NOTATION

a = interfacial area, cm²/cm³

 C_A = concentration of species A, g mole/cm³

 C_1 = as defined by Equation (15) D_A = diffusion coefficient, cm²/s F = hypergeometric series

 k_1 = rate constant, 1/s [cm³/g mole]ⁿ⁻¹ m = Thiele modulus, $\delta \sqrt{k/D_A C_A^{*n-1}}$

n = order of reaction Q = liquid holdup, cm³/cm³ T = residence time, s

I = residence time, s

 w_A = dimensionless concentration, C_A/C_A^*

x = distance parameter, cm $y = \text{dimensionless distance, } x/\delta$

Greek Letters

β = dimensionless gas-liquid parameter defined by Equation (5)

 δ = film thickness, cm

 θ = dimensionless residence time, $Q\delta^2/D_AT$

 $\psi_0, \psi_1 = \text{concentration parameters defined by Equation}$ (17)

Superscript

= condition at the interface

Subscript

c = condition in the bulk

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On the Importance of the Inertial Terms in the Modeling of Flow Maldistribution in Packed Beds

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In recent years there has been a growing interest in the development of modeling equations for representing flow maldistribution in packed beds. The main motivation for this work is provided by its relevance to a broad range of problems in chemical reaction engineering (namely, hot spot formation) and in metals processing (namely, the iron blast furnace). There appears to be general agreement that the mathematical models of such systems have made use of the differential, vectorial form of the Ergun equation, that is, Radestock and Jeschar (1970), Stanek and Szekely (1972, 1973, 1974). Moreover, in recent papers, Szekely et al. (1975) presented direct experimental proof for the validity of this approach.

In a recent paper, addressed to nonuniform flow in the iron blast furnace, Kitaev et al. (1975) suggested that even the differential vectorial form of the Ergun equation is an oversimplification, because in this form no allowance is made for inertial effects which could be significant in nonuniform flows. Unfortunately, they did not present a (numerical) solution of the full set of equations, containing these inertial terms, but rather assumed irrotational flow, the appropriateness of which is questionable, so that it is impossible to make a direct comparison between the results obtained from these two different formulations.

The purpose of this note is to present numerical solutions to some selected flow maldistribution problems by using both these approaches so that the practical importance of retaining the inertial terms may be critically assessed.

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FORMULATION

The vectorial form of the Ergun equation (Ergun, 1952) may be written as

$$\nabla P + V(f_1 + f_2 V) = 0 \tag{1}$$

where f_1 and f_2 are defined as

$$f_1 = \frac{150\mu (1 - \epsilon)^2}{(\phi dp)^2 \epsilon^3}$$
 (2)

$$f_2 = \frac{1.75 \,\rho \,\left(1 - \epsilon\right)}{\left(\phi dv\right) \,\epsilon^3} \tag{3}$$

In recent papers Shvydkii et al. (1974) and Kitaev (1975) suggested that in the proper representation of nonuniform flow through packed beds, allowance should be made for the inertial terms.

Written in terms of the superficial velocity and with two-dimensional Cartesian coordinates used, the equations proposed by Shvydkii and Kitaev take the following form:

$$V_{x} \frac{\partial V_{x}}{\partial x} + V_{y} \frac{\partial V_{x}}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} - \frac{f_{1}}{\rho} V_{x} - \frac{f_{2}}{\rho} V_{x} V$$
(4)

$$V_{x} \frac{\partial V_{y}}{\partial x} + V_{y} \frac{\partial V_{y}}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} - \frac{f_{1}}{\rho} V_{y} - \frac{f_{2}}{\rho} V_{y} V$$
(5)

where

$$V = \sqrt{V_x^2 + V_y^2}$$
 (6)

The comparison of Equations (1) (4) and (5) clearly shows the presence of the inertial terms on the left-hand side. This latter formulation is certainly appealing and represents a logical extension of earlier work on flow through porous media in which inertial terms were used in conjunction with the vectorial form of the Darcy equation.

The practical question arises, however, whether the allowance for the inertial terms does alter significantly the computed flow patterns. It is of interest to note that in contrast to the laminar Navier-Stokes equations, where one would expect the inertial terms to predominate at high velocities (and at a distance from solid surfaces), the terms on left-and right-hand sides of equations (4) and (5) are both of the order of (V^2) , so that conclusions may not be readily drawn regarding the magnitudes of these terms.

In the following, we shall present computed results which will allow the direct comparison of the streamline patterns and the velocity profiles obtained from the numerical solution of Equation (1) and Equations (4) and (5). Before we proceed further, it should be noted that a minor programming error was discovered in the numerical solution of Equation (1) reported in the earlier paper by Poveromo et al. (1975). As shown in Figure 1, upon correcting for this programming error, the agreement between predictions and measurements based on Equation (1) is further improved.

In the following we shall refer to the results obtained from the solution of Equation (1) and Equations (4) and (5) as formulation 1 and formulation 2, respectively. The specific configurations considered are sketched in Figure 2; these configurations were selected for their practical significance (for example, in blast furnace technology) and for the fact that these would seem to provide a critical test for the inclusion of the inertial terms. Figure 3 shows the computed streamline patterns for flow through a uniformly packed bed where the inlet gas stream was introduced through a side stream nozzle. The curves drawn with the continuous line correspond to formulation 1, while the curves drawn with the broken line represent the results from formulation 2, which includes the inertial terms. It is seen that the two flow patterns are quite similar. We note, moreover, that, as perhaps expected, the two solutions are essentially identical for parallel flow through uniformly packed beds; this plot is not reproduced here.

It follows that a critical test of the appropriateness of neglecting inertial terms is to consider a packing configuration where abrupt changes occur in the streamline pattern. Figure 4 shows a plot of the streamlines computed for a bed which contains alternating 'V' shaped layers of packing of different sizes and where the fluid was introduced through a side stream nozzle (shown in Fig 2b). Inspection of Figure 4 shows that the computed streamline patterns are similar, but there are some differences in detail in the wall region and at the interfaces between adjacent layers of packing. It is seen that the principal differences occur in locations where there is an abrupt change in the resistance to flow. The physical characteristics of these interfacial regions are as yet incompletely understood, so one cannot state unequivocally whether there is a sound physical basis for these differences.

Computed results were also obtained for the velocity profiles of the gas exiting the bed for 'V' shaped packing configurations, such that the interface between two different packings was close to the upper free surface. As seen in the computed streamline patterns, the two models exhibit the maximum discrepancy in these regions.

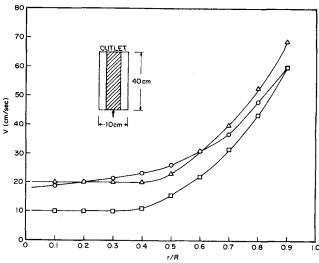


Fig. 1. Comparison of experimental and predicted velocity profiles for parallel flow through a bed packed with a high resistance core from Szekely and Poveromo (1975).

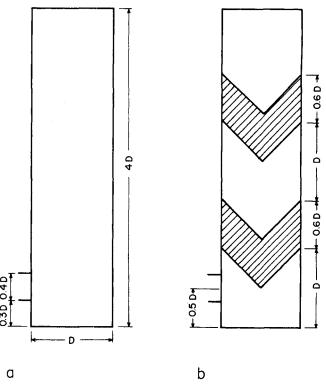


Fig. 2. (a). Uniform bed with air injection through the side. dp=0.0054D, $\epsilon=0.50$, $\phi=1$, Re=300. (b). Bed packed with V shaped layers and air injection through the side, Re=300. Hatched portion packing, dp=0.0018D, $\epsilon=0.40$, $\phi=1$ Interfacial region, dp=0.0036D, $\epsilon=0.35$, $\phi=1$ Remainder of the bed, dp=0.0054D, $\epsilon=0.50$, $\phi=1$.

It was found that the two formulations give quite similar results, and the differences between the computed point values of the velocity ranged from about 2 to 12%. As expected, the inertial formulation 2 predicted consist-

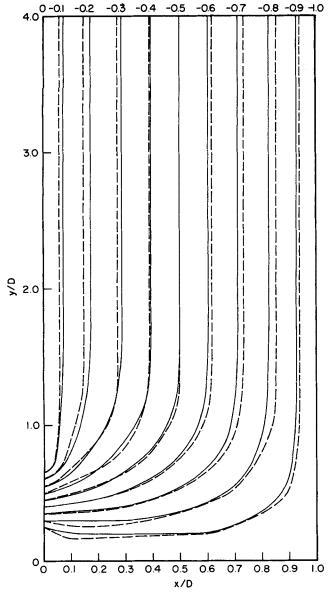


Fig. 3. Comparison between formulation 1 shown with solid lines and formulation 2 shown with dashed lines for configuration given in Figure 2a.

ently lower velocities, but in terms of average mass flow rates the discrepancy was only 3 to 5%.

CONCLUSIONS

The question has been raised whether it is necessary to include the inertial terms in the vectorial form of the Ergun equation in the formulation of flow maldistribution problems in packed beds. It is suggested that while the inclusion of the inertial terms would result in a formally more correct formulation, as a practical matter the error introduced in neglecting the inertial term is likely to be small, which would be difficult to detect experimentally.

The inclusion of the inertial terms greatly increases the computational labor, and it is questionable whether the refinement thus afforded is justified for the majority of chemical reaction engineering calculations. It should be noted, however, that the iron blast furnace consists of numerous (up to say twenty to twenty five) 'V' shaped layers where coke and ore particles alternate. Under these conditions, the inertial terms could well be important in both affecting the nature of flow maldistribution and in affecting the overall pressure drop mass flow rate relationship. Further experimental work in this area would seem to be justified.

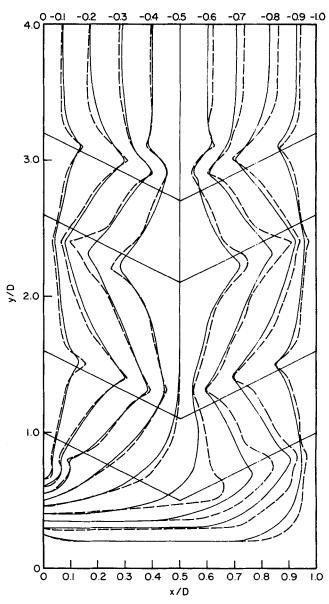


Fig. 4. Comparison between formulation 1 shown in solid lines and formulation 2 shown by dashed lines for configuration given in Figure 2b.

NOTATION

D = column diameter

dp = particle diameter

 f_1, f_2 = resistance parameters defined in Equations (2)

and (3), respectively.

 ∇ = gradient

 \underline{V} , V_x , V_y = velocity vector, absolute magnitude value and component value, respectively

P = pressure

 $Re = \text{Reynolds number } (\rho V dp/\mu)$

x, y = rectangular coordinates

 μ = viscosity

 $\rho = \text{density}$

= porosity

 ϕ = shape factor

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The Effect of a Pure Surfactant on the Damping of Liquid-column Oscillations

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In a previous communication (McComb, 1974) it was reported that polyethyleneoxide (PEO: Polyox grades WSR301 and N3000) in aqueous solution reduced the damping of manometer types of oscillations in a 1.25 cm bore PVC tube. It was concluded that this form of drag reduction was probably due to an adsorbed layer of PEO on the wall of the pipe. During a further investigation of this phenomenon, it was observed that the PEO additive also improved the wetting of the PVC tube wall above the liquid meniscus. This suggested trying the effect of a wetting agent which did not act as a drag reducer in shear flow. The surfactant chosen was Aerosol OT which, although it is used to disperse drag reducing fiber suspensions (Radin et al., 1975), does not itself affect turbulent flow (Lee et al., 1974).

The experimental setup and methods were described by McComb, but, briefly, a 1.25 cm bore PVC tube was formed into a semicircle of 29 cm radius. In each experi-

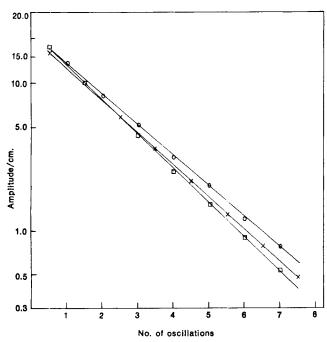


Fig. 1. Amplitude of oscillation against time for Aerosol OT in a semicircular PVC tube. \square Water. \bigcirc 150 p.p.m. Aerosol OT. imes10 000 p.p.m. Aerosol OT.

ment the length of liquid column was 88 cm, and this was given an initial displacement of 25 cm. The time period of the subsequent oscillations was 1.8 s.

Tests were carried out for a range of concentrations of Aerosol OT in water. In each case the rate of decay of manometer oscillations was reduced, relative to pure water. Also, in each case it was observed that Aerosol OT had the same effect as PEO in wetting the tube wall, above the meniscus.

In Figure 1 the logarithm of amplitude of oscillation is plotted against number of oscillations for water and two representative concentrations of Aerosol OT. It is clear that at 150 p.p.m. the Aerosol OT (like the Polyox additives) reduced the damping of the oscillations. Results are also given for a 1% solution of Aerosol OT as this is a typical concentration when it is used as a dispersant in drag reducing suspensions. Again, there was similar behavior to PEO (McComb, 1974), but this time at high concentrations where there was initially a more rapid decay followed by a decrease in damping in the final stages of the decay.

When these observations are put on a more quantitative basis, it may be seen that the effect of the surfactant is much smaller than the Polyox additives. If the total num-

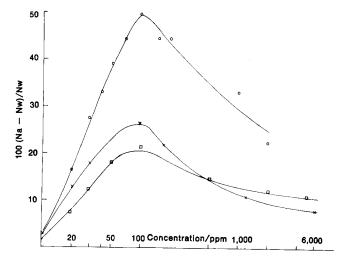


Fig. 2. Variation of damping reduction with additive concentrations (1) in a semicircular PVC tube. O Polyox WSR N3000. X Aerosol OT. (2) in a U shaped PVC tube
Aerosol OT.