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Some remarks on channelling and on radial dispersion in packed beds

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RADIAL DISPERSION IN PACKED BEDS

In order to describe radial dispersion in packed beds the relationship

$$D_r = \delta_{so} + \frac{u_o d}{PE_\infty\,(D/d \to \infty) f(D/d)} \tag{1}$$

is usually used. Inserting dimensionless quantities in eq. (1)

$$\frac{1}{PE} = \frac{\delta_{so}/\delta}{Pe} + \frac{1}{PE_\infty\,(D/d \to \infty) f(D/d)} \tag{2}$$

is obtained, with

$$PE = \frac{u_o d}{D_r}, \quad Pe = \frac{u_o d}{\delta}. \tag{3a, b}$$

The meaning of the symbols is as follows: u_o = superficial velocity, δ = diffusion coefficient in an unconfined gas space, δ_{so} = effective diffusion coefficient in the bed without fluid flow, D_r = effective coefficient for radial dispersion, D = tube diameter, d = particle diameter, PE = effective Péclet number defined with the dispersion coefficient D_r, and Pe = Péclet number defined with the diffusion coefficient δ.

The first term on the right-hand side of eq. (2) accounts for the influence of molecular diffusion and the second one for the influence of convective mixing on radial dispersion.

$PE_\infty\,(D/d \to \infty)$ is the limiting value of the effective Péclet number in an unconfined packed bed. This limiting value can be theoretically estimated using a mixing-cell model (Schlünder, 1966) or a statistical approach ("random walk theory", Baron, 1952) and is about 8.

$f(D/d)$ is a correction factor accounting for the influence of the tube wall [$f(D/d) > 1$]. In general, two different mechanisms can give rise to this influence:

(i) The reflection of stream lines and the resulting reduction of mixing intensity near the wall (index "W"). It is: $PE_{\infty,W} = 2PE_\infty(D/d \to \infty)$.

(ii) The flow maldistribution (channelling) caused by increased porosity (void fraction) in the vicinity of the wall.

Regarding the first mechanism Schlünder (1966) assumed that the width of the region of reduced mixing is equal to one particle diameter. Interpolating between the asymptotic values [$f(D/d) = 2$ for $D/d = 2$ and $f(D/d) = 1$ for $D/d \to \infty$] he obtained the relationship

$$f(D/d) = 2 - [1 - 2(d/D)]^2 \tag{4}$$

for the correction factor.

Curiously, eq. (4) has been compared almost exclusively and with astonishing success to radial dispersion data gained by injection measurements [see the comparison of eq. (4) with measurements of Fahien and Smith (1955), Zehner (1972) and Bauer (1976) given by Bauer in *Heat Exchanger Design Handbook* (1983) as well as in *VDI-Wärmeatlas* (1984)]. Such measurements take place by injecting a tracer or hot gas at the axis of the tube and recording the steady-state radial profiles at some cross-section downstreams. In most cases the profiles do not reach the wall of the tube. Consequently, the reason for the D/d dependence should be the flow maldistribution and not the reflection at the wall as implied by the use of eq. (4). To overcome this ambiguity is the main objective of the present contribution. In order to achieve this, a relationship between the flow maldistribution in packed beds and the correction factor $f(D/d)$ is derived. Using several equations proposed in the literature for the velocity profiles correction factors are calculated and compared to eq. (4) [in this context eq. (4) is regarded as empirical and representative for injection measurements]. Finally the influence of flow maldistribution on the form of the curve $PE = PE(Pe)$ is discussed.

DERIVATION OF THE CORRECTION FACTOR

Because of the increased porosity in the immediate vicinity of the container wall of a circular packed bed increased flow velocities appear there (channelling). As a consequence, the average superficial velocity u_o is greater than the actual superficial velocity in the core of the bed u_c. Because of the flatness of velocity profiles in the core of the bed u_c can be approximated by the velocity at the axis of the tube: $u_c = u(r = 0)$. For injection measurements taking place in this region of almost constant flow velocity the relationship

$$D_r = \delta_{so} + \frac{u_c d}{PE_\infty\,(D/d \to \infty)} \tag{5}$$

should be used instead of eq. (1). With the Péclet numbers as defined in eqs (3)

$$\frac{1}{PE} = \frac{\delta_{so}/\delta}{Pe} + \frac{1}{(u_o/u_c) PE_\infty\,(D/d \to \infty)} \tag{6}$$

is obtained. Comparison of eqs (6) and (2) yields

$$f(D/d) = u_o/u_c. \tag{7}$$

In order to calculate $f(D/d)$ from eq. (7) relationships proposed by various authors for the velocity profiles can be used. A brief review of such relationships is given in the following section.

RELATIONSHIPS FOR THE VELOCITY PROFILE

(i) *The equations of Hennecke and Schlünder*: Hennecke and Schlünder (1973) proposed the following equations for the calculation of velocity profiles in tubular packed beds of spherical particles:

$$\frac{u}{u_o} = \frac{K + [(P+2)/2](r/R)^P}{K+1} \tag{8a}$$

with

$$K = 1.5 + 0.0006[(D/d) - 2]^3 \tag{8b}$$

$$P = 1.14[(D/d) - 2]^{1/3} \tag{8c}$$

where R is the radius of the tube.

Setting u_c equal to $u(r = 0)$

$$\frac{u_c}{u_o} = \frac{K}{K+1} \tag{9}$$

is obtained.

Equations (8a)–(8c) have been fitted to the classical measurements of Schwartz and Smith (1953). These measurements were obtained using ring anemometers placed at some distance from the exit plane of the bed. The same data have been used by Fahien and Stankovic (1979). The relationship proposed by these authors for the velocity profile fulfills [contrary to eq. (8a)] the boundary condition $u(r/R = 1) = 0$.

(ii) *The bypass model of Martin*: Martin (1978) divided the packed bed into a core section (index c) of porosity ψ_c and a bypass section (index b) of porosity $\psi_b(\psi_b > \psi_c)$. Assuming radially constant velocities and the validity of the Ergun equation in each of the flow sections the ratio u_0/u_c can be obtained:

$$u_o/u_c = 1 - \varphi + \omega\varphi \qquad (10a)$$

where ω is the ratio of the superficial velocities in the two flow sections:

$$\omega \equiv u_b/u_c = f(\psi_c, \psi_b, \varphi, Re). \qquad (10b)$$

The exact functional dependence is given in the original paper cited above. φ is the relative area of the bypass cross-section and can be related to D/d by means of the equation

$$\varphi = 1 - [1 - (d/D)]^2. \qquad (10c)$$

For the calculations appearing in the next section $\psi_c = 0.40$ and $\psi_b = 0.50$ have been used.

(iii) *The equations of Vortmeyer and Schuster*: The equations proposed by Vortmeyer and Schuster (1983) for the calculation of velocity profiles in tubular packed beds of spherical particles are repeated here in order to correct several typographical mistakes appearing in the original paper. They are:

$$\frac{u}{u_o} = \beta\left\{1 - \exp\left[aR^*\left(1 - \frac{r}{R}\right)\right]\right]\left[1 - nR^*\left(1 - \frac{r}{R}\right)\right]\right\} \qquad (11a)$$

with

$$\beta = \frac{R^{*2}}{2}\left[\frac{R^{*2}}{2} - \frac{(nR^* - 1)(aR^* + 1)}{a^2} + n\left(\frac{R^{*2}}{a} + \frac{2R^*}{a^2} + \frac{2}{a^3}\right)\right.$$

$$\left. - \frac{\exp(aR^*)}{a^2}\left(1 - nR^* + \frac{2n}{a}\right)\right]^{-1} \qquad (11b)$$

with

$$R^* = R/d \qquad (11c)$$

$$a = \frac{4n}{4 - n} \qquad (11d)$$

and

$$n = 112.5 - 26.31Re + 10.97Re^2 - 0.1804Re^3 \quad 0.1 \leqslant Re < 1 \qquad (11e)$$

$$n = -1803 + 201.62(\ln Re + 4) - 3737(\ln Re + 4)^{0.5} + 5399(\ln Re + 4)^{1/3} \quad 1 \leqslant Re \leqslant 1000 \qquad (11f)$$

$$n = 27 \quad Re > 1000. \qquad (11g)$$

In order to elucidate eqs (11a)–(11f) some calculated velocity profiles are given in Fig. 1. Equations (11a)–(11f) were fitted to numerical results obtained by solving an extended Brinkman equation for the pressure loss. The extent as well as the location of the predicted velocity peaks are different from those measured by Schwartz and Smith. Vortmeyer and Schuster argue, that the reason for this disagreement is the distortion of velocity profiles between the exit plane of the bed and the actual plane, where the measurements of Schwartz and Smith were taken. In the paper of Vortmeyer and Schuster cited above experimental and theoretical evidence is given, which seems to support this argument.

COMPARISON BETWEEN CALCULATED CORRECTION FACTORS

In Fig. 2 correction factors $f(D/d)$ calculated according to eq. (7) and to the velocity distributions briefly discussed in the previous section are depicted. In the same picture $f(D/d)$ according to eq. (4) is shown. This equation can be regarded as representative for injection measurements in tubular beds of spherical particles. Consequently, the graph of Fig. 2 is a kind of test for the compatibility of the various velocity profiles with radial dispersion data gained by the injection method.

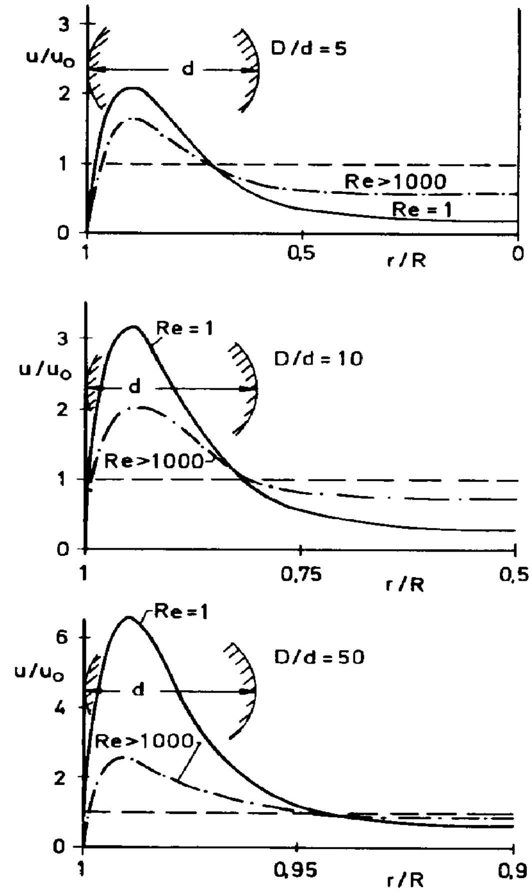

Fig. 1. Velocity profiles in a tubular packed bed of spherical particles according to Vortmeyer and Schuster [eqs 11(a)–11(f)].

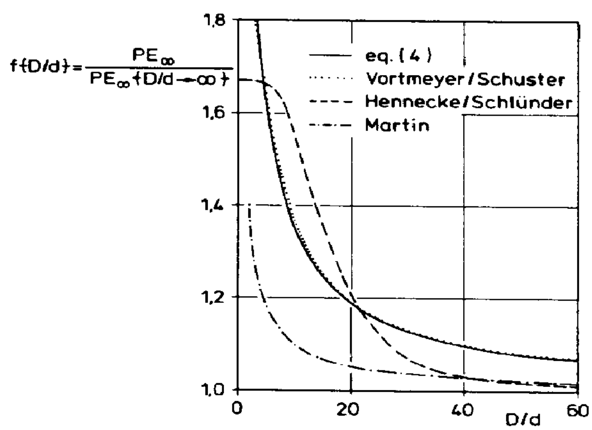

Fig. 2. The correction factor $f(D/d) = PE_\infty/PE_\infty(D/d \to \infty)$ according to eq. (4) as well as according to eq. (7) with the velocity profiles of Hennecke and Schlünder, and Martin as well as Vortmeyer and Schuster.

The best agreement is obtained when using the equation of Vortmeyer and Schuster for the velocity profiles.

THE INFLUENCE OF CHANNELLING ON THE FORM OF THE CURVE $PE = PE(Pe)$

In Figs 3 and 4 the functional dependence between the effective and the molecular Péclet numbers according to eq. (6) is depicted. The ratio u_o/u_c has been calculated from the velocity profiles of Vortmeyer and Schuster. The limiting value of the effective Péclet number for the unconfined packed bed $PE_\infty\,(D/d \to \infty)$ has been set equal to 8. For δ_{so}/δ the value 0.2254 has been used {from the empirical equation $\delta_{so}/\delta = 1 - \sqrt{1-\psi}$ with $\psi = 0.40$ [see Tsotsas and Martin (1988)]}. The calculations of Fig. 3 have been carried out with $Sc = 1$ (gaseous fluid phase) and those of Fig. 4 with $Sc = 1000$ (liquid fluid phase). A maximum of the curve $PE = PE(Pe)$ is predicted. The appearance of this maximum is caused by the dependence of channelling on the Reynolds number [eqs (11e)–(11g)]. Its extent varies with D/d as well as with the Schmidt number. Similar results can be obtained using the bypass model of Martin. The equations of Hennecke and Schlünder do not include any dependence of the velocity profiles on the Reynolds number; they yield a monotonously increasing $PE(Pe)$ function.

$PE(Pe)$ curves with a maximum have been observed by various authors during measurements of radial dispersion in packed beds [see the data collected by DeLigny (1970)]. All the mechanisms proposed previously in order to explain this behaviour [e.g. coupling between molecular diffusion and convective mixing (Bernard and Wilhelm, 1950), residual turbulence (DeLigny, 1970) etc.] refer to phenomena taking place in the core of the bed. The calculations of this paper point out for the first time that channelling can appreciably contribute to the formation of a maximum of the $PE(Pe)$ curve in the region of medium molecular Péclet numbers.

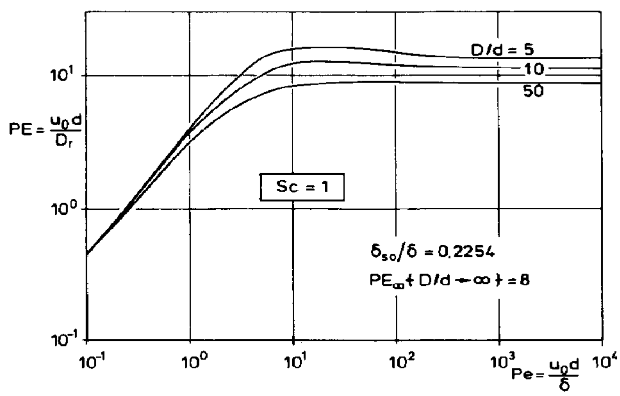

Fig. 3. Effective Péclet number, $PE = u_o d/D_r$, vs the molecular Péclet number, $Pe = u_o d/\delta$; calculated according to eq. (6) with u_c/u_o from eq. (11a), $PE_\infty(D/d \to \infty) = 8$, $\delta_{so}/\delta = 0.2254$ and $Sc = 1$ (gaseous fluid phase).

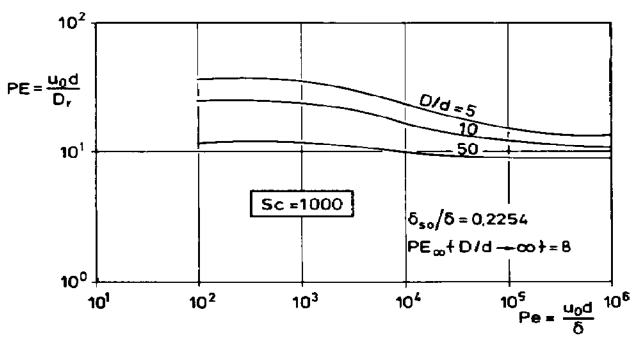

Fig. 4. Same as Fig. 3 with $Sc = 1000$ (liquid fluid phase).

SUMMARY

Reduced flow velocities in the central region of packed beds give rise to increased effective Péclet numbers during radial dispersion. Using the equations of Vortmeyer and Schuster for the velocity profile good agreement with the correction factors according to eq. (4) and with the results of injection measurements is obtained. In the region of medium molecular Péclet numbers a maximum of the effective Péclet number is predicted. The question whether a further correction factor taking into account the reflection at the wall should be used in connection with a boundary condition of the third kind at $r = R$ remains at the time being open.

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NOTATION

d	particle diameter, m
D	tube diameter, m
D_r	coefficient for radial dispersion, m²/s
r	radial coordinate, m
R	tube radius, m
u	local superficial velocity, m/s
u_c	superficial velocity in the core of the bed, m/s
u_o	average superficial velocity, m/s
δ	molecular diffusion coefficient, m²/s
δ_{so}	effective diffusion coefficient of the bed without fluid flow, m²/s
ν	kinematic viscosity, m²/s
ψ	porosity (void fraction)
Pe	molecular Péclet number ($= u_o d/\delta$)
PE	effective Péclet number for radial dispersion ($= u_o d/D_r$)
PE_∞	lim PE for $Pe \to \infty$
Re	Reynolds number ($= u_o d/\nu$)
Sc	Schmidt number ($= \nu/\delta$)

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Streaming potentials in inhomogeneous packed beds

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INTRODUCTION

Smoluchowski's equation provides the basic relationships between electrostatic potential gradients and pressure gradients across capillaries. This relationship was generalized to show its applicability to capillaries of any arbitrary cross-section (Overbeek, 1952). More recently, more exact equations for streaming potentials in fine capillaries at high zeta-potentials have been derived so that the limitation $\kappa a \gg 1.0$ no longer needs to be satisfied (Levine *et al.*, 1975).

In all of the above analyses the results derived for a single capillary tube are applied directly to a porous medium. While this may be a good assumption for a homogeneous packing of particles with the same zeta-potential, it is certainly not valid for an inhomogeneous mixture of particles. This study aims at addressing this problem and obtaining approximate results for inhomogeneous porous media.

Streaming potentials are very often measured for mixtures of mineral substrates. Such measurements are made in self-potential profiling for mineral exploration and logging of oil and gas wells. No systematic method exists for their interpretation. It would therefore be desirable to develop a method to better interpret streaming potentials of solid mixtures in terms of the zeta-potentials of each individual component.

THEORY

The pore space formed by the packing of particles is represented as a network of sites (pore bodies) and bonds (pore throats). The pore throats being the narrow constrictions in the converging–diverging pore cross-section. Similar representations of pore structure have been used by several other researchers in the past few years (Koplik, 1981; Heiba *et al.*, 1982). The network of interconnected bonds and sites is characterized by a coordination number (z) (defined as the number of bonds emanating from a site). The radii of the pore throats in the network conform to a pore throat size distribution $[f_p(R)]$ which can approximately be determined from mercury injection data or from any drainage capillary pressure curve. The microscopic flow distribution of fluid through the pores when a pressure gradient is imposed across the network is controlled by the pore throat size distribution.

Let us assume that the zeta-potential, instead of being uniform everywhere, is a function of the pore radius, $\zeta(R)$. Then, for each capillary the conduction and convection currents are given by

$$I_{\text{cond},R} = \frac{\pi R^2 \lambda E_R}{l} \tag{1}$$

$$I_{\text{conv},R} = \frac{\varepsilon \zeta(R) R^2 P_R}{4\mu l}. \tag{2}$$

A cylindrical geometry has been assumed for each pore throat, but in principle, any geometry could be assumed and the appropriate expressions arrived at. E_R and P_R are the potential drop and pressure drop across a pore of radius R. Equating the two currents at steady state would yield Smoluchowski's equation:

$$\zeta(R) = \frac{4\pi\mu\lambda}{\varepsilon}\left(\frac{E_R}{P_R}\right)_{I_R=0}. \tag{3}$$

This would be valid for a single capillary of radius R subject to the usual limitations for Smoluchowski's equation, i.e. $\kappa a \gg 1.0$. For a network of such capillaries, the overall conduction current through the network must be equal to the overall convection current at steady state. The total convection current is given by

$$I_{\text{conv}} = N \int_0^\infty I_{\text{conv},R} f_p(R)\,dR \tag{4}$$

where N is the number of pores at any cross-section normal to the direction of bulk fluid flow. Equivalently, if u_R is the fluid velocity in a pore of radius R, the total flow rate is given by

$$Q = \int_0^\infty u_R f_p(R) R^2\,dR. \tag{5}$$

Each pore may be assigned an electrical conductance, g_{Re}, given by