespie, Crandall, and Carberry [20] measured local and overall heat transfer coefficients in two random packed beds of 1 in. diameter brass spheres. Air was passed through the packing at flows corresponding to a Reynolds number range of 120 to 1700, based on superficial velocity and sphere diameter. Local heat transfer coefficients were measured in the first, second and nineteenth layers of packing. Average heat transfer coefficients were determined at 25 places in the bed. By examining the local heat transfer distribution the existence of a laminar boundary layer was verified. Highest values of heat transfer coefficient were obtained

for the surface perpendicular to the bulk flow in the bed. It was also observed from heat transfer coefficient profiles that at high Reynolds numbers the flow may rejoin the sphere and begin to build another boundary layer which subsequently separates. The effect of repacking of the bed was to change the range of local heat transfer coefficients, but the variation within the range was about the same. The entrance effect of the bed has been shown to result in a lower heat transfer coefficient in the top layer than in the bulk of the bed. This has been attributed to a lower incident flow rate and turbulence intensity. The effect of lateral position on average heat transfer coefficient showed higher coefficients near the wall than at the center of the bed.

Wilkins and Thodos [58] studied the evaporation of n-decane into air from the surface of 0.1 in. diameter celite spheres in both a random packed bed and a fluidized bed. Using their results and those of other investigators they obtained the relationship:

$$\varepsilon J_d = 0.589/Re_p^{0.427}$$

Jolls and Hanratty [27] used electrochemical techniques and studied details of flow around an instrumented 1 in. diameter nickel plated brass-bronze ball located 7 to 8 inches from the top in a dumped bed (voids fraction = 0.41) of 1 in. diameter glass spheres. Reynolds number (based on empty cross-section) ranged from 5 to 1100 and the Schmidt number of the flowing fluid was 1700. A transition from laminar to turbulent flow was found to occur in this system over a Reynolds number range from 110 to 150. The electrochemical reaction consisted of the reduction of the ferricyanide ion on the nickel cathode (test sphere) and oxidation of the ferrocyanide ion on a nickel pipe anode located outside the column. Electrode lead wires were placed at various points around the sphere. With the exception of the very rearward portion of the sphere the effect of Reynolds number on the local mass transfer rate was the same as that predicted by boundary layer theory. At the rear of the sphere local mass transfer measurements indicated a larger variation with Reynolds number, apparently due to separation. The effect of Reynolds number on the overall mass transfer to a sphere in either a bed of inert or active spheres indicates a slightly higher power on the Reynolds number dependency than that predicted by boundary theory. This research showed that the flow pattern varied from sphere to sphere. In order to make meaningful results it was necessary to average measurements from a large number of experiments. Reasonable correlation was obtained by assuming the Sherwood number varied with Re $_{0.57}^{0.57}$  and Sc $_{0.33}^{0.33}$ .

Galloway and Sage [17] used an instrumented 1.5 in. diameter copper sphere in a 12 in. diameter, 20 in. long column containing a rhombohedral array of 1.5 in. uniform diameter spheres in order to make local heat transfer measurements. Inert spheres were made of celluloid and partial spheres were used on the inside surface of the cylindrical wall to fill out the array and reduce wall effects. The study concerned determination of local heat transfer coefficients as a result of steady flow of air and covered a range of superficial Reynolds numbers from 875 to 3618 with the effect of turbulence being noted. Local air velocities in flow passages were measured directly. Analyzing available literature data their model provided an analytical expression which was found to represent transport from single cylinders and spheres, and arrays of cylindrical, spherical, and commercial packing. Overall deviation was 9.8%. The model also predicted the height of a gas phase transfer unit in commercial packed columns being irrigated with liquid within 12% for twelve cases involving absorption and vaporization. The basis of their boundary layer model was that the local Frössling number (Fs, equivalent to  $[Sh-2]/[Re^{1/2}Sc^{1/3}]$ ) was independent of surface shape and configuration of packing. Consequently such a model should apply equally well to any packing material. Their general equation was:

$$u/k_c = (H_t)a = \text{ReSc/Sh} = \text{Re}^{1/2}\text{Sc}^{2/3}/[\text{Fs} + 2/(\text{Re}^{1/2}\text{Sc}^{1/3})]$$

Galloway [15] presented results of earlier analyses of data using uniform spheres, cylinders and commercial packing. The expression given for mass transfer in beds of spheres was:

$$Sh_{p} = 2/[1 - (1 - \epsilon_{p})^{1/3}] + 0.55[(D_{p}G/\mu)(\epsilon_{p} - \epsilon_{b})]^{1/2}Sc^{1/3}$$
$$+ 0.30 Z_{t}(Z_{t} + 0.05)(D_{p}G/\mu\epsilon_{p})Sc^{1/3}$$

in whick  $\varepsilon_p$  is the voids fraction of the packing,  $\varepsilon_b$  is the voids fraction of relatively stagnant regions in the bed, and  $Z_t$  is the turbulence level.

Haring and Greenkorn [23] developed a statistical model of a porous medium with non-uniform pores which matched experimental capillary pressure, permeability and dispersion data. The model was constructed with two parameter distribution functions for pore radius and pore length. Orientation of pores was considered random in all directions. Various properties of a porous medium were found by integrating over joint distributions resulting from the model. Dimensionless quantities were used for pore length and radius so they varied from 0 to 1. To make the model non-uniform the dimensionless terms were each assumed to be distributed according to the beta function. The permeability of the model was found by relating the average velocity in an individual pore to the average velocity of all pores. The permeability-porosity ratio, which causes dissipation due to entrance-exit effects, was found to be a function of the average pore radius squared and the pore radius distribution. For most flow situations of interest to engineers, the residence time of the fluid in the individual pore is much smaller than the time needed for appreciable mixing due to molecular diffusion within that pore. Neglecting molecular diffusion, expressions for dispersion coefficient were found by determining the probability distribution of the position of a marked particle after a random walk of independent steps through the model. The dispersion coefficient was found to be dependent on both pore radius and length distributions.

Wegner, Karabelas, Hanratty [56] made studies of the motion of dye streamers in a rhombohedral array (voids fraction = 0.26) of 3 in. diameter Plexiglas spheres. The test sphere containing the dye taps was located in the tenth layer of a fifteen layer bed. Similar flow patterns were observed at superficial Reynolds numbers of 82 and 200. Nine distinct regions of reverse flow were noted. Flow was described as steady at the lower flow rate and unsteady at the higher one.

Van Der Merwe and Gauvin [55] investigated flow development in packed beds by setting up an experimental apparatus using a regular

arrangement of ten banks of seven centimeter diameter spheres. A skewed arrangement was also tested where the spheres were arranged on 0.375 in. rods at an angle where the mean flow direction made equal angles with the three principal axes of the packing. The pressure drag coefficients on the central sphere of each bank were determined for air having Reynolds numbers of 27,000 and 10,000. It was found from the distribution of local pressure measurements, which allowed determinations of the separation and reattachment points of the boundary layer on the central sphere of each bank, that the boundary layer behavior on a sphere in a packing is similar to that of a single sphere. The skewed arrangement showed a lower pressure drag coefficient than did the regular arrangement at the same Reynolds number.

Karabelas, Wegner and Hanratty [28] studied the effect of Grashof, Reynolds and Schmidt numbers on mass transfer rates to liquids (Sc = 1600) from cubic arrays of spheres. For Reynolds below  $Re_{p} = 110$ , the correlation equation was:

$$Sh_p = 0.46 (Gr Sc) \cdot ^{25}$$

They also give a summary of other authors' correlations for heat and mass transfer data.

#### FLOW PHENOMENA

Graetz [21] in 1883 made the first analysis for the development of the temperature profile in a round tube. He assumed the velocity profile was fully developed at the tube entrance for the two cases of uniform and parabolic velocity. Nusselt substantiated Graetz's solutions independently in 1910. Pohlhausen [42] solved the problem of heat transfer to a fluid in laminar flow parallel to a flat plate. The velocities and temperatures are approximated by polynomials in y having coefficients that are functions of x. The coefficients are determined by satisfying the boundary conditions at the plate and at the edge of the boundary layer using integral forms of the equations of continuity, motion and energy for the boundary layer.

Leveque [33] modified the problem of heat transfer to a fluid in laminar flow in a pipe with constant temperature walls. He assumed the parabolic velocity profile to be completely developed before the fluid enters the section of pipe where the heating begins. A thermal boundary layer is then assumed to develop, superimposing itself on the already developed velocity profile. The following equation was formulated:

Nu = 1.077 [D Re 
$$Pr/L$$
]<sup>1/3</sup>

This equation gives the same values for Nusselt number in the region [D Re Pr/L] greater than 100 as the more complicated Graetz equation.

The Leveque equation is not valid beyond the length where the thermal boundary layer reaches the center of the pipe.

Norris and Streid [38] analyzed the problem for laminar flow in flat rectangular ducts and suggested that entrance region Nusselt numbers for simultaneously developing velocity and temperature profiles might be obtained using results for heat transfer from a flat plate.

Langhaar [32] postulated that the pressure gradient in the transition length of a tube is higher than in a region of laminar flow because of increased frictional loss and increased kinetic energy if fluid as it passes downstream. He used linear approximation methods to solve the Navier-Stokes motion equations involving frictional flow for the case of steady flow in the transition length of a straight tube. A family of velocity profiles was determined which were defined by means of Bessel functions. The pressure function was then derived from the computed velocity field by means of the general energy equation.

Sparrow [53] studied the simultaneous development of temperature and velocity profiles in flat rectangular ducts. Laminar flow and constant wall temperature were assumed. Thermal and velocity boundary layer calculations were made using the Pohlhausen method. Nusselt numbers were reported for the Prandtl range from 0.01 to 50. By plotting D Re Pr/L (Graetz number, Gz) versus Nusselt number it was found that there is a separate curve for each Prandtl number in the entrance region. In contrast when a parabolic profile is assumed at the entrance, there is a single curve which satisfies all Prandtl numbers. In order to compare his results with those of Norris and Streid, the Pohlhausen solution gave the equation:

Nu = 
$$[0.664/\phi]$$
 [D Re Pr/L]<sup>1/2</sup>

For Prandtl numbers equal to or greater than one, many investigators have found  $\phi = Pr^{1/6}$ . For Pr less than one Sparrow has a plot of  $\phi$  vs. Pr.

Kays [30] studied the problem where the thermal and hydrodynamic boundary layers develop at the same time by combining Langhaar's results for the developing velocity profile with a numerical solution of the differential energy balance. His solutions were limited to fluids with a Prandtl number of 0.7. Kays pointed out that for high Prandtl number fluids, such as oils, the assumption of a fully developed velocity profile at the tube entrance does not affect the heat transfer mechanism because the velocity profile is established much more rapidly than the temperature profile at the place where heating begins. However, for fluids with Prandtl numbers near unity, such as gases, the velocity and temperature profiles develop at nearly the same rate along the tube. As a result experimental data showed considerably higher Nusselt numbers than predicted by the assumption of a parabolic profile throughout the tube. The Graetz parabolic velocity solution provided lower limit Nusselt numbers, while the Graetz slug flow solution gave upper limiting values. Kays showed that the Pohlhausen flat plate solution using Langhaar velocity profiles gave intermediate Nusselt numbers to those with parabolic and slug flows. As D/L approaches zero, Nusselt number approaches a minimum value of 5.75 for slug flow and 3.656 for parabolic flow. Kays postulates that the Pohlhausen solution should approximate actual performance near the tube entrance.

### THEORETICAL ANALYSIS

### MODEL OF A PACKED BED

Packed beds are commonly made by packing tubes or cylindrical vessels with solid particles such as cylindrical catalyst pellets, Raschig rings, spheres, etc. These beds are generally used to effect mass transport between the bulk of a fluid flowing through the bed and the fluid-solid interface (or the interface with a second fluid which wets the solid). Usually the solid particles which make up the bed distribute themselves in a random fashion, but sometimes, especially in research on the characteristics of packed beds, the packing is placed in the bed in a regular pattern. Figure 14 and 15 in Appendix B show the spatial arrangement for two types of regular fixed beds.



Figure 1. Random Packed Bed of Spheres

The mass, momentum, and heat transport characteristics of packed beds have been investigated by others in a vast number of experiments resulting (after correction for wall and end effects) in a large
number of correlating equations for transport in the bulk of the packed bed. These equations are generally expressed in terms of a packed bed Reynolds number together with a Sherwood and Schmidt number (or alternatively a Nusselt and Prandtl number). The tacit assumption is commonly made that these correlating equations may be used to design beds with a different packing material and a different random packing arrangement as long as the dimensionless variables are in the same range as the experiments.

While such extension of the correlating equations could lead to erroneous results (for example, when cylindrical packing happens to arrange itself in a manner which blocks the fluid) they have been used in this manner with some success. As might be expected, the correlating equations are extended more successfully when the dimensionless variables are defined in terms of the average interstitial velocity  $u/\varepsilon$  rather than superficial velocity u, and interstitial hydraulic radius  $\varepsilon/a$ , or  $\varepsilon D_p/6(1 - \varepsilon)$ , rather than the spherical packing diameter  $D_p$ . Thus a packed bed may be viewed more appropriately as a network of channels of varying shapes and sizes rather than as an aggregate of solids. The active part of the bed is the voids. It is the solids which are inert.



Figure 2. Model of a Random Packed Bed

This thesis grows out of the concept that the transport characteristics of a random packed bed can be computed from a physical model consisting of a simplified network of channels. Al-Khudayri [1] assumed a network of uniform cylindrical channels with mass transport in the individual channels governed by the Graetz [21] equation. McCabe and Smith [35] use a similar model to derive the Ergun [12] equation for pressure drop in packed beds. The model used here is more sophisticated than these. It includes channels of varying diameters, thus simulating the stagnant and active flow regions which occur in real packed beds. And it provides for mass transfer in the regimes of boundary layer formation and separation, and incipient turbulence. Specifically, this model, or combination of models, may be described as follows:

- 1. For computing velocity distribution in the bed and for computing mass transfer at low velocities, the physical model used is a network of cylindrical channels all of a length equal to the diameter of equivalent spherical packing. On the average these channels are at an angle of 45° with the axis of the bed, and the distribution of diameters is described by a parameter XS. The void volume per unit bed volume and the surface per unit bed volume are the same as in the real bed.
- 2. The distribution of velocities in the bed is computed assuming that all channels have the same pressure drop and that that pressure drop may be computed from Langhaar's analysis [32] of the entrance of a circular pipe. This

gives very low velocities in low diameter channels, and high velocities in large diameter channels.

- 3. Mass transfer in the channels is computed in accordance with the type of flow occurring. At the lowest velocities with fully developed velocity and concentration profiles the asymptotic Sherwood number for cylindrical tubes is used. At somewhat higher velocities with developed velocities and developing concentrations the Leveque equation is used to compute the Sherwood number. Both of these equations derive from rigorous application of basic fluid dynamic and transport principles to the flow regimes described.
- 4. At higher velocities and diameters both the velocity profile and the concentration profiles are developing. The treatment developed by Blasius and Pohlhausen [42] for flow over a surface parallel to the direction of flow is applicable here except that the real surface formed by spheres and cylindrical packing curves in the direction of flow. Since boundary layer separation occurs at about half way around a sphere or cylinder, the length of the boundary layer in the Pohlhausen equation is taken as half the length of the channel.
- 5. At still higher velocities a somewhat different physical model is used to simulate mass transport in a packed bed. Instead of regarding the fluid as flowing through a network of cylindrical passages, it is regarded as flowing normal to a bank of cylinders, again with the same void fraction and surface as the real bed. This model gives incipient turbulence at much lower velocities than cylindrical passages

and in this respect behaves more like a real packed bed. The Colburn [9] equation developed for heat transfer in fluids flowing across banks of tubes is applicable to this model.

- 6. In this thesis a single equation is used to compute the Sherwood number in all the flow regimes described above and in the transition regions between them. This equation states that the Sherwood number in any case is equal to the fourth root of the sum of the fourth powers of Sherwood numbers computed by all the equations described above. This is a somewhat arbitrary combination of these equations, but it does give values which are in pretty good agreement with the transition between developing concentrations and developed concentrations as derived rigorously by Graetz [21].
- 7. Overall mass transfer in the bed is then computed on the basis that all the concentrations leaving a given layer of channels mix to an average concentration before entering the next layer of channels.

Obviously what is described above is not a rigorous derivation of transport in a random packed bed from the equations of continuity, motion, energy, and mass transfer. It is, however, a combination of rigorous analysis and reasonable approximation to the transport behavior of a fluid flowing through a physical model designed to simulate many of the phenomena which occur in packed beds. Mass transfer coefficients computed from this model are therefore a priori predictions as to how random packed beds should behave over a wide range of operating conditions. This is much different from

correlating equations which represent a posteriori fits to limited range data taken on a particular packed bed.

The model equations are derived on the basis of heat transfer for simplicity reasons and then converted to mass transfer by substituting the appropriate dimensionless variables.

## DERIVATION OF MODEL EQUATIONS

Primary units for quantities used in the derivations are: heat H, mass M, length L, time t, force F, and temperature T.

Consider that the flow cross-section is distributed among the various diameters so that:

$$S/S_m = (D/D_m)^S$$
(1)

- where: S = total cross-sectional area of passages having diameters less than D
  - $S_m$  = total cross-sectional area of all passages
  - D = diameter of a given passage
  - D<sub>m</sub> = maximum passage diameter present
  - s = exponent which depends upon the distribution
     of passages

The average passage diameter  $D_{av}$  is determined from equation 1 by multiplying 4 times the average hydraulic radius. Average hydraulic radius is calculated by dividing  $S_m$  by the total perimeter of all passages. Since the perimeter of a given circular cross-section is  $\pi D = 4S/D$ :

$$D_{av} = \frac{4 S_m}{\int_0^{S_m} \frac{4}{D} dS}$$
(2)

After integration (See Appendix A):

$$D_{av} = \frac{a-1}{a} D_{m}$$
(3)

Let: XS = 1/s

$$D_{av} = (1 - XS) D_{m}$$
 (4)

When XS = 0,  $s = \infty$ , all passages have the same diameter. When XS = 1,  $D_{av} = 0$ . This requires that substantially all of the surface to be located in passages of infinitesimal diameter.



Ordinary packed bed parameters are:

u = superficial fluid velocity, based on empty cross section (L/t)

- $\varepsilon$  = voids fraction, voids volume/total bed volume (L<sup>3</sup>/L<sup>3</sup>)
- a = packing surface area per unit bed volume  $(L^2/L^3)$

 $D_p$  = particle diameter (L)

 $\mu$  = fluid viscosity (M/Lt)

 $\rho$  = fluid density (M/L<sup>3</sup>)

k = thermal conductivity of fluid (H/LtT)

C = heat capacity of fluid (H/MT)

 $\mathbf{J}$  = diffusion coefficient of active component in fluid (L<sup>2</sup>/t)

Volumetric hydraulic radius in terms of fixed bed parameters is the volume of voids divided by the packing surface area. Therefore the average equivalent diameter of a cylindrical passage is:

$$D_{av} = 4\varepsilon/a$$
(5)

Consider the fluid to be perfectly mixed before entering a given layer of passages so that the entering temperature  $T_1$  is the same for all passages. Consider the wall temperature  $T_w$  constant throughout the layer so that  $(T_1 - T_w) = \Delta T_1$  is also uniform. However, since different temperatures are reached at the end of different passages,  $T_2$  and  $(T_2 - T_w) = \Delta T_2$  are not uniform. Assume the length of a passage L to be equal to a particle diameter  $D_p$ , and the average angle between the flow direction in the passages and the axis of the bed to be  $\theta$ .

In order to determine the  $\Delta T_2/\Delta T_1$  ratio for a given passage a heat energy balance per unit of time is made:

m C dT<sub>p</sub> = -h (T<sub>p</sub> - T<sub>w</sub>) = D dL (6) where: m = mass flow rate of fluid in a passage (M/t) T<sub>p</sub> = temperature of fluid at any point in a passage (T)

h = fluid film heat transfer coefficient  $(H/tL^2T)$ 



Figure 4. Flow in a passage

Rearranging equation (6) and integrating over the length of the passage:

$$m C \int_{T_1}^{T_2} \frac{dT_2}{(T_p - T_w)} = -h \pi D \int_{O}^{L} dL$$
(7)

$$\ln \left[\Delta T_2 / \Delta T_1\right] = -\frac{h \pi DL}{mc}$$
(8)

The mass velocity of the fluid is  $G = m/(\pi D^2/4)$ .

$$\ln \left[\Delta T_2 / \Delta T_1\right] = - \frac{4 h L}{G C D}$$
(9)

The dimensionless groups--Reynolds number,  $Re = DG/\mu$ ; Nusselt number, Nu = hD/k; and Prandtl number,  $Pr = C\mu/k$ --are then substituted into equation (9).

$$\ln \left[\Delta T_2 / \Delta T_1\right] = - \frac{4 \text{NuL}}{Pr D \text{Re}}$$
(10)

It is then convenient to introduce Y = D Re/L, a parameter given in Langhaar's article [32].

$$\ln \left[\Delta T_2 / \Delta T_1\right] = -\frac{4 N \kappa}{Y R_r}$$
(11)

Solving for  $\Delta T_2 / \Delta T_1$ :

$$\Delta T_2 / \Delta T_1 = e^{-\frac{4 N m}{V P_r}}$$
(12)

In terms of dimensionless groups the average Reynolds number of the fluid, based on the superficial velocity direction, is defined as:

$$Re_{av} = \frac{D_{av}}{D_{m}} \int_{0}^{1} Re \cos \frac{D_{m}}{D} d\frac{s}{s_{m}}$$
(13)

The average temperature change ratio is calculated by integrating equation (12) over the distribution of passages.

$$(\Delta T_2 / \Delta T_1)_{av} = \frac{\int_{0}^{1} e^{-\frac{A H_u}{Y F_r}}}{\int_{0}^{1} Re \cos \phi \frac{D_m}{D} d\frac{S}{Sm}}$$
(14)

A relationship for Y is determined from the mechanical energy balance of a fluid streamline at the entrance of a tube, the pressure loss equation for fully developed laminar flow, and a correction to account for the pressure loss in the transition length.

Disregarding elevation effects and assuming a fluid of constant density, the Bernoulli equation [35] for potential steady-state flow along a streamline is:

$$\frac{dP}{Q} + \frac{I}{g} w \, dw = 0 \tag{15}$$

- where: P = static pressure of fluid (F/L<sup>2</sup>)
  - e = density of fluid (M/L<sup>3</sup>)
  - w = velocity component perpendicular to the cross section of channel (L/t)
  - $g_{r}$  = gravitational constant (LM/Ft<sup>2</sup>)

Since the average velocity in the tubes is  $u/\varepsilon$  and w in the mixing sections between layers is negligible:

$$\frac{-\Delta P}{Q} = \frac{u^2}{26^2 g_0}$$
(16)

By dividing both sides of equation (16) by  $\frac{u^2}{2\epsilon^2 g_e}$  and defining V (the number of 'velocity heads') =  $\frac{-\Delta P}{P(u^2/2\epsilon^2 g_e)}$ , then

$$V = 1$$
 (17)

at the tube entrance.

Beyond the transition length where the laminar flow pattern is fully developed the Hagen-Poiseuille equation [35] for pressure loss in a round tube applies.

$$-\Delta P = \frac{32 / Lu}{g \in D^2}$$
(16)

Since Y = D Re/L =  $\frac{D^2 u e}{e L r}$ 

$$V = 64/Y$$
 (19)

Therefore the equation V = 1 + 64/Y or its equivalent,

 $Y = \sqrt{VY^2 + 1024} - 32$  (See Appendix A), satisfy the limiting conditions at high Y and at low Y, but in the intermediate region (transition length) a correction is needed. This region is important to the model because of the distribution of passages. Langhaar [32] made a theoretical study of the pressure losses in the flow developing region of a tube and his results are used in this thesis to make the needed correction.

Langhaar's analysis begins with the Navier-Stokes differential equation of motion for flow perpendicular to the channel cross section. He solves the differential equation using the equation of continuity and valid approximations. The solution is a family of velocity profiles defined by Bessel functions. The pressure function is then determined from the computed velocity field by means of the general energy equation. From these equations then Langhaar calculates a table of values for 4/Y versus V. For purposes of this thesis the table is converted into the equation:

$$Y = (\sqrt{VY^2 + 1024} - 32)(1 - \frac{B}{RT + A/RT})$$
(20)

where: B,A = constants

$$RT = (VY^2)^{.25}$$
(21)

By analyzing Langhaar's data the best fit seems to be when: B = 5.8, A = 175.

The Nusselt number in a given passage is determined by combining the limiting value and three other equations using the fourth power averaging method.

Nu = 
$$((3.656)^4 + (1.615)^4 (Y Pr)^{4/3} + (0.664(2 Y)^{1/2} Pr^{1/3})^4 + (22)$$
  
(0.33 Re<sup>.6</sup> Pr<sup>1/3</sup>)<sup>4</sup>)<sup>.25</sup>

Equation 22 is a continuous equation and represents a weighted average of the limiting Nusselt number for fully developed laminar flow in tubes [30], the Leveque equation for developed velocity and developing temperature laminar flow profiles [33], the Pohlhausen equation for developing laminar velocity and temperature profiles [42], and the Colburn equation for heat transfer in turbulent flow across tube banks [9]. The factor 2 in the Pohlhausen equation compensates for the formation of two boundary layers in one length of channel as previously described.



Figure 5. Nusselt Numbers in Tubes

As is seen in equation 22 the Nusselt number for boundary layer formation, developed laminar flow and turbulent flow is proportional to the one-third power of the Prandtl number times Reynolds number to a power which depends upon flow conditions. For the analogy between heat and mass transfer the following terms are defined:

Nu<sub>av</sub> = average Nusselt number,  $D_{av}h/k$   $k_c$  = mass transfer coefficient based on superficial velocity (L/t)  $Sh_{av}$  = average Sherwood number,  $D_{av}k_c/dP$   $Sh_p$  = Sherwood number based on particle diameter,  $D_pk_c/dP$  Sc = Schmidt number of fluid,  $\frac{M}{Q_c dP}$   $Re_p$  = Reynolds number based on particle diameter,  $D_puQ/\mu$ Relationships derived in Appendix A are:

$$Re_{p} = 1.5(1 - \varepsilon)Re_{av}$$
(23)

$$\frac{Re_{P}}{1-\epsilon} = \frac{6uR}{2\mu}$$
(24)

$$Sh_p = 1.5(1 - \epsilon)Sh_{av}/\epsilon$$
 (25)

$$Sh_p \stackrel{e}{\underbrace{l=e}} = \frac{6 \kappa_e \epsilon}{\lambda \sigma}$$
(26)

For mass transfer Sherwood number and Schmidt number are similar, respectively, to Nusselt number and Prandtl number of heat transfer. Therefore:

$$\mathrm{Sh}_{\mathrm{av}}/\mathrm{Sc}^{1/3} \simeq \mathrm{Nu}_{\mathrm{av}}/\mathrm{Pr}^{1/3}$$
<sup>(27)</sup>

In terms of mass transfer then:

$$\operatorname{Sh}_{av}/\operatorname{Sc}^{1/3} \alpha \operatorname{Re}_{av}^{x}$$
 (28)

with the value of x depending upon the type of flow. It then follows that:

. .

$$\frac{Sh_{p}}{Sc^{1/3}} \frac{\epsilon}{1-\epsilon} = C_{1} \left( \frac{R_{ep}}{1-\epsilon} \right)^{X}$$
(29)

where  $C_1$  is a proportionality constant.

Equation 29 expresses the mass transfer characteristics of a packed bed in terms of voids volume and voids surface area and many of the literature correlations use varying forms of this equation.

For a bed of spherical particles the following relationship is derived in Appendix A.

$$L = D_{p} = 6(1 - \epsilon)/a$$
(30)

## OPERATION OF THE MODEL

The general procedure used to mathematically solve for

$$\frac{Rep}{1-6}$$
 and  $\frac{Shp}{Sc''} \frac{\epsilon}{1-\epsilon}$  from the model is:

- (A) Bed porosity ( $\varepsilon$ ) and Pr (Sc) are set at desired values. The angle  $\Theta$  is assumed to be 45°, so  $\cos \Theta = 0.707$ .
- (B) XS is assigned a value of 0.3 (See Appendix B).
- (C) A value for  $(VY^2)_m$  is assumed, the magnitude of which depends upon the voids fraction and the desired value for  $\text{Re}_p/(1 - \epsilon)$ (See Appendix C).
- (D)  $\operatorname{Re}_{av}$  and  $(\Delta T_2/\Delta T_1)_{av}$  are evaluated from equations 13 and 14 by integration.  $D_{av}/D_m$  is calculated from equation 4. For each value of S/S<sub>m</sub>, the following sequence of equations is used:
  - (a)  $D/D_m$  from equation 1
  - (b)  $VY^2$  from  $(VY^2)_m (D/D_m)^4$  (31)

- (c) RT from equation 21
- (d) Y from equation 20

(e) From Appendix A: Re = 1.5 Y 
$$\frac{1-\epsilon}{\epsilon} \left(\frac{5m}{s}\right)^{(1-\times 5)}$$
 (32)

¥5

(f) Nu from equation 22

(E) 
$$\operatorname{Re}_{p}/(1-\varepsilon)$$
 is then determined from equation 23.

(F) Nu<sub>av</sub> is calculated from (See Appendix A):

$$Nu_{av} = -\frac{\epsilon P_{F} Re_{av}}{6(1-\epsilon)\cos\Phi} - \ln\left(\frac{\Delta T_{a}}{\Delta T_{i}}\right)_{av}$$
(33)

(G) Finally by combining equations 25 and 27:

$$\frac{Sh\rho}{Sc^{1/3}} \frac{\epsilon}{1-\epsilon} = \frac{1.5 \text{ Nuay}}{Pr^{1/3}}$$
(34)

Model equations are summarized in Appendix D.

The mass transfer coefficient can then be determined from equation 26.

$$k_{c} = \frac{\Delta \mathcal{B} S c^{1/3}}{6 \epsilon} \left[ \frac{Shp}{S c^{1/3}} \frac{\epsilon}{1 - \epsilon} \right]$$

The pressure loss per unit length of bed can be calculated from the model and the Ergun equation (See Appendix A).

$$-\Delta P/\Delta L = \frac{9 a^{2} \mu^{2} (1-\epsilon)^{2} (1-X5)^{4} (VY^{2})_{m}}{128 g_{c} \epsilon^{4} P D_{p}}$$
(35)

A correlation between mass transfer coefficient and pressure loss per unit length of bed can be made by combining equations 28 and 35:

$$k_{c} = \frac{-\Delta P}{\Delta L} \left[ \frac{64 \mathcal{D} e^{3} e g_{c} Sc^{1/3} D_{P}}{27 a \mu^{2} (1-e)^{2} (1-XS)^{4} (VY^{2})_{m}} \right] \left[ \frac{Sh_{P}}{Sc^{1/3}} \frac{e}{1-e} \right]$$
(36)

The heat transfer coefficient can be determined by combining the definition of  $Nu_{av}$  and equation 5.

$$h = Nu_{av}ka/4 \epsilon$$
 (37)

.

Computer programs showing the operational steps of the model are given in Appendix E.

## RESULTS

The principal advantages of the computerized model of this thesis compared to previous correlations are its flexibility and its coverage of larger ranges of Reynolds and Schmidt numbers and bed porosities. Literature correlations are generally for data obtained from specially constructed laboratory beds. Grdphs of data are usually in the form of Colburn 'J' factors versus Reynolds number which are easily compared with results of this model. Authors' equations containing Colburn 'J<sub>d</sub>' factors are changed to equations containing Sherwood number by:

 $J_{d} = k_{c}/(u \ Sc^{2/3})$ Since:  $Re_{p} = D_{p} u \rho/\mu$  $Sc = \mu/(\rho B)$  $Sh_{p} = D_{p} k_{c}/B$ Then:  $Sh_{p}/(Re_{p} \ Sc) = k_{c}/\mu$ 

 $J_{d} = Sh_{p} / (Re_{p} Sc^{1/3})$ 

Correlation equations often contain specially defined axial mixing or turbulence correction factors and apply only for limited ranges of packed bed parameters. Data have been obtained by evaporating various liquids from porous solid particles into gas streams, dissolving pellets of slightly soluble solids into flowing liquids or extracting liquids from porous solids into flowing water.

Correlations for gases at relatively low Reynolds numbers (below 250) are most difficult because mixing in the axial direction becomes increasingly significant and it is hard to avoid essentially equilibrium conditions at the exit even in a short packed bed.

In this work boundary layer theory is considered by using the Pohlhausen equation in the model to account for the development of temperature, concentration and velocity profiles in the entrance region of a conduit. The model also contains the Leveque equation for developing temperature and developed velocity profiles. These are important for gases because the temperature, concentration and velocity profiles develop simultaneously whereas for viscous liquids the velocity profile develops first. For gases, therefore, heat and mass transfer occur at a much greater rate in this region than downstream where profiles are fully developed.

Figure 6 shows the effect of a low Schmidt number (gases) on the model at low Reynolds numbers. It can be seen that mass transfer is much greater than for a liquid with a high Schmidt number.

Figure 7 shows the effect of distributed cross-sections on the rate of heat and mass transfer. A distribution index (XS) of 0.3 gives Nusselt and Sherwood numbers at extremely low Reynolds numbers which are only about one-third of the amount they would be if all passages were of the same diameter. Data for the graph are given in Table 41 in Appendix F.

An equation to account for turbulence is also incorporated into the model. It is based on the Colburn equation for turbulent flow



$$\frac{Rep}{1-e} = \frac{GuP}{AP}$$

Figure 6. Effect of Schmidt Number on Mass Transfer at Low Reynolds Numbers





heat transfer across tube banks. Jolls and Hanratty [27] and Karabelas, Wegner and Hanratty [28], using electrochemical techniques report that in a dumped bed of 1 in. spheres having a voids fraction of 0.41 that a transition from laminar to turbulent flow occurred over the Reynolds number range of 110 to 150  $(\text{Re}_{\rm D}/(1 - \epsilon) = 186 - 255)$ .

Table 1 shows the results of the model not using the turbulence equation. The model equations used were identical with those of Table 2 with the exception of the omission of the turbulence equation. Comparison of the two tables shows that turbulence affects the results above a Reynolds number of 260.

Tables1 to 33 compare  $\operatorname{Sh}_p/\operatorname{Sc}^{1/3}[\varepsilon/(1-\varepsilon)] = \frac{d \, \kappa_e \, \varepsilon}{A \, d \sigma \, 5 \, \epsilon^{1/5}} = 6 \, \text{KE/ADS}$ (computer print-out) values from the model with those obtained by using various authors' equations and graphs. The Reynolds numbers given are  $\operatorname{Re}_p/(1-\varepsilon) = 6 \, \mathrm{u} \, \mathbb{C}/a \, \mu = 6 \, \mathrm{UR/AZ}$  (computer print-out). Table 39 is an example computer program used to compute Table 2 and is found in Appendix E.  $(\mathrm{VY}^2)_m$  values were selected from Appendix C to produce the Reynolds number range desired at the voids fraction of the bed. The equations listed in the headings are those of the authors and the Reynolds number ranges given are in terms of  $\operatorname{Re}_p/(1-\varepsilon)$ .

Tables 2 and 3 compare the model results with those of Chu, Kalil and Wetteroth [8]. Their correlation equation is for mass transfer in packed and fluidized beds to a gas, Schmidt number of 2.57, covering a  $\text{Re}_p/(1 - \epsilon)$  range from 30 to 5000 and bed porosities of 0.38 and 0.64.

$$J_{d} = 1.77 [Re_{p}/(1 - \epsilon)]^{-.44}$$

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TABLE 1. COMPARISON OF MODEL WITH CHU, KALIL AND WETTEROTH [8]

CHU + KALIL + WETTEROTH (1953) EQUATION J = 1.77/REE\*\*.44 SCHMIDT NUMBER = 2.57 (GASES) VOIDS FRACTION = 0.38 REYNOLDS NUMBER RANGE = 30 - 5000 XS = 0.3

REYNOLDS	MODEL	СНИ	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
~~ 7677	5 3150	( (075	0 1275
29.15/1	5.2150	4.47/5	0.15/5
40.4643	5.9654	5.3421	0.1044
54.3287	6.7986	6.3004	0.0732
72.0920	7.7186	7.3819	0.0436
94.6633	8.7323	8.5984	0.0153
123.1697	9.8490	9.9641	-0.0116
159.0187	11.0793	11.4965	-0.0376
203.9735	12.4354	13.2165	-0.0628
260.2463	13.9321	15.1485	-0.0873
330.6098	15.5866	17.3210	-0.1112
418.5302	17.4186	19.7662	-0.1347
528.3253	19.4506	22.5206	-0.1578
665.3528	21.7076	25.6251	-0.1804
836.2363	24.2168	29.1246	-0.2026
1049.1404	27.0080	33.0692	-0.2244
1314.1057	30.1131	37.5136	-0.2457
1643.4611	33.5668	42.5189	-0.2666
2052.3297	37.4066	48.1521	-0.2872
2559.2521	41.6733	54.4879	-0.3075
3186.9540	46.4115	61.6094	-0.3274
3963.2883	51.6702	69.6094	-0.3471
4922.3948	57.5034	78.5915	-0.3667

•

TABLE 2. COMPARISON OF MODEL WITH CHU, KALIL AND WETTEROTH [8]

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CHU + KALIL + WETTEROTH (1953) EQUATION J = 1.77/REE\*\*.44 SCHMIDT NUMBER = 2.57 (GASES) VOIDS FRACTION = 0.38 REYNOLDS NUMBER RANGE = 30 - 5000 XS = 0.3

REYNOLDS	MODEL	СНО	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
29.7577	5.3352	4.4975	0.1570
40.4643	6.1447	5.3421	0.1306
54.3287	7.0588	6.3004	0.1074
72.0920	8.0872	7.3819	0.0872
94.6633	9.2432	8.5984	0.0697
123.1697	10.5422	9.9641	0.0548
159.0187	12.0020	11.4965	0.0421
203.9735	13.6425	13.2165	0.0312
260.2463	15.4874	15.1485	0.0218
330.6098	17.5643	17.3210	0.0138
418.5302	19.9058	19.7662	0.0070
528.3253	22.5495	22.5206	0.0012
665.3528	25.5381	25.6251	-0.0034
836.2363	28.9198	29.1246	-0.0070
1049.1404	32.7488	33.0692	-0.0097
1314.1057	37.0850	37.5136	-0.0115
1643.4611	41.9954	42.5189	-0.0124
2052.3297	47.5545	48.1521	-0.0125
2559.2521	53.8453	54.4879	-0.0119
3186.9540	60.9609	61.6094	-0.0106
3963.2883	69.0052	69.6094	-0.0087
4922.3948	78.0956	78.5915	-0.0063

TABLE 3. COMPARISON OF MODEL WITH CHU, KALIL AND WETTEROTH [8]

CHU + KALIL + WETTEROTH (1953) EQUATION J = 1.77/REE\*\*.44 SCHMIDT NUMBER = 2.57 (GASES) VOIDS FRACTION = 0.64 REYNOLDS NUMBER RANGE = 30 - 5000 XS = 0.3

REYNOLDS	MODEL	СНО	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
30.6966	8.5324	7.7076	0.0966
40.0189	9.6402	8.9417	0.0724
51.7523	10.8636	10.3265	0.0494
66.4739	12.2154	11.8805	0.0274
84.9081	13.7110	13.6258	0.0062
107.9628	15.3684	15.5878	-0.0142
136.7743	17.2084	17.7957	-0.0341
172.7587	19.2550	20.2824	-0.0533
217.6751	21.5353	23.0848	-0.0719
273.6998	24.0789	26.2438	-0.0899
343.5172	26.9188	29.8046	-0.1072
430.4298	30.0909	33.8172	-0.1238
538.4942	33.6344	38.3366	-0.1398
672.6872	37.5924	43.4238	-0.1551
839.1108	42.0125	49.1464	-0.1698
1045.2445	46.9470	55.5795	-0.1838
1300.2556	52.4542	62.8071	-0.1973
1615.3801	58.5991	70.9229	-0.2103
2004.3909	65.4544	80.0319	-0.2227
2484.1720	73.1013	90.2516	-0.2346
3075.4214	81.6313	101.7137	-0.2460
3803.5146	91.1471	114.5663	-0.2569
4699.5597	101.7643	128.9749	-0.2673

.

This equation converts to:

$$Sh_p/Sc^{1/3}[\epsilon/(1 - \epsilon)] = 1.77 \epsilon [Re_p/(1 - \epsilon)]^{.56}$$

Table 4 shows a comparison of one equation of Thoenes and Kramers [54] and the model. They measured the rate of mass transfer between a flowing fluid and the surface of one active sphere in the middle of a regular bed of spheres. Eight different geometric configurations of spherical packing were used. They present graphs interpreting their data, but do not list the data in tabular form. One equation given is:

$$Sh_p ε/(1 - ε) = 1.26 [Re_p/(1 - ε)]^{1/3} Sc^{1/3} + 0.054 [Re_p/(1 - ε)]^{.8} Sc^{.4}$$
  
+ 0.8[Re\_p/(1 - ε)]<sup>.2</sup>

The first term is said to be for laminar convective transfer, the second for turbulent convective transfer and the third for diffusion in the stagnant regions near contact points of adjacent spheres. The last term is said to account for a large part of mass transfer in gases at Reynolds numbers less than 500. Another equation listed in this same article is:

$$Sh_p \epsilon / (1 - \epsilon) = 1.0 [Re_p / (1 - \epsilon)]^{1/2} Sc^{1/3}$$

which they say checks within ± 10% for all of their 438 mass transfer measurements. The ranges for this equation are given as: voids fraction, 0.25 to 0.50; Schmidt number, 1 to 4000; Reynolds number, 40 to 4000. Tables 5 through 8 compare this equation with the model.

Table 9 shows the equation of Bradshaw and Bennett [5] who measured mass transfer coefficients for air passing through various TABLE 4. COMPARISON OF MODEL WITH THOENES AND KRAMERS [54]

THDENES & KRAMERS (1958) EQUATION SH/SC\*\*1/3 = 1.26 REE\*\*1/3 + .054 REE\*\*.8 SC\*\*.067 + .8 REE\*\*.2/SC\*\*1/3 SCHMIDT NUMBER = 1.0 (GASES) VOIDS FRACTION = 0.32 REYNOLDS NUMBER RANGE = 40 - 4000 XS = 0.3

REYNOLDS	MODEL	THOENES	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
39.9038	5.4498	7.0087	-0.2860
54.1952	6.2858	7.8628	-0.2508
72.6815	7.2529	8.8089	-0.2145
96.3457	8.3596	9.8574	-0.1791
126.3956	9.6171	11.0220	-0.1460
164.3293	11.0419	12.3193	-0.1156
212.0186	12.6556	13.7704	-0.0880
271.8090	14.4823	15.4002	-0.0633
346.6431	16.5496	17.2393	-0.0416
440.2082	18.8897	19.3235	-0.0229
557.1130	21.5400	21.6954	-0.0072
703.0961	24.5441	24.4050	0.0056
885.2755	27.9519	27.5106	0.0157
1112.4486	31.8200	31.0800	0.0232
1395.4568	36.2119	35.1921	0.0281
1747.6302	41.1983	39.9385	0.0305
2185.3349	46.8582	45.4261	0.0305
2728.6450	53.2794	51.7792	0.0281
3402.1703	60.5602	59.1428	0.0234
4236.0747	68.8104	67.6867	0.0163

TABLE 5. COMPARISON OF MODEL WITH THOENES AND KRAMERS [54]

```
THOENES & KRAMERS (1958)
EQUATION SH = 1.0 RE**1/2 SC**1/3
SCHMIDT NUMBER = 1.0 (GASES)
VOIDS FRACTION = 0.40
REYNOLDS NUMBER RANGE = 40 - 4000
XS = 0.3
```

REYNOLDS	MODEL	THOENES	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
	( 2001	4 3744	0.0124
40.0017	0.2981	0.3/00	-0.0124
24.2909	1.2104	1.5134	-0.0220
71.9472	8.2533	8.4821	-0.0277
94.2029	9.4165	9.7058	-0.0307
122.2702	10.7198	11.0575	-0.0315
157.5324	12.1816	12.5511	-0.0303
201.7237	13.8236	14.2029	-0.0274
257.0198	15.6701	16.0318	-0.0230
326.1454	17.7488	18.0594	-0.0175
412.5041	20.0921	20.3101	-0.0108
520.3302	22.7369	22.8107	-0.0032
654.8720	25.7253	25.5904	0.0052
822.6120	29.1049	28.6812	0.0145
1031.5341	32.9285	32.1175	0.0246
1291.4520	37.2553	35.9367	0.0353
1614.4116	42.1509	40.1797	0.0467
2015.1856	47.6885	44.8908	0.0586
2511.8839	53.9497	50.1186	0.0710
3126.7029	61.0260	55.9169	0.0837
3886.8476	69.0199	62.3445	0.0967

TABLE 6. COMPARISON OF MODEL WITH THOENES AND KRAMERS [54]

THOENES & KRAMERS (1958) EQUATION SH = 1.0 RE\*\*1/2 SC\*\*1/3 SCHMIDT NUMBER = 4000. (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 40 - 4000 XS = 0.3

.

REYNOLDS	MODEL	THOENES	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
40-6615	6.5896	6.3766	0.0323
54.3969	7,5172	7,3754	0.0188
71.9472	8.5594	8,4821	0.0090
94.2029	9.7288	9.7058	0.0023
122.2702	11.0404	11.0575	-0.0015
157.5324	12.5116	12.5511	-0.0031
201.7237	14.1628	14.2029	-0.0028
257.0198	16.0181	16.0318	-0.0008
326.1454	18.1055	18.0594	0.0025
412.5041	20.4576	20.3101	0.0072
520.3302	23.1118	22.8107	0.0130
654.8720	26.1103	25.5904	0.0199
822.6120	29.5005	28.6812	0.0277
1031.5341	33.3357	32.1175	0.0365
1291.4520	37.6747	35.9367	0.0461
1614.4116	42.5833	40.1797	0.0564
2015.1856	48.1347	44.8908	0.0673
2511.8839	54.4106	50.1186	0.0788
3126.7029	61.5023	55.9169	0.0908
3886.8476	69.5127	62.3445	0.1031

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TABLE 7. COMPARISON OF MODEL WITH THOENES AND KRAMERS [54]

```
THOENES & KRAMERS (1958)
EQUATION SH = 1.0 RE**1/2 SC**1/3
SCHMIDT NUMBER = 1.0 (GASES)
VOIDS FRACTION = 0.50
REYNOLDS NUMBER RANGE = 40 - 4000
XS = 0.3
```

REYNOLDS	MODEL	THOENES	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
39.6532	7.3841	6.2970	0.1472
52.2723	8.3994	7.2299	0.1392
68.2434	9.5265	8.2609	0.1328
88.3577	10.7772	9.3998	0.1278
113.6052	12.1676	10.6585	0.1240
145.2278	13.7167	12.0510	0.1214
184.7829	15.4457	13.5934	0.1199
234.2199	17.3790	15.3042	0.1193
295.9704	19.5443	17.2037	0.1197
373.0563	21.9731	19.3146	0.1209
469.2186	24.7011	21.6614	0.1230
589.0736	27.7678	24.2708	0.1259
738.3027	31.2173	27.1717	0.1295
923.8861	35.0983	30.3954	0.1339
1154.3883	39.4648	33.9762	0.1390
1440.3116	44.3770	37.9514	0.1447
1794.5291	49.9018	42.3618	0.1510
2232.8186	56.1140	47.2527	0.1579
2774.5188	63.0978	52.6737	0.1652
3443.3339	70.9478	58.6799	0.1729
4268.3221	79.7704	65.3323	0.1809

TABLE 8. COMPARISON OF MODEL WITH THOENES AND KRAMERS [54]

THOENES & KRAMERS (1958) EQUATION SH = 1.0 RE\*\*1/2 SC\*\*1/3 SCHMIDT NUMBER = 4000. (LIQUIDS) VOIDS FRACTION = 0.50 REYNOLDS NUMBER RANGE = 40 - 4000 XS = 0.3

REYNOLDS	MODEL	THOENES	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
39.6532	7.6487	6.2970	0.1767
52.2723	8.6622	7.2299	0.1653
68.2434	9.7893	8.2609	0.1561
88.3577	11.0424	9.3998	0.1487
113.6052	12.4365	10.6585	0.1429
145.2278	13.9894	12.0510	0.1385
184.7829	15.7218	13.5934	0.1353
234.2199	17.6582	15.3042	0.1333
295.9704	19.8265	17.2037	0.1322
373.0563	22.2586	19.3146	0.1322
469.2186	24.9899	21.6614	0.1331
589.0736	28.0603	24.2708	0.1350
738.3027	31.5139	27.1717	0.1377
923.8861	35.3994	30.3954	0.1413
1154.3883	39.7710	33.9762	0.1457
1440.3116	44.6887	37.9514	0.1507
1794.5291	50.2196	42.3618	0.1564
2232.8186	56.4388	47.2527	0.1627
2774.5188	63.4301	52.6737	0.1695
3443.3339	71.2884	58.6799	0.1768
4268.3221	80.1198	65.3323	0.1845

size naphthalene spheres and cylinders. Beds were randomly packed,4 in. diameter and 5 to 10 in. high. Their correlation equation is:

$$J_d = 2.0/Re_p Sc^{1/3} + 1.97/Re_p^{1/2}$$

which is said to cover the  $Re_p$  range from 400 to 10,000. In terms of this work the equation is:

$$Sh_{p}/Sc^{1/3}[\epsilon/(1 - \epsilon)] = 2.0 \epsilon/(1 - \epsilon)Sc^{1/3} + 1.97 \epsilon/(1 - \epsilon)^{1/2}$$

$$[Re_{p}/(1 - \epsilon)]^{.5}$$

with a  $Re_D/(1 - \epsilon)$  range from 667 to 16,667.

A theoretical study of gaseous diffusion rates in packed beds using a free surface model (spherical particle surrounded by a spherical envelope of fluid) and boundary layer theory was made by Kusik and Happel [31]. They give the equation:

$$Sh_p/Sc^{1/3} Re_p^{1/2} = 0.93/(\epsilon - 0.75(1 - \epsilon)(\epsilon - .2))^{0.5}$$

which they say is applicable for  $\operatorname{Re}_p/\varepsilon$  range of from 100 to 1000 and a voids fraction range from 0.3 to 1.0. The Reynolds number range converts to  $\operatorname{Re}_p/(1 - \varepsilon)$  between 67 and 667 at a porosity of 0.4 and between 233 and 2330 at a porosity of 0.7. Tables 10 and 11 are for voids fractions of 0.4 and 0.7.

Liquid mass transfer coefficients for randomly packed beds of benzoic acid spheres and water were measured by Williamson, Bazaire and Geankoplis [59]. Two equations are reported, each covering a different Reynolds number range.

The equation:

St Sc<sup>.58</sup> = 2.4(
$$\text{Re}_{p}/\epsilon$$
)<sup>-.66</sup>

TABLE 9. COMPARISON OF MODEL WITH BENNETT AND BRADSHAW [3]

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BRADSHAW & BENNETT (1961) EQUATION J = 2.0/(RE SC++1/3) + 1.97/RE++.5 SCHMIDT NUMBER = 2.57 (GASES) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 667 - 16667 XS = 0.3

REYNOLDS	MODEL	BRADSHAW	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
673.5189	26, 2911	27.3747	-0.0412
845 8481	20 7285	20 5601	-0.0270
			-0.0219
1000.4570	33.0109	34.1015	-0.0144
1327.4116	38.0163	38.0375	-0.0005
1659.0617	42.9933	42.4097	0.0135
2070.5549	48.6220	47.2641	0.0279
2580.4587	54.9854	52.6506	0.0424
3211.5306	62.1762	58.6243	0.0571
3991.6634	70.2983	65.2462	0.0718
4955.0464	79.4691	72.5835	0.0866
6143.5903	89.8206	80.7107	0.1014
7608.6738	101.5020	89.7104	0.1161
9413.2845	114.6816	99.6743	0.1308
11634.6421	129.5498	110.7038	0.1454
14367.4106	146.3218	122.9116	0.1599
17727.6347	165.2408	136.4224	0.1744

TABLE 10. COMPARISON OF MODEL WITH KUSIK AND HAPPEL [31]

KUSIK & HAPPEL (1962) EQUATION SH = 0.93/(E-0.75(1-E)(E-0.2))\*\*.5 RE\*\*.5 SC\*\*1/3 SCHMIDT NUMBER = 1.0 (GASES) VDIDS FRACTION 0.40 REYNOLDS NUMBER RANGE = 67 - 667 XS = 0.3

•

REYNOLDS	MODEL	KUSIK	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
66.1489	7.9246	7.0153	0.1147
76.9430	8.5270	7.5660	0.1127
89.2338	9.1685	8.1480	0.1113
103.2058	9.8513	8.7627	0.1105
119.0673	10.5783	9.4120	0.1102
137.0542	11.3526	10.0979	0.1105
157.4337	12.1777	10.8226	0.1112
180.5085	13.0574	11.5887	0.1124
206.6214	13.9954	12.3986	0.1140
236.1608	14.9961	13.2553	0.1160
269.5664	16.0640	14.1618	0.1184
307.3356	17.2039	15.1214	0.1210
350.0301	18.4214	16.1376	0.1239
398.2840	19.7220	17.2140	0.1271
452.8119	21.1121	18.3546	0.1306
514.4185	22.5984	19.5634	0.1343
584.0083	24.1880	20.8447	0.1382
662.5978	25.8885	22.2029	0.1423

TABLE 11. COMPARISON OF MODEL WITH KUSIK AND HAPPEL [31]

KUSIK & HAPPEL (1962) EQUATION SH = 0.93/(E-0.75(1-E)(E-0.2))\*\*.5 RE\*\*.5 SC\*\*1/3 SCHMIDT NUMBER = 1.0 (GASES) VDIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 233 - 2330 XS = 0.3

REYNOLDS	MODEL	KUSIK	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
232 1225	25.0388	23,6251	0.0564
262 9783	26.6128	25.1464	0.0551
202 • 7969	28 2942	26 7589	0 0539
291 1000			0.0520
337.0403	30.0389	20.4000	0.0529
381.2897	31.9433	30.2791	0.0520
431.1519	33.9440	32.1982	0.0514
487.3167	36.0679	34.2311	0.0509
550.5560	38.3225	36.3845	0.0505
621.7330	40.7154	38.6650	0.0503
701.8132	43.2549	41.0796	0.0502
791.8767	45.9495	43.6360	0.0503
893.1315	48.8034	46.3419	0.0505
1006.9285	51,8412	49.2057	0.0508
1134.7789	55.0582	52.2362	0.0512
1278.3733	58.4704	55.4428	0.0517
1439.6023	62-0892	58,8352	0.0524
1620.5811	65,9269	62.4240	0.0531
1022 4754	60 0067	66 2201	0.0530
1023.0130	07.9901	00.2201	0.0559
2051.5325	74.3124	70.2353	0.0548
2307.1125	78.8888	74.4819	0.0558

is said to cover a  $\operatorname{Re}_p/\varepsilon$  range from 0.08 to 125 for a bed porosity of 0.4 and a Schmidt number of 1000. This converts to:

$$h_p/Sc^{1/3}[\epsilon/(1-\epsilon)] = 2.4 Sc^{.09} \epsilon^{1.66}/(1-\epsilon)^{.66} [Re_p/(1-\epsilon)]^{.34}$$

for  $\operatorname{Re}_p/(1 - \varepsilon)$  from 0.053 to 83. Table 12 analyzes this equation. The other equation listed is:

St Sc<sup>.58</sup> = 
$$0.442(\text{Re}_p/\epsilon)^{-.31}$$

covering a  $\operatorname{Re}_p/\varepsilon$  range from 125 to 5000. This equation converts to:  $\operatorname{Sh}_p/\operatorname{Sc}^{1/3}[\varepsilon/(1-\varepsilon)] = 0.442 \operatorname{Sc}^{.09} \varepsilon^{1.31}/(1-\varepsilon)^{.31} [\operatorname{Re}_p/(1-\varepsilon)]^{.69}$ at a  $\operatorname{Re}_p/(1-\varepsilon)$  range between 83 and 3333 for a voids fraction of 0.4. Table 13 compares the equation with the model.

Two equations are reported by Wilson and Geankoplis [60] for mass transfer from randomly packed beds of benzoic acid spheres to water and propylene glycol solutions. They report the equation:

$$\varepsilon J_{d} = 1.09 Re_{p}^{-2/3}$$

for the  $\text{Re}_{p}$  range from 0.0016 to 55, Schmidt numbers varying from 950 to 70,600 and bed porosities between 0.35 and 0.75. This converts to the equation:

$$h_p/Sc^{1/3} [\epsilon/(1 - \epsilon)] = 1.09/(1 - \epsilon) Re_p^{1/3}$$

for a  $\operatorname{Re}_p/(1 - \varepsilon)$  range from 0.0027 to 92 at a bed porosity of 0.4 and 0.0053 to 183 at a bed porosity of 0.7. Tables 14 through 18 compare the model results with this equation. The other equation:

$$\varepsilon J_d = 0.25 \text{ Rep}^{-.31}$$

TABLE 12. COMPARISON OF MODEL WITH WILLIAMSON,<br/>BAZAIRE AND GEANKOPLIS [59]

WILLIAMSON & BAZAIRE & GEANKOPLIS (1963) EQUATION ST SC\*\*.58 = 2.4 (RE/E)\*\*-.66 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 0.053 - 83 XS = 0.3

REYNOLDS	MODEL	WILLIAMSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
0 0528	0 5484	0 5034	0 0820
0.0789	0 6309	0 5769	0.0855
0 1177	0.7269	0.6600	0.0005
0.1755	0 0 2 7 4	0.0007	0.0908
0.2616	0.0370	0.1510	0.0901
0.2014	0.9647	0.8009	0.1014
0.3889	1.1105	0.9922	0.1065
0.5778	1.2779	1.1352	0.1116
0.8569	1.4702	1.2979	0.1172
1.2675	1.6912	1.4827	0.1233
1.8690	1.9455	1.6920	0.1303
2.7443	2.2380	1.9280	0.1385
4.0072	2.5745	2.1929	0.1482
5.8102	2,9613	2.4881	0.1597
8.3509	3,4053	2.8147	0.1734
11.8776	3,9137	3,1729	0.1892
16 6027	4 4039	2 5422	0.1072
$10 \cdot 0757$	7.770		0.2073
23.1024	5.1552	3.9817	0.2213
31.7142	5.8997	4.4307	0.2489
42.8610	6.7420	4.9085	0.2719
57.2182	7.6897	5.4151	0.2957
75.5354	8.7540	5.9514	0.3201
# TABLE 13. COMPARISON OF MODEL WITH WILLIAMSON, BAZAIRE AND GEANKOPLIS [59]

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WILLIAMSON & BAZAIRE & GEANKOPLIS (1963) EQUATION ST SC\*\*.58 = 0.442 (RE/E)\*\*-.31 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 83 - 3333 XS = 0.3

REYNOLDS	MODEL	WILLIAMSON	DEVIATION
(GUR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
83.6600	9.1886	6.1578	0.3298
108.9902	10.4353	7.3908	0.2917
140.8616	11.8335	8.8218	0.2545
180.8422	13.4021	10.4816	0.2179
230.8992	15.1635	12.4066	0.1818
293.4984	17.1440	14.6400	0.1460
371.7243	19.3742	17.2324	0.1105
469.4210	21.8891	20.2428	0.0752
591.3615	24.7289	23.7395	0.0400
743.4491	27.9387	27.8008	0.0049
932.9637	31.5691	32.5162	-0.0300
1168.8604	35.6763	37.9883	-0.0648
1462.1372	40.3230	44.3338	-0.0994
1826.2865	45.5790	51.6864	-0.1339
2277.8505	51.5220	60.1985	-0.1684
2837.1057	58.2389	70.0451	-0.2027
3528.9034	65.8272	81.4264	-0.2369

TABLE 14. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 1.09/RE\*\*2/3 SCHMIDT NUMBER = 950 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 0.0027 - 92 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
0.0027	0.2416	0.2134	0.1166
0.0053	0.2785	0.2686	0.0357
0.0107	0.3314	0.3379	-0.0195
0.0213	0.4059	0.4250	-0.0468
0.0424	0.5082	0.5343	-0.0511
0.0841	0.6446	0.6713	-0.0414
0.1665	0.8214	0.8431	-0.0262
0.3290	1.0459	1.0578	-0.0113
0.6473	1.3298	1.3255	0.0032
1.2662	1.6898	1.6576	0.0190
2.4532	2.1472	2.0665	0.0376
4.6819	2.7284	2.5632	0.0605
8.7345	3.4650	3.1555	0.0893
15.7971	4.3926	3.8445	0.1247
27.5323	5.5482	4.6266	0.1661
46.1803	6.9723	5.4971	0.2115
74.7931	8.7131	6.4556	0.2590

TABLE 15. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 1.09/RE++2/3 SCHMIDT NUMBER = 70600 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 0.0027 - 92 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
0.0027	0.2070	0.2134	-0.0309
0.0053	0.2633	0.2686	-0.0200
0.0107	Ó.3342	0.3379	-0.0111
0.0213	0.4234	0.4250	-0.0037
0.0424	0.5355	0.5343	0.0023
0.0841	0.6764	0.6713	0.0075
0.1665	0.8537	0.8431	0.0124
0.3290	1.0770	1.0578	0.0178
0.6473	1.3591	1.3255	0.0247
1.2662	1.7163	1.6576	0.0341
2.4532	2.1701	2.0665	0.0477
4.6819	2.7475	2.5632	0.0670
8.7345	3.4805	3.1555	0.0933
15.7971	4.4049	3.8445	0.1272
27.5323	5.5579	4.6266	0.1675
46.1803	6.9799	5.4971	0.2124
74.7931	8.7192	6.4556	0.2596

TABLE 16. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 1.09/RE + 2/3SCHMIDT NUMBER = 950 (LIQUIDS) VOIDS FRACTION = 0.70REYNOLDS NUMBER RANGE = 0.0053 - 183XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
0.0050	0.3839	0.4183	-0.0896
0.0101	0.4783	0.5260	-0.0996
0.0200	0.6051	0.6610	-0.0924
0.0397	0.7706	0.8302	-0.0774
0.0786	0.9814	1.0420	-0.0616
0.1548	1.2478	1.3062	-0.0467
0.3034	1.5850	1.6345	-0.0312
0.5896	2.0120	2.0396	-0.0137
1.1306	2.5520	2.5339	0.0071
2.1237	3.2320	3.1264	0.0326
3.8752	4.0802	3.8204	0.0636
6.8225	5.1235	4.6130	0.0996
11.5576	6.3869	5.4992	0.1389
18.8821	7.8977	6.4767	0.1799
29.9160	9.6911	7.5505	0.2208
46.2762	11.8153	8.7322	0.2609
70.3346	14.3362	10.0399	0.2996
105.5814	17.3412	11.4957	0.3370
157.1198	20.9410	13.1245	0.3732

TABLE 17. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 1.09/RE\*\*2/3 SCHMIDT NUMBER = 70600 (LIQUIDS) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 0.0053 - 183 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
0.0050	0.3979	0.4183	-0.0513
0.0101	0.5035	0.5260	-0.0446
0.0200	0.6362	0.6610	-0.0390
0.0397	0.8030	0.8302	-0.0339
0.0786	1.0129	1.0420	-0.0286
0.1548	1.2777	1.3062	-0.0223
0.3034	1.6122	1.6345	-0.0137
0.5896	2.0358	2.0396	-0.0018
1.1306	2.5721	2.5339	0.0148
2.1237	3.2483	3.1264	0.0375
3.8752	4.0932	3.8204	0.0666
6.8225	5.1335	4.6130	0.1013
11.5576	6.3946	5.4992	0.1400
18.8821	7.9037	6.4767	0.1805
29.9160	9.6958	7.5505	0.2212
46.2762	11.8191	8.7322	0.2611
70.3346	14.3394	10.0399	0.2998
105.5814	17.3441	11.4957	0.3371
157.1198	20.9436	13.1245	0.3733

TABLE 18. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 0.25/RE\*\*.31 SCHMIDT NUMBER = 950 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 92 - 2500 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
92.6051	9.6456	6.6633	0.3091
115.0941	10.7156	7.7417	0.2775
142.2887	11.8924	8.9619	0.2464
175.1088	13.1871	10.3417	0.2157
214.6648	14.6124	11.9022	0.1854
262.2967	16.1827	13.6672	0.1554
319.6189	17.9146	15.6642	0.1256
388.5730	19.8266	17.9245	0.0959
471.4868	21.9396	20.4836	0.0663
571.1448	24.2767	23.3812	0.0368
690.8685	26.8637	26.6621	0.0075
834.6116	29.7285	30.3764	-0.0217
1007.0720	32.9020	34.5799	-0.0509
1213.8246	36.4179	39.3351	-0.0801
1461.4782	40.3129	44.7115	-0.1091
1757.8623	44.6272	50.7870	-0.1380
2112.2491	49.4048	57.6484	-0.1668
2535.6173	54.6939	65.3929	-0.1956

TABLE 19. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 0.25/RE\*\*.31 SCHMIDT NUMBER = 70600 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 92 - 2500 ' XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
92.6051	9.6513	6.6633	0.3095
115.0941	10.7209	7.7417	0.2778
142.2887	11.8973	8.9619	0.2467
175.1088	13.1917	10.3417	0.2160
214.6648	14.6169	11.9022	0.1857
262.2967	16.1870	13.6672	0.1556
319.6189	17.9188	15.6642	0.1258
388.5730	19.8305	17.9245	0.0961
471.4868	21.9439	20.4836	0.0665
571.1448	24.2807	23.3812	0.0370
690.8685	26.8679	26.6621	0.0076
834.6116	29.7328	30.3764	-0.0216
1007.0720	32.9061	34.5799	-0.0508
1213.8246	36.4223	39.3351	-0.0799
1461.4782	40.3172	44.7115	-0.1089
1757.8623	44.6318	50.7870	-0.1379
2112.2491	49.4093	57.6484	-0.1667
2535.6173	54.6977	65.3929	-0.1955

TABLE 20. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 0.25/RE\*\*.31 SCHMIDT NUMBER = 950 (LIQUIDS) VDIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 183 - 5000 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
181.3178	22.4266	13.1327	0.4144
227.8180	25.0308	15.3733	0.3858
285.7430	27.9346	17.9744	0.3565
357.8186	31.1730	20.9922	0.3265
447.3915	34.7842	24.4910	0.2959
558.5660	38.8100	28.5439	0.2645
696.3739	43.2961	33.2348	0.2323
866.9824	48.2931	38.6597	0.1994
1077.9505	53.8570	44.9288	0.1657
1338.5433	60.0503	52.1685	0.1312
1660.1180	66.9420	60.5240	0.0958
2056.5974	74.6098	70.1625	0.0596
2545.0501	83.1405	81.2761	0.0224
3146.4014	92.6312	94.0858	-0.0157
3886.3040	103.1907	108.8460	-0.0548
4796.2047	114.9411	125.8496	-0.0949

TABLE 21. COMPARISON OF MODEL WITH WILSON AND GEANKOPLIS [60]

WILSON & GEANKOPLIS (1966) EQUATION E J = 0.25/RE\*\*.31 SCHMIDT NUMBER = 70600 (LIQUIDS) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 183 - 5000 XS = 0.3

REYNOLDS	MODEL	WILSON	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
181.3178	22.4291	13.1327	0.4144
227.8180	25.0332	15.3733	0.3858
285.7430	27.9367	17.9744	0.3566
357.8186	31.1755	20.9922	0.3266
447.3915	34.7864	24.4910	0.2959
558.5660	38.8115	28.5439	0.2645
696.3739	43.2987	33.2348	0.2324
866.9824	48.2949	38.6597	0.1995
1077.9505	53.8578	44.9288	0.1657
1338.5433	60.0525	52.1685	0.1312
1660.1180	66.9437	60.5240	0.0958
2056.5974	74.6112	70.1625	0.0596
2545.0501	83.1416	81.2761	0.0224
3146.4014	92.6330	94.0858	-0.0156
3886.3040	103.1971	108.8460	-0.0547
4796.2047	114.9396	125.8496	-0.0949

is for a  $\operatorname{Re}_p$  ranging from 55 to 1500 with Schmidt numbers and voids fractions being the same as for the other equation. This equation converts to:

$$Sh_p/Sc^{1/3}[\epsilon/(1 - \epsilon)] = 0.25/(1 - \epsilon) Re_p^{.69}$$

for a  $\text{Re}_p/(1 - \epsilon)$  range from 92 to 2500 at a porosity of 0.4 and 183 to 5000 at a bed porosity of 0.7. Tables 18 through 21 show comparison of results of the model with the equation.

In his thesis Galloway [15] reports equations containing turbulence factors and graphs of  $\varepsilon$  J<sub>d</sub> versus Re<sub>p</sub> for beds of spheres, cylinders and commercial packing. Tables 22 through 30 show results obtained by estimating equations from his graphs and using these equations for comparison with the model. Estimated equations for spheres are:

$$\varepsilon J_d = 0.85 Re_p^{-.50}$$

for a  $\text{Re}_{p}$  range between 3 and 10,000 and a Schmidt number of 1000. This converts to:

$$Sh_p/Sc^{1/3}[\epsilon/(1-\epsilon)] = 0.85(1-\epsilon)^{-.5}[Re_p/(1-\epsilon)]^{.5}$$

for a  $\text{Re}_p/(1 - \epsilon)$  range between 5 and 16,700 for a bed porosity of 0.4 and between 10 and 33,333 for a voids fraction of 0.7.

$$\varepsilon J_{d} = 0.95 Re_{p}^{-.51}$$

for a Rep range between 10 and 10,000 and a Schmidt number of 1. This converts to:

$$h_p/Sc^{1/3}[\epsilon/(1-\epsilon)] = 0.95(1-\epsilon)^{-.51}[Re_p/(1-\epsilon)]^{.49}$$

for a  $\text{Re}_p/(1 - \epsilon)$  range between 17 and 16,700 for a bed porosity of 0.4 and between 33 and 33,333 for a voids fraction of 0.7. Tables 22 to 25 analyze these equations.

Estimated equations for commercial packing are:

$$\epsilon J_{d} = 0.7 Re_{p}^{-.48}$$

for a Rep range between 35 and 2000 and a Schmidt number of 1. This converts to:

$$Sh_p/Sc^{1/3} [\epsilon/(1 - \epsilon)] = 0.7(1 - \epsilon)^{-.48} [Re_p/(1 - \epsilon)]^{.52}$$

for a  $\operatorname{Re}_p/(1 - \varepsilon)$  range between 58 and 3333 for a bed porosity of 0.4 and between 117 and 6667 for a voids fraction of 0.7.

$$\varepsilon J_{d} = 0.23 Rep^{-.32}$$

for a Rep range between 2000 and 10,000 and a Schmidt number of 1000. This converts to:

$$Sh_p/Sc^{1/3}[\epsilon/(1-\epsilon)] = 0.23(1-\epsilon)^{-.32}[Re_p/(1-\epsilon)]^{.68}$$

for a  $\operatorname{Re}_p/(1 - \varepsilon)$  range between 3333 and 16,667 for a bed porosity of 0.4.

$$\varepsilon J_{d} = 0.50 Re_{p}^{-.41}$$

for a Rep range between 35 and 2000 and a Schmidt number of 1000. This converts to:

$$Sh_p/Sc^{1/3}[\epsilon/(1 - \epsilon)] = 0.50(1 - \epsilon)^{-.41}[Re_p/(1 - \epsilon)]^{.59}$$

TABLE 22. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, SPHERES [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR BEDS OF SPHERES E J = 0.95/RE\*\*.51 SCHMIDT NUMBER = 1 (GASES) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 17 - 16700 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AŽ)	(6KE/ADS)	(6KE/ADS)	FRACTION
16.0226	4.2321	4.7993	-0.1340
27.8987	5.3202	6.2980	-0.1837
46.7518	6.7193	8.1108	-0.2070
75.6586	8.4574	10.2685	-0.2141
118.9646	10.5737	12.8180	-0.2122
182.9820	13.1487	15.8287	-0.2038
276.9902	16.2933	19.3942	-0.1903
414.6284	20.1469	23.6330	-0.1730
615.7833	24.8866	28.6870	-0.1527
909.1413	30.7331	34.7212	-0.1297
1335.7102	37.9542	41.9242	-0.1046
1953.7778	46.8719	50.5120	-0.0776
2845.9635	57.8739	60.7349	-0.0494
4129.2699	71.4299	72.8860	-0.0203
5969.3868	88.1137	87.3116	0.0091
8600.9973	108.6299	104.4228	0.0387
2356.5448	133.8460	124.7084	0.0682
17706.9452	164.8315	148.7499	0.0975

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TABLE 23. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, SPHERES [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR BEDS OF SPHERES E J = 0.95/RE++.51 SCHMIDT NUMBER = 1 (GASES) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 33 - 33333 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
34.3932	10.0932	9.9371	0.0154
52.8744	12.3347	12.2682	0.0053
80.0105	14.9978	15.0291	-0.0020
119.7385	18.1788	18.3116	-0.0073
177.7973	21.9951	22.2256	-0.0104
262.4626	26.5873	26.8989	-0.0117
385.5627	32.1195	32.4771	-0.0111
563.9079	38.7822	39.1276	-0.0089
821.3252	46.7982	47.0439	-0.0052
1191.5570	56.4309	56.4531	-0.0003
1722.3868	67.9957	67.6232	0.0054
2481.4956	81.8735	80.8725	0.0122
3564.7579	98.5255	96.5798	0.0197
5107.9823	118.5122	115.1950	0.0279
7303.5199	142.5150	137.2532	0.0369
10423.7565	171.3632	163.3893	0.0465
14854.3412	206.0669	194.3568	0.0568
21141.1899	247.8578	231.0495	0.0678
30056.9690	298.2387	274.5268	0.0795

TABLE 24. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, SPHERES [15]

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GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR BEDS OF SPHERES E J = 0.85/RE\*\*.50 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 5 - 16700 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
7.2776	3.2283	2.9603	0.0830
13.2947	4.0952	4.0011	0.0229
23.4360	5.1789	5.3123	-0.0257
39.7536	6.5186	6.9188	-0.0613
65.0221	8.1595	8.8485	-0.0844
103.1153	10.1587	11.1430	-0.0968
159.6190	12.5910	13.8639	-0.1010
242.7263	15.5542	17.0962	-0.0991
364.4930	19,1772	20,9501	-0.0924
542.5527	23.6257	25.5602	-0.0818
802.4290	29.1067	31.0846	-0.0679
1180.7022	35.8728	37.7062	-0.0511
1729.4439	44.2276	45.6348	-0.0318
2522.5093	54.5361	55,1137	-0.0105
3664,5050	67.2397	66.4279	0.0120
5303,5616	82.8762	79,9147	0.0357
7649.4773	102,1049	95.9752	0,0600
10999.4387	125.7371	115-0876	0.0846
15774.4283	154.7732	137.8224	0.1095

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TABLE 25. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, SPHERES [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR BEDS OF SPHERES E J = 0.85/RE\*\*.50 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 10 - 33333 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
13.3576	6.7951	5.6718	0.1653
21.6167	8.3831	7.2152	0.1393
33.9899	10.2660	9.0475	0.1186
52.2805	12.4967	11.2209	0.1020
79.1400	15.1469	13.8056	0.0885
118.4652	18.3106	16.8909	0.0775
175.9381	22.1053	20.5844	0.0688
259.7546	26.6711	25.0115	0.0622
381.6315	32.1721	30.3165	0.0576
558.2222	38.7982	36.6658	0.0549
813.1324	46.7716	44.2526	0.0538
1179.7914	56.3548	53.3041	0.0541
1705.5391	67.8620	64.0898	0.0555
2457.4278	81.6717	76.9305	0.0580
3530.4414	98.2436	92.2088	0.0614
5059.1272	118.1347	110.3814	0.0656
7234.0508	142.0238	131.9924	0.0706
10325.0707	170.7337	157.6902	0.0763
14714.2601	205.2717	188.2467	0.0829
20942.4748	246.8614	224.5806	0.0902
29775.2226	296.9975	267.7847	0.0983

# TABLE 26. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, COMMERCIAL PACKING [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR COMMERCIAL PACKING E J = 0.7/RE\*\*.48 SCHMIDT NUMBER = 1 (GASES) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 58 - 3333 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(GUR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
		-	
59.4799	7.5302	7.4861	0.0058
78.4085	8.6058	8.6427	-0.0042
102.3652	9.8115	9.9280	-0.0118
132.5366	11.1626	11.3553	-0.0172
170.4078	12.6788	12.9407	-0.0206
217.8417	14.3824	14.7034	-0.0223
277.1744	16.2989	16.6654	-0.0224
351.3298	18.4574	18.8519	-0.0213
443.9556	20.8915	21.2912	-0.0191
559.5844	23.6398	24.0146	-0.0158
703.8279	26.7462	27.0562	-0.0115
883.6104	30.2597	30.4537	-0.0064
1107.4541	34.2353	34.2479	-0.0003
1385.8291	38.7340	38.4834	0.0064
1731.5826	43.8238	43.2091	0.0140
2160.4675	49.5802	48.4786	0.0222
2691.7937	56.0881	54.3509	0.0309
3349.2280	63.4420	60.8915	0.0402

# TABLE 27. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, COMMERCIAL PACKING [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR COMMERCIAL PACKING E J = 0.7/RE\*\*.48 SCHMIDT NUMBER = 1 (GASES) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 117 - 6667 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(GUR/AZ)	(GKE/ADS)	(6KE/ADS)	FRACTION
120.1870	18.2114	15.0524	0.1734
151.5724	20.3618	16.9825	0.1659
190.7316	22.7569	19.1381	0.1590
239.5497	25.4265	21.5459	0.1526
300.3476	28.4033	24.2350	0.1467
375.9781	31.7229	27.2373	0.1413
469.9422	35.4241	30.5874	0.1365
586.5336	39.5495	34.3235	0.1321
731.0155	44.1459	38.4876	0.1281
909.8388	49.2648	43.1262	0.1246
1130.9102	54.9635	48,2905	0,1214
1403.9211	61.3058	54.0378	0.1185
1740.7517	68.3626	60.4314	0.1160
2155.9658	76.2135	67.5419	0.1137
2667.4182	84.9474	75.4479	0.1118
3296.9977	94.6639	84.2367	0.1101
4071.5381	105.4746	94.0057	0,1087
5023.9338	117.5047	104-8630	0,1075
6194.5064	130.8944	116.9292	0.1066

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# TABLE 28. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, COMMERCIAL PACKING [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR COMMERCIAL PACKING E J = 0.50/RE\*\*.41 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 58 - 3333 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(GUR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
59.4799	7.8287	6.8676	0.1227
78.4085	8.9100	8.0835	0.0927
102.3652	10.1229	9.4605	0.0654
132.5366	11.4831	11.0180	0.0404
170.4078	13.0089	12.7792	0.0176
217.8417	14.7218	14.7717	-0.0033
277.1744	16.6471	17.0275	-0.0228
351.3298	18.8143	19.5839	-0.0409
443.9556	21.2574	22.4832	-0.0576
559.5844	24.0153	25.7732	-0.0731
703.8279	27.1319	29.5075	-0.0875
883.6104	30.6564	33.7459	-0.1007
1107.4541	34.6437	38.5549	-0.1128
1385.8291	39.1548	44.0085	-0.1239
1731.5826	44.2578	50.1891	-0.1340
2160.4675	50.0283	57.1888	-0.1431
2691.7937	56.5509	65.1107	-0.1513
3349.2280	63.9206	74.0705	-0.1587

### TABLE 29. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, COMMERCIAL PACKING [15]

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GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR COMMERCIAL PACKING E J = 0.23/RE\*\*.32 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 3333 - 16667 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
3419.3315	64.6694	68.5171	-0.0594
3770.5474	68.3292	73.2275	-0.0716
4156.7638	72.1945	78.2479	-0.0838
4581.3815	76.2764	83.5982	-0.0959
5048.1279	80.5869	89.2993	-0.1081
5561.0876	85.1385	95.3735	-0.1202
6124.7370	89.9444	101.8448	-0.1323
6743.9821	95.0186	108.7383	-0.1443
7424.1993	100.3758	116.0810	-0.1564
8171.2809	106.0317	123.9015	-0.1685
8991.6844	112.0026	132.2304	-0.1806
9892.4867	118.3061	141.1000	-0.1926
10881.4438	124.9604	150.5449	-0.2047
11967.0551	131.9852	160.6019	-0.2168
13158.6356	139.4007	171.3100	-0.2289
14466.3931	147.2289	182.7108	-0.2409
15901.5144	155.4928	194.8487	-0.2531
17476.2585	164.2157	207.7707	-0.2652

# TABLE 30. COMPARISON OF MODEL WITH GALLOWAY AND SAGE, COMMERCIAL PACKING [15]

GALLOWAY & SAGE (1967) ESTIMATED EQUATION FOR COMMERCIAL PACKING E J = 0.50/RE\*\*.41 SCHMIDT NUMBER = 1000 (LIQUIDS) VOIDS FRACTION = 0.70 REYNOLDS NUMBER RANGE = 117 - 6667 XS = 0.3

REYNOLDS	MODEL	GALLOWAY	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
120.1870	18.4361	13.8186	0.2504
151.5724	20.5849	15.8458	0.2302
190.7316	22.9782	18.1467	0.2102
239.5497	25.6457	20.7583	0.1905
300.3476	28.6203	23.7218	0.1711
375.9781	31.9377	27.0829	0.1520
469.9422	35.6369	30.8927	0.1331
586.5336	39.7602	35.2081	0.1144
731.0155	44.3547	40.0928	0.0960
909.8388	49.4720	45.6183	0.0778
1130.9102	55.1695	51.8648	0.0599
1403.9211	61.5108	58.9226	0.0420
1740.7517	68.5671	66.8936	0.0244
2155.9658	76.4176	75.8925	0.0068
2667.4182	85.1519	86.0486	-0.0105
3296.9977	94.8687	97.5080	-0.0278
4071.5381	105.6806	110.4352	-0.0449
5023.9338	117.7119	125.0161	-0.0620
6194.5064	131.1033	141.4601	-0.0789

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for a  $\text{Re}_p/(1 - \epsilon)$  range between 58 and 3333 for a bed porosity of 0.4 and between 117 and 6667 for a voids fraction of 0.7. Tables 26 to 30 show these equations.

Data for mass transfer in randomly packed beds of spheres to gases at low Reynolds numbers is given by Petrovic and Thodos [40]. The values given are corrected for axial mixing. Their recommended equation is:

$$\varepsilon J_d = 0.357/Re_p^{.359}$$

and is recommended for a  $Re_p$  between 3 and 230. This converts to the equation:

$$Sh_p/Sc^{1/3}[\epsilon/(1 - \epsilon)] = 0.357 \text{ Re}_p \cdot \frac{641}{(1 - \epsilon)}$$

with a  $\text{Re}_p/(1 - \epsilon)$  range from 5 to 390. Comparison of this equation with the model is in Table 31.

Table 32 compares the model with the equation of Jolls and Hanratty [27]. They used electrochemical techniques to study mass transfer rates to an active sphere in a dumped bed. They report the equation:

$$Sh_p/Sc^{1/3} = 1.44 Re_p^{.58}$$

to be good for a Schmidt number of 1700, voids fraction of 0.41 and a Re<sub>p</sub> range between 35 and 140. This converts to:

$$\operatorname{Sh}_{p}/\operatorname{Sc}^{1/3}[\varepsilon/(1 - \varepsilon)] = 1.44 \varepsilon/(1 - \varepsilon) \operatorname{Re}_{p}^{.58}$$

at a  $\text{Re}_{\text{p}}/(1 - \epsilon)$  range between 59 and 237.

TABLE 31. COMPARISON OF MODEL WITH PETROVIC AND THODOS [40]

PETROVIC & THODOS (1968) EQUATION E J = 0.357/RE\*\*.359 SCHMIDT NUMBER = 3 (GASES) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 5 - 390 XS = 0.3

REYNOLDS	MODEL	PETROVIC	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
4 0722	2 6707	1 1001	0 5525
4.7133	2.0191		0.5525
7.1760	3.0551	1.5168	0.5035
10.2537	3.5051	1.9067	0.4560
14.4859	4.0366	2.3794	0.4105
20.2101	4.6556	2.9456	0.3672
27.8271	5.3662	3.6159	0.3261
37.8124	6.1719	4.4012	0.2868
50.7344	7.0783	5.3138	0.2492
67.2819	8.0954	6.3678	0.2134
88.3002	9.2360	7.5800	0.1792
114.8381	10.5147	8.9707	0.1468
148.2052	11.9482	10.5641	0.1158
190.0427	13.5558	12.3895	0.0860
242.4094	15.3604	14.4813	0.0572
307.8858	17.3888	16.8798	0.0292
389.6970	19.6724	19.6321	0.0020

TABLE 32. COMPARISON OF MODEL WITH JOLLS AND HANRATTY [27]

JOLLS & HANRATTY (1969) EQUATION SH/SC\*\*1/3 = 1.44 RE\*\*.58 SCHMIDT NUMBER = 1700 (LIQUIDS) VOIDS FRACTION =0.41 REYNOLDS NUMBER RANGE = 59 - 237 XS = 0.3

REYNOLDS	MODEL	JOLLS	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
58.8424	7.9148	7.8308	0.0106
66.6772	8.3873	8.4196	-0.0038
75.3981	8.8847	9.0418	-0.0176
85.0932	9.4082	9.6990	-0.0309
95.8594	9.9591	10.3928	-0.0435
107.8039	10.5389	11.1254	-0.0556
121.0455	11.1491	11.8986	-0.0672
135.7153	11.7914	12.7149	-0.0783
151.9587	12.4674	13.5765	-0.0889
169.9367	13.1792	14.4862	-0.0991
189.8276	13.9287	15.4467	-0.1089
211.8288	14.7182	16.4611	-0.1184
236.1587	15.5500	17.5326	-0.1274

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TABLE 33. COMPARISON OF MODEL WITH WILKINS AND THODOS [58]

WILKINS & THODOS (1969) EQUATION E J = 0.589/RE\*\*.427 SCHMIDT NUMBER = 3 (GASES) VOIDS FRACTION = 0.40 REYNOLDS NUMBER RANGE = 33 - 3333 XS = 0.3

REYNOLDS	MODEL	WILKINS	DEVIATION
(6UR/AZ)	(6KE/ADS)	(6KE/ADS)	FRACTION
30.5378	5.5967	5.1958	0.0716
41.3359	6.4317	6.1801	0.0391
55.2624	7.3700	7.2988	0.0096
73.0485	8.4226	8.5643	-0.0168
95.5950	9.6028	9.9915	-0.0404
124.0220	10.9258	11.5989	-0.0616
159.7301	12.4092	13.4086	-0.0805
204.4754	14.0731	15.4469	-0.0976
260.4610	15.9415	17.7445	-0.1131
330.4458	18.0426	20.3371	-0.1271
417.8749	20.4093	23.2650	-0.1399
527.0341	23.0791	26.5740	-0.1514
663.2337	26.0949	30.3151	-0.1617
833.0319	29.5045	34.5448	-0.1708
1044.5050	33.3614	39.3260	-0.1787
1307.5790	37.7251	44.7281	-0.1856
1634.4369	42.6617	50.8281	-0.1914
2040.0195	48.2448	57.7118	-0.1962
2542.6420	54.5568	65.4746	-0.2001
3164.7524	61.6895	74.2231	-0.2031

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TABLE NUMBER	VOIDS FRACTION	REYNOLDS NUMBER RANGE	DEVIATION FRACTION RANGE	AVERAGE DEVIATION FRACTION
31	0.40	5-390	.55 🔶 0	+0.15
22	0.40	17-16,700	132110	-0.02
2	0.38	30-5000	.16 🔶01	+0.03
3	0.64	30-5000	.1027	-0.15
33	0.40	33-3333	. 07 🔶 20	-0.10
23	0.70	33-33,333	0 🔶 . 07	+0.02
4	0.40	40-4000	2902	-0.04
5	0.40	40-4000	0310	+0.04
7	0.50	40-4000	.141218	+0.14
26	0.40	58-3333	0	+0.01
10	0.40	67-667	.11 -> .14	+0.12
27	0.70	117-6667	.17 -> .11	+0.13
. 11	0.70	233-2330	.05 ->.06	+0.05
9	0.40	667-16,667	0417	+0.08

TABLE 34. SUMMARY OF RESULTS FOR GASES

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AVERAGE PERCENTAGE DEVIATION = +3%

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TABLE 35. SUMMARY OF RESULTS FOR LIQUIDS

		REYNOLDS	DEVIATION	AVERAGE
TABLE	VOIDS	NUMBER	FRACTION	DEVIATION
NUMBER	FRACTION	RANGE	RANGE	FRACTION
14	0.40	0.0027-92	.120526	+0.06
		Sc=950		
15	0.40	0.0027-92	0326	+0.06
		<b>Sc=7</b> 0600		
16	0.70	0.0053-183	0937	+0.05
		Sc=950		•
17	0.70	0.0053-183	0537	+0.06
		Sc=70600		
12	0.40	0.053-83	.0832	+0.15
24	0.40	5 16 700	09. N. 10. N. 11	+0 02
24	0.40	5-10,700	.001011	+0.02
25	0.70	10-33,333	.160510	+0.08
6	0.40	40-4000	.03 010	+0.04
8	0.50	40-4000	.18-+.13 -+.18	+0.15
28	0 40	58-3333	12	-0.04
20	0140			-0.04
32	0.41	59-237	.01	-0.03
13	0.40	83-3333	. 33 🛶 24	+0.03
18	0.40	92-2500	. 30	+0.05
30	0 70	117 6667	25 . 09	.0.05
50	0.70	11/-000/	, 23 , 00	+0.05
20	0.70	183-5000	.41 🔶10	+0.14
29	0.40	3333-16,667	0627	-0.15

AVERAGE PERCENTAGE DEVIATION = +5%

In order to demonstrate the usefulness of the computer model the results of an example problem, taken from Satterfield [48], are shown in Table 36. Table 40 in Appendix E is the program listing for Table 36. This program calculates h,  $k_c$  and pressure loss per unit length of bed by reading in the standard packed bed parameters and fluid properties. Actual Reynolds number (REI) is the Re<sub>p</sub>/(1 -  $\varepsilon$ ) calculated from bed parameters and fluid properties. Calculated Reynolds number (REE) is the Re<sub>p</sub>/(1 -  $\varepsilon$ ) calculated from (VY<sup>2</sup>)<sub>m</sub>. The (VY<sup>2</sup>)<sub>m</sub> used is calculated from the actual REI. Since the relationship between (VY<sup>2</sup>)<sub>m</sub> and the Reynolds number changes with the porosity of the bed, the constants Al through A9 have to be changed accordingly. The values for these constants are given in Table 37, Appendix C. 88

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# GIVEN BED CHARACTERISTICS

DIFFUSION COEFFICIENT (DIF) = 0.0296 SQ FT/HR

BED POROSITY (EP) = 0.40 SPECIFIC SURFACE (ASP) = 311 SQ FT/(CU FT) PARTICLE DIAMETER (DPA) = 0.01285 FT

VISCOSITY (VIS) = 0.092 LB/(FT,HR)

DENSITY (RHO) = 1.05 LB/(CU FT)

HEAT CAPACITY (CP) = 0.90 BTU/(LB,DEG F) SUPERFICIAL VELOCITY (VEL) = 1320 FT/HR

### COMPUTER RESULTS

		ACTUAL	CALCULATED Reynolds
	SCHMIDT	REYNOLDS	
VYSM	NUMBER	NUMBER	NUMBER
165593.6539	2.9601	322.6467	322.1269

HEAT	MASS	
TRANSFER	TRANSFER	DP/DL
COEFFICIENT	COEFFICIENT	PSI/FT
433.9091	98.0404	0.0397

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# GIVEN FLUID PROPERTIES

THERMAL CONDUCTIVITY (AK) = 0.131 BTU/(FT,HR,DEG F)

### TABLE 36. EXAMPLE USING MODEL

#### DISCUSSION OF RESULTS

The model equations of this thesis simulate heat and mass transfer rates in a randomly packed bed better over a wide range parameters than any of the empirical equations we found in the literature. This is because the equations are derived from basic fluid dynamics and transport phenomena principles. Other authors' equations are obtained by drawing arbitrary straight lines through scattered data points and in some cases using special mixing or turbulence factors to fit their data. Some of the earlier authors did not recognize that  $J_d$  was inversely proportional to voids fraction.  $\varepsilon J_d$ , and not  $J_d$ , is shown to be a function of Reynolds number by Thoenes & Kramers [54], Gupta & Thodos [22], Wilson & Geankoplis [60], and others. The model equations also cover the entire range of Reynolds numbers, Schmidt or Prandtl numbers, and voids fractions whereas literature equations are for limited ranges.

Comparisons between the model and empirical equations are given in Tables 2 to 33 and summarized in Tables 34 and 35.

The equation of Chu, Kalil and Wetteroth [8] is analyzed in Tables 2 and 3. Their equation is said to apply to both packed and fluidized beds and shows no dependency of  $J_d$  on voids fraction. In the article they show data for fixed beds with voids fractions of about 0.4 and expanded beds of higher porosities. Table 2, which is for a voids fraction of 0.38, shows a much better correlation than Table 3, which is for a porosity of 0.64. The equation of Chu,

et. al., gives mass transfer rates that are proportional to voids fraction compared to the model equations which indicate less dependency. For example, at an interstitial Reynolds number of 3900, the increase in mass transfer by the Chu equation is 0.64/0.38 whereas the model equations show an increase of only the square root of this ratio. In addition mass transfer rates are necessarily higher in fluidized beds due to the increased surface contact between solid and fluid which is the case in Table 2.

Thoenes and Kramers [54] present the equation shown in Table 4, which contains three additive terms. One term is for mass transfer in laminar flow, one for turbulent flow and one for stagnant areas. The packing was arranged in a body-centered cubic configuration. Analysis of results indicates that mass transfer was better in the bed at low Reynolds numbers than the model shows. This could be accountable to regular packing. In a regular packed bed there are bottlenecks in which the fluid flows at a much higher rate than the average velocity. Consequently mass transfer is greater in these areas. The effect on overall transfer rate would reasonably be greatest at lower Reynolds numbers.

Tables 5 to 8 compare a simplified formula presented by Thoenes and Kramers in the same article which they say has a mean deviation of  $\pm$  10%. Agreement is reasonably good for beds with porosities of 0.4 but model results average about 15% higher than the given formula for a voids fraction of 0.5. No tabular data is listed, but lines on graphs presented for packed beds with porosities of 0.48 generally show higher rates of mass transfer than for the lower porosities.

The equation of Bradshaw and Bennett [5] shown in Table 9 is in terms of  $J_d$  instead of  $\varepsilon J_d$ . Also the data from which the equation was derived shows a 25% standard deviation.

Kusik and Happel [31] use a free surface model to derive their equation which is compared to the model in Tables 10 and 11. They used boundary layer theory in the derivation. As the Tables indicate, correlation is better at a voids fraction 0.7 than for 0.4. This would seem reasonable for a free surface model which is described as a sphere surrounded by a spherical envelope of fluid.

Williamson, Bazaire and Geankoplis [59] present two equations, one for low and one for high Reynolds numbers. These comparisons are shown in Tables 12 and 13. Agreement is not too good, especially in the Reynolds number region where the two equations coincide. There is considerable scattering of the data and these two equations seemed to be the best fit.

Wilson and Geankoplis [60] used the data of the previous article by the senior author and new data to present two new equations which are analyzed in Tables 14 to 21. The first four Tables are for void fractions of 0.4 and the others for 0.7. It can be seen that changing the Schmidt number from 950 to 70,600 affects the results only at low Reynolds numbers. Figures 8 and 9, which follow, show graphically the answers in Tables 14 and 18. The model results follow closely the authors' equations, except in the intersecting region. Again in order to divide the data into two correlating equations, it was necessary to have larger deviations at intermediate Reynolds numbers. Similar graphs would result by plotting Tables 15 and 19, etc.



$$\frac{Rep}{1-e} = \frac{6uq}{AP}$$

Figure 8. Comparison of Model with Wilson and Geankoplis [60] Low Reynolds Numbers



Figure 9. Comparison of Model with Wilson and Geankoplis [60] High Reynolds Numbers

Galloway [15] presents graphs in his thesis that are correlations of his data and other authors. The equations presented contain turbulence intensity factors and are difficult to compare with the model. Two of the graphs given are plots of  $Sh/Sc^{1/3}$  versus Reynolds number; so equations were estimated from them that are comparable to the model. Tables 22 to 25 are for beds of spheres and the results compare reasonably well with the model. Tables 26 to 30 are for commercial packing. Again the results compare favorably.

Petrovic and Thodos [40] give an equation for mass transfer to gases. Table 31 shows poor correlation at low Reynolds numbers but the data presented in the article shows considerable scattering especially at low Reynolds numbers. He also uses axial mixing factors of Epstein [11] in his analyses.

Wilkins and Thodos [58] use the previous data of the senior author and others and give a new equation for mass transfer to gases which varies considerably from the previous equation. These results are given in Table 33. This equation gives higher mass transfer rates at corresponding Reynolds numbers.

Jolls and Hanratty [27] give an equation for mass transfer for an isolated sphere in a bed of inert spheres. Table 32 shows that mass transfer is slightly better than for the model. This would seem logical since the model is for a randomly packed bed of active spheres.

Figures 10, 11, and 12 compare the model results with literature equations for gases and liquids at voids fractions of 0.4 and 0.7. These Figures show that the model equations agree with the various



Rep = bul

Figure 10. Comparison of Model with Literature Correlations



Figure 11. Comparison of Model with Literature Correlations


Figure 12. Comparison of Model with Literature Correlations

authors' correlations better than the correlations do with each other. For this reason the deviation fractions in Tables 2 to 33 are based on results of the model equations. As is indicated in Tables 34 and 35 the average deviation for gases and liquids are +3% and +5%, respectively. Root mean square deviation, which is a measure of data scattering, is not applicable. Root mean square deviations were determined to be 13.0% for gases and 14.2% for liquids.

Satterfield [48] uses the equation of Petrovic and Thodos [40] and calculates heat and mass transfer coefficients for a hydrodesulfurization reactor packed with cylindrical catalyst pellets. Table 36 shows results using the model of this thesis. Units for the answers are: heat transfer coefficient--Btu/ft<sup>2</sup>hr<sup>o</sup>F; mass transfer coefficient--ft/hr; pressure drop per unit length of bed--pounds force per square inch per foot. Agreement between the computer answers and those of Satterfield is about 10% due to the use of the Petrovic equation.

#### SUMMARY

Through the years a very large number of articles have appeared in the literature, representing a huge expenditure of research time and effort in the study of heat, mass and momentum transfer in packed beds. Many of the authors have presented correlation equations for mass transfer coefficients covering varying ranges of fluid flow rates, physical properties and bed characteristics. The method of computing mass transfer coefficients developed here differs from most of these correlations, since it is based on a physical model and does not employ arbitrary empirical constants to fit a specific set of data.

If we compare the values predicted by the literature correlations with those computed by this new model, we find that the root-meansquare deviation for the literature correlations studied is about 13.5%, whereas the average deviation between the physical model results of this thesis and these same correlations is about 4%. In other words the mass transfer results from the model agree better with authors' results than a comparison of authors' results with one another.

The physical model is derived from basic principles of fluid flow and transport phenomena. The bed is considered to be randomly packed with spheres. The channels between the spheres are treated at low Reynolds numbers as parallel cylindrical tubes with different

cross sections. The distribution of cross sections is described by a distribution index, XS. The bed is assumed to be divided into layers of these parallel passages with the length of each passage equal to the diameter of the spheres used. The fluid from all of the tubes in each layer mix before entering the next layer. Flow in the passages is treated as laminar and the pressure drop across each layer is the same through each of the parallel conduits.

Mass transfer coefficients computed using this model are the ones for equimolal counter-diffusion, for low concentrations, or for other cases where J is equal to N. These coefficients are therefore entirely analogous to heat transfer and the latter may be computed by substituting Pr for Sc and Nu for Sh. Also in deriving the model most of the basic transport phenomena equations used--Leveque, Pohlhausen, Colburn--were originally derived for heat transfer. For simplicity, therefore, the model was derived on the basis of heat transfer and converted to mass transfer by substitution of the appropriate dimensionless variables.

Starting equations are heat and mechanical energy balances across a passage with constant temperature walls. A correction is added to account for the higher pressure gradient in the transition length. Musselt number is calculated (a) from a weighted average of the limiting value for fully developed laminar flow, (b) from the Leveque equation for developed velocity and developing temperature profiles, (c) from the Pohlhausen equation for developing velocity and temperature profiles and (d) from the Colburn equation for heat transfer across tube banks. These are all combined into a continuous equation which smooths out the transition ranges between the regimes

described by the individual equations. Average Nusselt and Reynolds numbers are then determined by integrating over the distribution of the cross sections in the layer. Overall Nusselt and Prandtl numbers of heat transfer are converted to Sherwood and Schmidt numbers of mass transfer. Since most of the literature correlations are in terms of Sherwood number divided by Schmidt number to the one-third power, they are easily compared with the model.

Due to the complexity of doing the mathematics of the model equations, they are solved by means of a computer program.

The model equations cover a much broader range of Reynolds and Schmidt numbers and bed porosities than do any of the literature correlations. The Colburn equation is used to account for turbulent heat and mass transfer at high Reynolds numbers. At low Reynolds numbers the distribution of cross sections is particularly important since uniform passages would give higher Sherwood numbers than experimental results show. This should be particularly important for gas chromatography where mass transfer occurs at extremely low flow rates in packed beds containing finely divided particles.

## CONCLUSIONS

The results and conclusions of this research are summarized as follows:

- a. Overall mass and heat transfer coefficients and pressure loss per unit length of bed can be predicted with reasonable accuracy using the physical model of this thesis. Fluid properties that need to be specified are: viscosity, heat capacity, superficial velocity, thermal conductivity, density, diffusion coefficient of active component through the fluid. Bed characteristics which have to be known are: porosity, particle size, specific surface per unit volume and an index defining the distribution of passage crosssections within the bed.
- b. The model equations cover wider Reynolds and Schmidt number ranges than do any of the literature correlations.
- c. Mass transfer results using the model equations show deviations from literature correlations of 3% for gases and 5% for liquids in the Reynolds and Schmidt number ranges reported.
- d. Mass transfer values calculated in Reynolds and Schmidt number ranges not corroborated by experimental investigators are believed to be reasonably accurate because basic principles of fluid dynamics and transport phenomena are used in developing the model.

- e. The distribution of cross-sections introduced into the model has an effect upon coefficients computed over the entire Reynolds number range. The effect is greatest, however, at extremely low Reynolds numbers where it gives Sherwood and Nusselt numbers which are much lower for the bed than for the limiting values for individual passages.
- f. Treatment of the passages between the spheres as layers of parallel tubes with mixing between layers proved to be satisfactory and convenient.
- g. The Pohlhausen and Leveque equations adequately describe transfer in the flow developing regions and the Colburn equation simulates the turbulence flow results. For simplicity reasons the model was derived on the basis of heat transfer.

## RECOMMENDATIONS FOR FUTURE WORK

After analyzing the results of this thesis the following suggestions are made for future investigations:

- a. Design carefully controlled experiments to cover a wide range of Schmidt, Reynolds numbers and bed porosities to further verify the results of the model. Investigate Reynolds number regions not previously explored. With more controlled experiments we would be justified in making a more sophisticated model.
- b. Using turbulent boundary layer theory or some other theoretical method, investigate the turbulent region in more detail to obtain a better theoretical model.
- c. Determine the effect of distributed cross sections on results using cylinders or commercial packing, such as Raschig rings, instead of spheres.
- d. Refine the fourth power method of evaluating the transition regions when calculating Nusselt number.
- e. Investigate the effect of particle shape on the distribution coefficient, XS, at low Reynolds numbers. Design experiments for gas flow mass transfer in beds of finely divided particles.
- f. Assume venturi shaped cross sections or passages with flat walls to see if a better model can be formulated.

g. A theoretical model could be attempted assuming passages with non-isothermal walls. The partial differential equations involved, however, would be more difficult to solve.

## APPENDICES

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APPENDIX A

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## APPENDIX A

## DERIVATION OF MODEL EQUATIONS

$$\frac{\text{DERIVATION OF } D_{av}}{D_{av}} = \frac{4 S_m}{\int_0^{s_m} \frac{4}{D} dS}$$

$$\text{Total perimeter from: } \Sigma m D = \int_0^{s_m} \frac{4}{D} dS$$
Since:  $S = \frac{S_m}{D_m} D^s$ 

$$dS = \frac{S_m}{D_m} S D^{s-1} dD$$

$$D_{av} = \frac{4 S_m}{(D_m / 4) / (S_m) + D^{s-1} dD}$$

$$D_{av} = \frac{\int_{m}^{D_{m}} \left(\frac{4}{D}\right) \left(\frac{5m}{D_{m}}\right) s D^{s-1} dD}{\int_{m}^{S/s} \int_{0}^{S_{m}} D^{s-2} dD}$$

$$D_{av} = \frac{D_{m}^{S/s}}{D_{m}^{S-2} dD}$$

$$D_{av} = \frac{D_{m}^{S/s}}{D_{m}^{S-1}} (s-1)$$

 $D_{av} = [(s - 1)/s] D_{m}$ 

.

•

(3)

(1)

V = 1 + 64/Y  $VY^{2} = Y^{2} + 64 Y$   $Y^{2} + 64 Y + 1024 = VY^{2} + 1024$   $(Y + 32)^{2} = VY^{2} + 1024$   $Y = (VY^{2} + 1024)^{1/2} - 32$ 

## MODEL EQUATIONS ASSUMING PARTICLES ARE SPHERES

The parallel cylindrical passage model is related to spherical particles using the subscript p to represent such particles.

 $\frac{\text{Volume of sphere}}{\text{Surface area of sphere}} = \frac{1}{\pi} \frac{\pi}{D_p^3} = \frac{1-\epsilon}{\Delta}$ 

$$D_{p} = 6(1 - \varepsilon)/a \tag{30}$$

Since:  $a = 4 \epsilon / D_{av}$  (5)

$$D_{p} = 1.5 D_{av} (1 - \epsilon)/\epsilon$$
(38)

$$Re_{p} = \frac{6(1-2)nq}{2}$$
(24)

Since:  $Re_{av} = D_{av} u Q/\epsilon \not$ 

 $D_{av} = 4 \epsilon/a$  (5)

$$Re_{av} = \frac{4 u \ell}{k / k}$$
(39)

$$Re_{p} = 1.5(1 - \varepsilon)Re_{av}$$
(23)

Since: 
$$Sh_{av} = D_{av} k_c / B$$

•

$$D_{av} = \frac{D_{e} \epsilon}{1.5(1-\epsilon)}$$
(38)

$$Sh_p = D_p k_c / \Delta$$

$$Sh_{av} = \frac{\ell Sh_{p}}{1.5(1-\ell)}$$
(25)

Since: 
$$D_{p} = 6(1 - \epsilon)/a$$
 (30)

$$Sh_p \stackrel{\bullet}{\underset{1-\bullet}{\underbrace{\bullet}}} = \stackrel{\bullet}{\underset{\bullet}{\underbrace{\bullet}}} \stackrel{\bullet}{\underset{\bullet}{\underbrace{\bullet}}} \stackrel{\bullet}{\underset{\bullet}{\underbrace{\bullet}}} (26)$$

Re = Y L/D

.

>

1

Since: 
$$L = D_p = 1.5 D_{av} (1-4)$$
 (38)

$$Re = \frac{1.5 D_{ev} Y}{D} \left(\frac{1-6}{6}\right)$$

Since:  $D_{av} = (1 - XS)D_m$  (4)

.

$$Re = 1.5 Y(1 - XS)[(1 - \varepsilon)/\varepsilon](D_m/D)$$

Since: 
$$D/D_m = (S/S_m)^{XS}$$
 (1)

Re = 1.5 Y(1 - XS) [(1 - 
$$\epsilon$$
)/ $\epsilon$ ] (S<sub>m</sub>/S)<sup>XS</sup> (32)

The average Nusselt number is calculated from an energy balance over a layer of passages. For one passage at the angle  $\theta$  it has been previously shown that:

$$Nu = - [(D \ Re \ Pr)/(4 \ L)][ln(\Delta T_2/\Delta T_1)]$$
(10)

A similar equation can be written for the average Nusselt number of heat flow perpendicular to the superficial velocity direction.

$$Nu_{av} = - \left[ \left( \frac{D}{av} \frac{Re}{av} \frac{Pr}{4} \right) / \left( \frac{4 L \cos \theta}{2} \right) \right] \left[ \ln \left( \frac{\Delta T}{2} / \frac{\Delta T}{1} \right) \right]$$
(40)

Since: 
$$L = 1.5 D_{av} [(1 - \varepsilon)/\varepsilon]$$
 (38)

$$Nu_{av} = - \left\{ \frac{[Re_{av}Pr \epsilon]}{[6 \cos \theta(1 - \epsilon)]} \frac{[\ln(\Delta T_2/\Delta T_1)]}{[\ln(\Delta T_2/\Delta T_1)]} \right\}$$
(33)

The average Stanton number is defined as:  $St_{av} = Nu_{av}/(Re_{av}Pr)$ .

$$St_{av} = - \left\{ \epsilon / \left[ 6 \cos \theta (1 - \epsilon) \right] \right\} \left[ \ln \left( \Delta T_2 / \Delta T_1 \right)_{av} \right]$$
(41)

L

The pressure loss per unit length in terms of the parameters of the model is determined by the following procedure from the Ergun [12] equation.

Ergun equation: 
$$\frac{-\Delta P \oint_c D_p e^3}{\mathbb{E} L \cos \phi u^2(1-\theta)} = \frac{150(1-\theta)}{Re_p} + 1.75$$

Let: EY = 
$$\frac{-\Delta P f_{c} D_{p} e^{3}}{P L \cos \bullet u^{4}(1-\epsilon)}$$

Since: 
$$VY^2 = \left(\frac{-\Delta P 2 f_{1} e^{2}}{e^{2} u^{2}}\right) \left(\frac{D^4 u^4 e^{2}}{e^{2} \mu^{2} L^{2}}\right)$$

$$(VY^2)_{\rm m} = VY^2 (D_{\rm m}/D)^4$$
 (31)

.

$$(VY^2)_{\rm H} = \frac{-\Delta P 2 4 c P D_{\rm H}}{\mu^2 L^2}$$

$$EY = \frac{(VY^{2})_{m} / L D_{p} e^{3}}{2 e^{2} D_{m}^{4} \cos * u^{2}(1-6)}$$

Since: 
$$L = D_p = 6(1 - \epsilon)/a$$
 (30)

$$EY = \frac{18(VY^{5})_{m} / e^{3}(1-e)}{e^{2} D_{m} u^{2} a^{2} \cos \Phi}$$

Since: 
$$D_{av}/D_{m} = (1 - XS)$$
 (4)

$$EY = \frac{18 (VY^{*})_{M} e^{3} (1-e) (1-Xs)^{4} \mu^{2}}{D_{M}^{4} cos + A^{2} \mu^{2} e^{2}}$$

Since: 
$$D_{av} = 4 \epsilon/a$$
 (5)

$$EY = \frac{9(VY^{2})_{M}(1-6)(1-XS)^{4}A^{2}\mu^{2}}{128 \ C \ c \ s \ \phi \ u^{2} \ q^{2}}$$

I

The Ergun Equation in terms of the model is then:

$$\frac{-\Delta P \oint_{e} D_{p} e^{3}}{P L \cos \theta u^{+}(1-e)} = \frac{q (hV)_{n} (1-e)(1-x3)_{a}^{a} / a^{+}}{158 e \cos \theta u^{+} (1-e)} = \frac{150(1-e)}{Re_{p}} + 1.15 (42)$$

Solving for pressure loss per unit length of bed:

$$-\Delta P/\Delta L = \frac{q \Delta^{+} / (1 - \epsilon)^{+} (1 - \kappa s)^{+} (/ \gamma^{+})_{m}}{128 g_{0} \epsilon^{+} (2 D_{p})}$$
(35)

APPENDIX B

I.

## APPENDIX B

#### DISTRIBUTION INDEX

XS was assigned a value of 0.3 by comparing model results with other authors' results from random packed beds. Figure 13 compares the equation of Wilson and Geankoplis with the model for XS values of 0, 0.25 and 0.50. After studying this graph and other similar plots from other authors it was decided to use XS = 0.3 in all calculations.  $D_m/O_p$  ratios for simple cubic (Figure 14) and rhombohedral (Figure 15) arrays or any other regular arrangement of spherical packing can be approximated by the following method.

$$D_{av} = (1 - XS)D_{m}$$
 (4)  
XS = 1 -  $D_{av}/D_{m}$ 

Since: 
$$D_p = 1.5 D_{av} (1 - \epsilon)/\epsilon$$
 (38)

$$XS = 1 - \frac{4}{L^{c}(1-4)} \frac{Dp}{Dn}$$

Since in regular packing the passage cross sections would be uniformly distributed (XS=0):

$$D_m/D_p = \frac{4}{1.5(1-4)}$$
(43)



 $\frac{Rep}{1-e} = \frac{6uQ}{aP}$ 





Figure 14. Simple Cubic Array of Spheres

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Figure 15. Rhombohedral Array of Spheres



## APPENDIX C

## APPENDIX C

# $(VY^2)_m$ variation with reynolds number

As is shown in Table 38 the  $(VY^2)_m$  value to use to produce a desired Reynolds number depends upon the porosity of the bed. Equation 44, which is in the form:

 $\ln (VY^2)_{m} = A1 + A2 (\ln REI) + A3 (\ln REI)^2 + \dots + A9(\ln REI)^8$ 

can be used to predict the correct  $(VY^2)_m$ . Using the data from Table 38 the average constants--Al, A2, A3, ..., A9--were determined by a least squares technique using the Gauss-Jordan elimination method.

#### TABLE 37

## **CONSTANTS FOR EQUATION 44**

	EP = 0.3	EP = 0.4	EP = 0.5	EP = 0.6	EP = 0.7
A1	.41243E+01	.45844E+01	.50061E+01	.55116E+01	.58816E+01
A2	.10406E+01	.10358E+01	.10360E+01	.12308E+01	.10583E+01
A3	85468E-02	61421E-02	.10438E-02	78292E-02	.27823E-01
A4	30444E-04	.40949E-02	.72698E-02	90507E-02	.11183E-01
A5	.26067E-02	.23634E-02	.18841E-02	.32217E-02	.49379E-03
<b>A6</b>	56269E-04	18728E-03	26065E-03	.89163E-04	30353E-03
A7	62718E-04	43577E-04	27265E-04	59663E-04	.63015E-06
<b>A8</b>	.69841E-05	.61836E-05	.53091E-05	.39252E-05	.35445E-05
A9	22253E-06	21780E-06	20741E-06	76254E-07	18853E-06

TABLE 38.  $(VY^2)_m$  VARIATION WITH REYNOLDS NUMBER

## VOID FRACTIONS (EP) OF 0.3,0.4,0.5,0.6,0.7

4# 7.2m 7.44

VYSM EP=0.3 EP=0.4EP=0.5 EP=0.6 EP=0.7 0.500E 00 0.872E-02 0.561E-02 0.374E-02 0.249E-02 0.160E-02 0.100E 01 0.173E-01 0.111E-01 0.744E-02 0.496E-02 0.319E-02 0.200E 01 0.345E-01 0.222E-01 0.148E-01 0.987E-02 0.634E-02 0.400E 01 0.686E-01 0.441E-01 0.294E-01 0.196E-01 0.126E-01 0.800E 01 0.136E 00 0.875E-01 0.583E-01 0.389E-01 0.250E-01 0.160E 02 0.269E 00 0.173E 00 0.115E 00 0.770E-01 0.495E-01 0.320E 02 0.532E 00 0.342E 00 0.228E 00 0.152E 00 0.978E-01 0.640E 02 0.104E 01 0.673E 00 0.449E 00 0.299E 00 0.192E 00 0.128E 03 0.204E 01 0.131E 01 0.877E 00 0.585E 00 0.376E 00 0.256E 03 0.396E 01 0.254E 01 0.169E 01 0.113E 01 0.728E 00 0.512E 03 0.756E 01 0.486E 01 0.324E 01 0.216E 01 0.138E 01 0.102E 04 0.140E 02 0.905E 01 0.603E 01 0.402E 01 0.258E 01 0.204E 04 0.254E 02 0.163E 02 0.108E 02 0.726E 01 0.466E 01 0.409E 04 0.441E 02 0.284E 02 0.189E 02 0.126E 02 0.811E 01 0.819E 04 0.739E 02 0.475E 02 0.317E 02 0.211E 02 0.135E 02 0.163E 05 0.119E 03 0.768E 02 0.512E 02 0.341E 02 0.219E 02 0.327E 05 0.187E 03 0.120E 03 0.805E 02 0.536E 02 0.345E 02 0.655E 05 0.288E 03 0.185E 03 0.123E 03 0.825E 02 0.530E 02 0.131E 06 0.436E 03 0.280E 03 0.187E 03 0.124E 03 0.802E 02 0.262E 06 0.653E 03 0.420E 03 0.280E 03 0.186E 03 0.120E 03 0.524E 06 0.970E 03 0.624E 03 0.416E 03 0.277E 03 0.178E 03 0.104E 07 0.143E 04 0.921E 03 0.614E 03 0.409E 03 0.263E 03 0.209E 07 0.210E 04 0.135E 04 0.902E 03 0.601E 03 0.386E 03 0.419E 37 0.307E 04 0.197E 04 0.131E 04 0.879E 03 0.565E 03 0.838E 07 0.448E 04 0.288E 04 0.192E 04 0.128E 04 0.823E 03 0.167E 08 0.650E 04 0.418E 04 0.278E 04 0.185E 04 0.119E 04 0.335E 08 0.940E 04 0.604E 04 0.402E 04 0.268E 04 0.172E 04 0.671E 08 0.135E 05 0.870E 04 0.580E 04 0.387E 04 0.248E 04 0.134E J9 0.194E 05 0.125E 05 0.834E 04 0.556E 04 0.357E 04 0.268E 09 0.278E 05 0.179E 05 0.119E 05 0.796E 04 0.512E 04 0.536E 09 0.398E 05 0.256E 05 0.170E 05 0.113E 05 0.732E 04 0.107E 10 0.569E 05 0.365E 05 0.243E 05 0.162E 05 0.104E 05 0.214E 10 0.810E 05 0.521E 05 0.347E 05 0.231E 05 0.148E 05 0.429E 10 0.115E 06 0.741E 05 0.494E 05 0.329E 05 0.211E 05 0.858E 10 0.164E 06 0.105E 06 0.703E 05 0.468E 05 0.301E 05 0.171E 11 0.233E 06 0.149E 06 0.998E 05 0.665E 05 0.428E 05 0.343E 11 0.330E 06 0.212E 06 0.141E 06 0.945E 05 0.607E 05 0.687E 11 0.469E 06 0.301E 06 0.201E 06 0.134E 06 0.861E 05 0.137E 12 0.665E 06 0.427E 06 0.285E 06 0.190E 06 0.122E 06 0.274E 12 0.942E 06 0.606E 06 0.404E 06 0.269E 06 0.173E 06

The values in the 5 columns to the right are Reynolds numbers,

 $\operatorname{Re}_p/(1-\varepsilon)$ , calculated from the model using  $(VY^2)_m$  values in the left column.

APPENDIX D

## APPENDIX D

SUMMARY OF MODEL EQUATIONS

Assume a value for  $(VY^2)_m$  depending upon the  $\operatorname{Re}_p/(1 - \varepsilon)$  desired. By graphical integration solve for: ŀ

$$Re_{av} = (1 - XS) \cos \phi \int_{0}^{1} Re \left(\frac{S_{m}}{S}\right)^{XS} d\left(\frac{S}{S_{m}}\right)$$
(13)

$$(\Delta T_{2}/\Delta T_{1})_{av} = \frac{\int_{0}^{1} e^{-\frac{4M_{u}}{\sqrt{R_{r}}}} \operatorname{Re}\left(\frac{S_{m}}{S}\right)^{\times S} d\left(\frac{S}{S_{m}}\right)}{\int_{0}^{1} \operatorname{Re}\left(\frac{S_{m}}{S}\right)^{\times S} d\left(\frac{S}{S_{m}}\right)}$$
(14)

The sequence used for the graphical integration is: For  $S/S_m$  values between 0 and 1, determine:

$$VY^2 = (VY^2)_{\rm m} (S/S_{\rm m})^4 (XS)$$
 (31)

$$RT = (VY^2)^{.25}$$
 (21)

$$Y = (VY^{2} + 1024 - 32)(1 - 5.8/(RT + 175/RT))$$
(20)

$$Re = 1.5 Y(1 - XS) \left(\frac{1 - 6}{6}\right) \left(\frac{S_{h_1}}{5}\right)^{XS}$$
(32)

Nu = 
$$((3.656^{4} + 1.615^{4} (Y Pr)^{4/3} + (.664 (2 Y)^{1/2} Pr^{1/3})^{4})^{4/3}$$
 (22)  
+  $(.33 \text{ Re}^{.6} Pr^{1/3})^{4})^{.25}$ 

After  $\text{Re}_{av}$  and  $(\Delta T_2/\Delta T_1)_{av}$  have been determined:

$$Re_{p}/(1-\varepsilon) = 1.5 Re_{av}$$
(23)

$$Nu_{av} = - \frac{e \operatorname{Pr} \operatorname{Re}_{bv}}{6(1-4) \cos \theta} \quad \ln \left(\frac{\Delta T_{b}}{\Delta T_{l}}\right)_{Av} \tag{33}$$

$$\frac{Sh_p}{Se^{43}} \stackrel{\ell}{\longrightarrow} = \frac{1.5 \text{ Nu}_{AV}}{P_{F}^{1/3}}$$
(34)

$$k_{c} = \frac{h d' S_{c}^{\prime \prime 3}}{6 d} \left[ \frac{Shp}{S_{c}^{\prime \prime 3}} \frac{d}{1-d} \right]$$
(26)

$$-\Delta P/\Delta L = \frac{q \lambda^2 f^2 (1-\epsilon)^2 (1-xs)^4 (VY^2)_m}{128 s_c \epsilon^4 \ell D_p}$$
(35)

$$h = Nu_{av} k a/(4 \epsilon)$$

(37)

ŀ

APPENDIX E

#### APPENDIX E

```
TABLE 39. COMPUTER PROGRAM LISTING FOR TABLE 2
      WRITE(5,1)
      FORMAT(1H1)
  1
      WRITE(5.2)
  2
      FORMAT(14(/)21X'CHU + KALIL + WETTEROTH (1953)',/21X
     1'EQUATION J = 1.77/REE++.44',/21X
     2'SCHMIDT NUMBER = 2.57 (GASES)',/21X
     3'VOIDS FRACTION = 0.38'./21X
     4'REYNOLDS NUMBER RANGE = 30 - 5000',/21X
     5^{XS} = 0.3^{I}////)
      WRITE(5.3)
  3
     FORMAT(9X
     1'REYNOLDS
                                                            DEVIATION
                           MODEL
                                              CHU
     21/9X
                        (6KE/ADS)
                                         (6KE/ADS)
                                                            FRACTION'
     3 ( 6 UR / AZ )
     4,//)
      FORMAT(4F17.4)
  4
С
      COSINE THETA
      CT=.707
C
      CONSTANT IN LANGHAAR CORRECTION
      8=5.8
С
      SCHMIDT NUMBER EQUALS VISCOSITY DIVIDED BY
С
      DENSITY AND DIFFUSIVITY
      PR=2.57
С
      BED VOIDS FRACTION
      EP=.38
      EPR=(1.-EP)/E^{p}
С
      DISTRIBUTION INDEX
      XS=.3
С
      V TIMES Y SQUARED MAXIMUM
      VYSM=2600.
      DO 12 N=1.22
      VYSM=VYSM+1.5
      S DIVIDED BY S SUBSCRIPT M
С
      SR = 1.0625
С
      START GRAPHICAL INTEGRATION TO FIND
С
      AVERAGE REYNOLDS NUMBER AND
С
      AVE TEMPERATURE DIFFERENCE RATIO
      DO \ 10 \ I = 1, 16
      SR=SR-.0625
С
      D DIVIDED BY D SUBSCRIPT M
      DR = SR + XS
С
      V TIMES Y SQUARED
      VYS= VYSM + DR++4
      VARIABLE IN LANGHAAR CORRECTION
С
      RT = VYS + 25
С
      Y EQUALS DIAMETER TIMES REYNOLDS NUMBER
С
      DIVIDED BY LENGTH
      Y = ((1024.+VYS)**.5 - 32.)*(1. - B/(RT + 175./RT))
С
      REYNOLDS NUMBER IN A PASSAGE
      RE=1.5+Y+EPR/DR+(1.-XS)
```

## TABLE 39 (cont'd,)

С		NUSSELT NUMBER IN A PASSAGE				
		AA=3.656**4+1.615**4*(Y*PR)**1.33333				
		BB=(.664*(2.*Y)**.5*PR**.33333)**4				
		CC=(.33*RE**.6*PR**.33333)**4				
		GNU = (AA + BB + CC) * * .25				
		IF(I-1)15.15.9				
С		LOGARITHM OF MAXIMUM TEMPERATURE DIFFERENCE RATIO. SR = 1				
	15	ALXM=-4.*GNU/PR/Y				
С		STARTING VALUE FOR INTEGRAL TO FIND AVERAGE REYNOLDS NUMBER				
		SUMR=-RE/2.				
С		STARTING VALUE FOR INTEGRAL TO FIND AVERAGE TEMPERATURE RATIO				
		SXOMR=-RE/2.				
С		SUM OF REYNOLDS NUMBERS				
	2	SUMR=SUMR+RE/DR				
С		TEMPERATURE DIFFERENCE RATIO DIVIDED BY MAXIMUM RATIO				
		XOXM=EXP(-4.*GNU/PR/Y-ALXM)				
С		SUM OF TEMPERATURE DIFFERENCE RATIOS DIVIDED BY MAXIMUM RATIO				
	10	SXOMR=SXOMR+XOXM*RE/DR				
С		CORRECTION FOR THE INITIAL VALUE				
		SUMR=SUMR+RE/DR/2.				
С		CORRECTION FOR THE INITIAL VALUE				
		SXOMR=SXOMR+RE/DR/2.				
С		AVERAGE REYNOLDS NUMBER FOR A GIVEN VYSM				
		REA=(1XS)*CT*SUMR/16.				
С		AVERAGE TEMPERATURE DIFFERENCE RATIO DIVIDED BY MAXIMUM RATIO				
		DTAOM=SXOMR/SUMR				
С		AVERAGE TEMPERATURE DIFFERENCE RATIO FOR A GIVEN VYSM				
		XX=-(ALOG(DTAOM)+ALXM)				
С		AVERAGE STANTON NUMBER				
		STA=XX/6./EPR/CT				
С		PARTICLE REYNOLDS NUMBER DIVIDED BY (1 - VOIDS FRACTION) = 6UR/AZ				
_		REE=1.5*REA				
С		AVERAGE NUSSELT NUMBER				
		GNUA=STA*REA*PR				
С		6KE/ADS FROM MODEL EQUATIONS				
~		SST=1.5*GNUA/PR**.33333				
C		6KE/ADS FROM THE EQUATION OF CHU, KALIL AND WETTEROTH				
c						
L		DEVIATION FRACTION BASED ON MODEL 6KE/ADS				
		UEV = (331 - UHU)/351				
	12	ПКТТЕ (3,4)КСС,331, СПО, ЛЕУС СОМТТИНК				
	12					
		UALL EXII				

END

TABLE 40. COMPUTER PROGRAM LISTING FOR TABLE 36 WRITE(5,1) FORMAT(1H1,12(/)) 1 WRITE(5.5) 5 FORMAT(27X'GIVEN FLUID PROPERTIES',//12X 2 VISCOSITY (VIS) = 0.092 LB/(FT,HR),/12X"HEAT CAPACITY (CP) = 0.90 BTU/(LB,DEG F)",/12X 3 'SUPERFICIAL VELOCITY (VEL) = 1320 FT/HR'./12X 4 'THERMAL CONDUCTIVITY (AK) = 0.131 BTU/(FT.HR.DEG F)') 5 WRITE(5.6) FORMAT(12X, 'DENSITY (RHO) = 1.05 LB/(CU FT) +/12X 6 'DIFFUSION COEFFICIENT (DIF) = 0.0296 SQ FT/HR',///25X 1 'GIVEN BED CHARACTERISTICS',//12X 2 3 \*BED PURDSITY (EP) = 0.40\*,/12X'SPECIFIC SURFACE (ASP) = 311 SQ FT/(CU FT)',/12X 4 'PARTICLE DIAMETER (DPA) = 0.01285 FT') 5 WRITE(5.7) 7 FORMAT(////30X'COMPUTER RESULTS') WRITE(5,2) 2 FORMAT(//11X 1' ACTUAL CALCULATED' 2,/11X31 SCHMIDT REYNOLDS **REYNOLDS**<sup>•</sup> 4,/10X 5ºVYSM NUMBER NUMBER NUMBER!) С COSINE THETA CT=.707 С CONSTANT IN LANGHAAR CORRECTION 8=5.8 С DISTRIBUTION INDEX XS=.3С **VISCOSITY** OF FLUID VIS=.092 С HEAT CAPACITY OF FLUID CP=.9С SUPERFICIAL VELOCITY OF FLUID VEL=1320. С THERMOCONDUCTIVITY OF FLUID AK=.131 С DENSITY OF FLUID RHU=1.05 С DIFFUSIVITY OF ACTIVE COMPONENT DIF = .0296С BED VOIDS FRACTION EP=.4С SPECIFIC SURFACE OF PACKING ASP=311.

C DIAMETER OF PARTICLE

TABLE 40 (cont'd.) DPA=.01285 GRAVITATIONAL CUNSTANT GC=4.17E+08EPR=(1.-EP)/EPSCHMIDT NUMBER EQUALS VISCOSITY DIVIDED BY DENSITY AND DIFFUSIVITY SC=VIS/DIF/RHO PR=SC ACTUAL PARTICLE REYNOLDS NUMBER REO=DPA+VEL+RHO/VIS ACTUAL REYNOLDS NUMBER = 6UR/AZ REI=REO/(1.-EP)CONSTANTS FROM TABLE 37 A1 = .458442E+01A2=.1035827E+01 A3 = -.6142123E - 02A4=.4094915E-02 A5=.2363402E-02 A6=-.187284E-03 A7=-.4357685E-04 A8=.6183554E-05 A9=-.2178007E-06 EQUATION TO FIND V TIMES Y SQUARED MAX FROM ACTUAL REYNOLDS NUMBER A=ALOG(REI) AZ=A1+A2+A+A3+A++2 AZ=AZ+A4+A++3+A5+A++4+A6+A++5 AZ=AZ+A7+A++6+A8+A++7+A9+A++8 V TIMES Y SQUARED MAX VYSM=EXP(AZ) S DIVIDED BY S SUBSCRIPT M SR = 1.0625START GRAPHICAL INTEGRATION TO FIND AVERAGE REYNOLDS NUMBER AND AVE TEMPERATURE DIFFERENCE RATIO DO 10 I = 1,16 SR=SR-.0625 С D DIVIDED BY D SUBSCRIPT M DR = SR + XSС **V TIMES Y SQUARED** VYS= VYSM + DR++4 С VARIABLE IN LANGHAAR CORRECTION RT = VYS + .25C Y EQUALS DIAMETER TIMES REYNOLDS NUMBER С DIVIDED BY LENGTH Y = ((1024.+VYS)\*\*.5 - 32.)\*(1. - B/(RT + 175./RT))С REYNOLDS NUMBER IN A PASSAGE RE=1.5+Y+EPR/DR+(1.-XS) C NUSSELT NUMBER IN A PASSAGE

C

С С

C

С

С

C C

С

С

TABLE 40 (cont'd.)

		AA=3.656**4+1.615**4*(Y*PR)**1.33333
		RB=(664*(2*Y)**5*DD**37373)**A
		$CC = ( 33 \times 10^{-1} \times 10$
		$CVU_{(,55,KL_{,0},0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0$
		$UNU = (AA+DD+UU)^{}.25$
_		1F(1-1)15,15,9
С		LOGARITHM OF MAXIMUM TEMPERATURE
С		DIFFERENCE RATIO, $SR = 1$
	15	ALXM=-4.*GNU/PR/Y
С		STARTING VALUE FOR INTEGRAL
С		TO FIND AVERAGE REYNOLDS NUMBER
		SUMR=-RE/2.
С		STARTING VALUE FOR INTEGRAL TO FIND
С		AVERAGE TEMPERATURE DIFFERENCE RATIO
		SXOMR=_RF/2
e		SIM OB DEVNOLDS MUMBEDS
	Q	
C	9	TENDEDATUDE DIFFEDENCE DATIO
č		ILMPERATURE DIFFERENCE RATIO
C		DIVIDED BY MAXIMUM RAITO
6		XUXM=E&P(-4. "GNU/PR/Y-ALXM)
		SUM OF TEMPERATURE DIFFERENCE RATIOS
C	_	DIVIDED BY MAXIMUM RATIO
	19	SXOMR=SXOMR+XOXM*RE/DR
C		CORRECTION FOR INITIAL VALUE
		SXOMR=SXOMR+RE/DR/2.
С		CORRECTION FOR INITIAL VALUE
		SUMR=SUMR+RE/DR/2.
С		AVERAGE REYNOLDS NUMBER FOR A GIVEN VYSM
		REA=(1,-XS)*CT*SUMR/16.
С		AVERAGE TEMPERATURE DIFFERENCE RATIO
С		DIVIDED BY MAXIMUM RATIO
		DTAOM=SXOMR/SUMR
С		AVERAGE TEMPERATURE DIFFERENCE RATIO
C		EOD & CIVEN VYSM
		$\mathbf{Y}_{\mathbf{X}} = (\mathbf{A} \cup \mathbf{C} (\mathbf{D} \top \mathbf{A} \cup \mathbf{M}) + \mathbf{A} \cup \mathbf{Y}_{\mathbf{M}})$
C		AVEDACE CTANTON AUBADED
$\sim$		AVERAGE STANION NUMBER
C		
č		PARTICLE REYNOLDS NUMBER DIVIDED
C		BY $(1 VOIDS FRACTION) = 6UR/AZ$
~		REE=1.5*REA
C		AVERAGE NUSSELT NUMBER
~		GNUA=STA*REA*PR
C		6KE/ADS FROM MODEL EQUATIONS
		SST=1.5*GNUA/PR**.33333
С		HEAT TRANSFER COEFFICIENT
		AH=GNUA*AK*ASP/4./EP
С		MASS TRANSFER COEFFICIENT
		AKC=ASP*DIF*SC**.33333/6./EP*SST
С		PRESSURE LOSS PER UNIT LENCTH OF RED
		DPDL=9.*ASP**2*VIS**2*(1_FD)**2
		$\frac{DPDL_{\pm}DPDI + (1 _ YS) + * 4 + 1/VSM / 129}{DPDL_{\pm}DPDI + (1 _ YS) + * 4 + 1/VSM / 129}$

		TABLE	40 (co	nt'd.)		
3 4 8	DPDL=DPDL/GC/EP**4/RHO/ WRITE(5,3)VYSM,PR,REI,R FORMAT(/4F17.4) WRITE(5,4) FORMAT(////6X 1'HEAT 2'TRANSFER 3'COEFFICIENT FORMAT(/9X3F17.4) WRITE(5,8)AH,AKC,DPDL CALL EXIT END		/DP <b>A/</b> REE	MASS TRANSFER CDEFFICIE	DP/DL",/7X PSI/FT")	
EAT EXT IOC	URES SUPP ENDED PRE S	ORTED CISION				
	REQUIREM MON	ENTS FOR O VARIABLES	172	PROGRAM	1312	
END	OF COMPIL	ATION				
// ×	EQ					

APPENDIX F
#### APPENDIX F

## TABLE 41. SHERWOOD NUMBERS, UNIFORM AND NON-UNIFORM PASSAGES

#### SCHMIDT NUMBER = 1 VOIDS FRACTION = .4

REYNOLDS	SHERWOOD	REYNOLDS	SHERWOOD
(4UR/AZ)	(XS=.3)	(4UR/AZ)	(XS=0)
0.0002	1.1300	0.0007	3.6560
0.0004	1.1302	0.0015	3.6560
0.0009	1.1310	0.0030	3.6560
0.0018	1.1320	0.0060	3.6560
0.0037	1.1337	0.0120	3.6560
0.0074	1.1364	0.0239	3.6561
0.0147	1.1410	0.0476	3.6563
0.0293	1.1493	0.0945	3.6568
0.0582	1.1646	0.1872	3.6580
0.1154	1.1937	0.3698	3.6611
0.2279	1.2459	0.7278	3.6690
0.4483	1.3294	1.4240	3.6890
0.8765	1.4542	2.7603	3.7392
1.6971	1.6377	5.2708	3.8611
3.2356	1.9065	9.8294	4.1339
6.0269	2.2956	17.7197	4.6595
10.8788	2.8416	30.6258	5.5049
18.9190	3.5732	50.6487	6.6785
31.6664	4.5129	80.5665	8.1774
51.1936	5.6792	124.4274	10.0291
80.4313	7.0988	188.4019	12.3023
123.6393	8.8263	261.8330	15.1029
187.0805	10.9363	418.5266	18.5683
279.9594	13.5222	618.4262	22.8646
415.6919	16.7032	909.9348	28.1877
613.6238	20.6271	1333.2542	34.7702
901.4041	25.4737	1945.2162	42.8924
1 318.3273	31.4590	2826.2189	52.8964
1920.0885	38.8428	4090.1040	65.2029
2785.5598	47.9403	5898.1543	80.3305
4026.4345	59.1366	8478.8974	98.9195
5800.9157	72.9045	12156.1121	121.7597
8333.1087	89.8261	17388.4383	149.8247
11940.4643	110.6193	24825.4019	184.3144
17072.5996	136.1690	35386.6635	226.7064

TABLE OF NOMENCLATURE

### TABLE OF NOMENCLATURE

## Primary Quantities

St. Line in

Symbol	Dimension Name
F	Force
Н	Heat
L	Length
М	Mass
Т	Temperature
t	Time

# Secondary Quantities

Symbol [Variable]	Name	Dimensions					
		F	Н	L	M	Т	t
a	Packing area per unit volume of bed			-1			
С	Heat capacity of flowing fluid		1		-1	-1	
D	Diameter of a given passage			1			
Dav	Average diameter of a passage			1			
D <sub>m</sub>	Maximum diameter of any passage			1			
Dp	Particle diameter			.1			
ø	Diffusivity of solute in flowing fluid			2			-1
G	Mass velocity of fluid in a given passage			-2	1		-1
Gav	Average mass velocity of fluid perpendicular to cross-section			-2	1		-1

.

Symbol	Name	Dimensions					
		F	H	L	м	Т	t
<sup>g</sup> c	Gravitational constant	-1		1	1		-2
h	Average Fluid film heat transfer coefficient parallel to the bed axis		1	-2		-1	-1
k	Thermal conductivity of fluid		1	-1		-1	-1
k c	Average mass transfer coefficient			1			-1
L	Length of parallel passages			1			
m	Mass flow rate in a given passage				1		-1
Р	Pressure exerted by fluid	1		-2			
S	Total cross-sectional area of all passages having diameters less than D			2			
Sm	Total cross-sectional area of all passages			2			
T <sub>1</sub>	Temperature of fluid entering a passage					1	
T <sub>2</sub>	Temperature of fluid leaving a passage					1	
т <sub>р</sub>	Temperature of fluid at any point in a passage					1	
Tw	Temperature of the passage wall					1	
u	Average linear velocity of fluid, based on empty cross-section, perpendicular to the cross- section of the bed			1			-1
W	Velocity component perpendicular to the cross-section			1			-1
ρ	Fluid density			-3	1		
μ	Fluid viscosity			-1	1		-1

## TABLE OF NOMENCLATURE (cont'd.)

## TABLE OF NOMENCLATURE (cont'd.)

## Other Terms

Symbol	Name
ε	Voids fraction (voids volume/total bed volume)
<b>Ð</b>	Average angle between passages and average flow direction in bed (degrees)
A,B	Constants in Langhaar [32] correction factor for Y
C <sub>1</sub> ,x	Constant and exponent in: $Sh_p/Sc^{1/3} [\epsilon/(1 - \epsilon)]$
	= $C_1[Re_p/(1 - \varepsilon)]^x$
S	Exponent which depends upon the distribution of passages
XS	1/s

Dimensionless Groups

Sy	mb	01

#### Name

Basic Formula

Gz	Graetz number	D Re Pr/L
Jd	Colburn mass transfer factor	Ke Scars
<b>յ</b>	Colburn heat transfer factor	h R 3/8
Nu	Nusselt number in a passage	h D/k
Nuav	Average Nusselt number in all passages	h D <sub>av</sub> /k
Pr	Prandtl number of fluid	Cµ/k
Re	Reynolds number in a passage	D G/µ
Re <sub>av</sub>	Average Reynolds number in all passage <b>s</b>	D <sub>av</sub> G <sub>av</sub> /µ
Rep	Reynolds number based on particle diameter	<sup>D</sup> ը ս <b>ę</b> /µ

## TABLE OF NOMENCLATURE (cont'd.)

## Dimensionless Groups

Symbol	Name	Basic Formula
RT	Variable in Langhaar [32] correction factor	(VY <sup>2</sup> ).25
Sc	Schmidt number	<u>+</u> • #
Sh <sub>av</sub>	Average Sherwood number	D <sub>av</sub> k <sub>c</sub> /D
Shp	Sherwood number based on particle diameter	D <sub>p</sub> k <sub>c</sub> /D
Stav	Average Stanton number	h/C G <sub>av</sub>
V	Velocity head	-4P (11-/24-4)
( <b>V</b> Y <sup>2</sup> ) <sub>m</sub>	Maximum VY <sup>2</sup> factor	$VY^2(D_m/D)^4$
¥ _	Parameter of Langhaar [32]	D Re/L

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