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CREEPING FLOW

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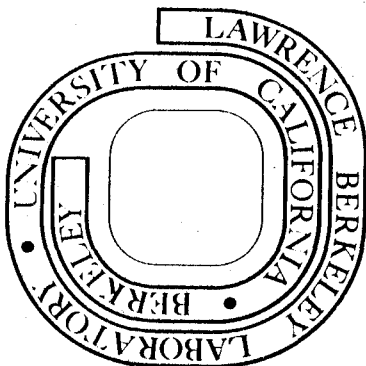
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Simulation of a Packed Bed as an Array of
Periodically Constricted Tubes
I: Creeping Flow

by

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July 1976

Abstract

A general method has been developed to solve the creeping-flow equations in a continuous, periodic, arbitrarily shaped tube. Interior collocation on a finite-difference grid was used to solve the Stokes stream function equation. Results are presented for a parabolic and a sinusoidal periodically constricted tube (PCT). A friction factor, Reynolds number relationship for a packed bed modeled as an array of sinusoidal PCT has been calculated.

Scope

The transfer rates across a packed bed can be predicted a priori if the exact geometry of flow channels can be described. This is usually impossible except for a uniformly structured bed. It then becomes necessary to introduce microscopic models for the bed. The simplest model considers the bed to be an array of straight cylinders. Recently, Payatakes et al. (1973a,b) introduced a new model for the flow channels in a packed bed. These authors consider the bed to consist of an array of periodically constricted tubes (PCT). The converging, diverging character of the flow in these tubes is a better approximation to the true nature of the flow in the actual bed. They have presented results of numerically solving the full Navier-Stokes equations for Reynolds numbers between 1 and 75. This paper extends their results to the creeping-flow regime. These results can be used to predict the Reynolds number, friction factor product for a packed bed as a function of the PCT geometry. Furthermore, the velocity profiles calculated are to be used in solving the mass-transfer problem in these PCT.

Conclusions and Significance

This study has presented a technique for solving the incompressible, Newtonian fluid, creeping-flow equations in a periodically constricted tube. Interior collocation on a finite-difference grid was used to reduce the partial differential stream function equation to a set of coupled, ordinary differential equations. This approach is much

more economical than solving the full elliptic equation by over-relaxation. The generalized coordinate system in which the problem is solved facilitates a straightforward calculation for the velocity field in any tube in the shape of a periodic, continuous body of revolution.

A packed bed can be modeled as an array of these tubes. Figure 7 shows the relationship between the bed friction factor and Reynolds number for a bed consisting of sinusoidal PCT. The results depend upon the two dimensionless geometry variables r_A and A/r_A (figure 1). The results can be used in solving the convective diffusion equation in a PCT.

Introduction

The behavior of packed beds can be simulated by utilizing a microscopic model for the flow channels in the bed. The appropriate equations can then be solved to predict transfer rates across the bed. The simplest model considers the flow channels to be an array of straight tube capillaries. Sheidegger (1957) and more recently Dullien (1975) have provided a review of this approach. Such a first order model cannot, however, satisfactorily correlate experimental data. The straight streamlines which result from applying the capillary model seem to be an inappropriate approximation to the twisting, converging, diverging character of the flow in a bed. Recently, a new microscopic model for a packed bed was introduced by Payatakes et al. (1973a,b). These authors envision the flow channels

to be an array of periodically constricted tubes (PCT) of random dimensions. The converging, diverging nature of the flow in these tubes is a better approximation to the true character of the flow in a packed bed. These authors show by statistical and heuristic arguments that the problem of modeling the flow behavior in an array of these randomly sized PCT reduces to considering one dimensionless PCT. They present a technique to calculate the model parameters.

The purpose of this series of work has been to calculate transfer rates across a bed modeled as an array of PCT. Creeping flow conditions have been assumed in the bed. This first paper specifically concerns itself with solving the creeping flow equations in a PCT. These results will be used as the velocity profiles in the subsequent work.

Since the Navier-Stokes equations become linear for creeping flow, interior collocation on a finite-difference grid was used to solve the fluid dynamics. This novel technique is more economical than the over-relaxation techniques generally used in solving elliptic equations. Furthermore, the velocity fields can be easily found for a tube in the shape of any continuous, periodic body of revolution.

Creeping Flow in a PCT

The PCT is generated by the surface of revolution of a cosine function about the axis of symmetry as shown in figure 1. (The wall function proposed by Payatakes et al. was parabolic. The

choice is immaterial to the concept of a PCT however.) All lengths are made dimensionless with the period of oscillation ℓ . The creeping-flow equations are to be solved in this geometry. Because no inertial effects are present, the radial velocity v_r will be zero at $z = 0, 0.5, \text{ and } 1.0$, and the streamwise velocity v_z will be an even function of z with the same frequency as the wall oscillation. These considerations make it clear that the governing equations need be solved only in $0 \leq z \leq 0.5$.

A packed bed is modeled as an array of these PCT. The fluid approaches the bed at a superficial approach velocity v_s . The average dimensional velocity $\langle v_{Ad} \rangle$ through each tube is defined such that the flow rate in each tube is equal to $\langle v_{Ad} \rangle \pi r_{Ad}^2$ where r_{Ad} is the length averaged dimensional radius. Geometrical considerations show that $\langle v_{Ad} \rangle$ can be written in terms of the approach velocity as

$$\langle v_{Ad} \rangle = \frac{v_s}{\epsilon} \left[1 + \frac{1}{2} (A/r_A)^2 \right]$$

where A is the dimensionless wall oscillation amplitude. The governing equations need be solved in a single PCT. These results can then be applied to the entire bed due to the assumed homogeneity and periodicity of the structure.

The dimensionless, incompressible Navier-Stokes equations for creeping-flow with axial symmetry can be reduced to a single, linear, fourth order partial differential equation by introducing the normalized stream function ψ as

$$E^4 \psi = 0 \quad (1)$$

where

$$E^2 = \frac{\partial^2}{\partial r^2} - \frac{1}{r} \frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2} \quad (2)$$

$$v_z = \frac{r_A^2}{2r} \frac{\partial \psi}{\partial r} \quad (3)$$

$$v_r = -\frac{r_A^2}{2r} \frac{\partial \psi}{\partial z}$$

The stream function equation is to be solved subject to the boundary conditions

$$\left. \begin{aligned} \psi &= 0 \\ \frac{\partial}{\partial r} \frac{1}{r} \frac{\partial \psi}{\partial r} &= 0 \end{aligned} \right\} r = 0 \quad \begin{array}{l} 4(i) \\ 4(ii) \end{array}$$

$$\left. \begin{aligned} \frac{1}{r} \frac{\partial \psi}{\partial r} &= 0 \\ \psi &= 1 \end{aligned} \right\} r = r_w(z) \quad \begin{array}{l} 4(iii) \\ 4(iv) \end{array}$$

and a periodicity condition

$$\frac{\partial^{(n)}}{\partial z^{(n)}} \psi(r, z) = \frac{\partial^{(n)}}{\partial z^{(n)}} \psi(r, z + m) \quad n, m = 0, 1, 2, \dots \quad (5)$$

The boundary conditions of equation 4 state that at the centerline

i) the radial velocity is zero, ii) the axial velocity is symmetric, and at the wall iii) there is no slip on the axial velocity, and

iv) the flow rate at each cross section is a constant, here referred to a straight cylinder of radius r_A .

No analytical solution for equations 1, 4, and 5 could be found. Boundary and interior collocation on a finite-difference grid was used. These approximation techniques are examined by Finlayson (1972), Villadsen (1970), and Villadsen and Stewart (1967).

Boundary collocation approximation for ψ

By considering the periodicity conditions, a separable solution of the form

$$\psi_j = f_j(r) \cos(\lambda_j z) \quad (6)$$

where

$$\lambda_j = 2\pi j, \quad j = 0, 1, 2, \dots$$

can be postulated. If equation 6 is substituted into equation 1, a governing equation for the $f_j(r)$ is obtained.

$$\begin{aligned} \frac{d^4 f_j}{dr^4} - \frac{2}{r} \frac{d^3 f_j}{dr^3} + \left(\frac{3}{r} - 2\lambda_j^2 \right) \frac{d^2 f_j}{dr^2} + \left(\frac{2\lambda_j^2}{r} - \frac{3}{r^3} \right) \frac{df_j}{dr} \\ + \lambda_j^4 f_j = 0 \end{aligned} \quad (7)$$

The general solution to this equation which remains finite at $r = 0$ is

$$f_j(r) = A_j r I_1(\lambda_j r) + B_j r^2 I_2(\lambda_j r) \quad (8)$$

It can be shown that the Hagen-Poiseuille solution for the stream function is recovered when $\lambda_j \rightarrow 0$. The approximate solution for the stream function can then be written as

$$\psi(r, z) = 2A_0 \left(\frac{r}{r_A}\right)^2 - B_0 \left(\frac{r}{r_A}\right)^4 - \sum_{j=1}^{NCF} \left[A_j r I_1(\lambda_j r) + B_j r^2 I_2(\lambda_j r) \right] \cos(\lambda_j z). \quad (9)$$

The first two terms on the right represent the stream function for a straight tube of radius r_A if $A_0 = B_0 = 1$. The summation of terms can be thought of as a correction function for the basic Hagen-Poiseuille flow.

Interior collocation approximation for ψ

By introducing a new set of coordinates (η, z) defined by

$$\eta = r/r_w(z) \quad (10)$$

the boundary conditions of equation 4 along the wall can be transferred to a coordinate curve $\eta = 1$. The interior collocation technique on a finite-difference grid can be used to approximate the hydrodynamics. Assume an approximate solution for the normalized stream function of the form

$$\psi(\eta, z) = 2\eta^2 - \eta^4 + \sum_{k=1}^{NCP} \eta^2 (1 - \eta^2)^2 A_k(z) \phi_{k-1}(\eta^2). \quad (11)$$

The first two terms on the right side represent the Hagen-Poiseuille solution. The summation of terms can again be considered as a correction

function to the basic parabolic flow. The functions $\phi_{k-1}(\eta^2)$ in the summation term can be any complete set of functions. The weighting factor $\eta^2(1-\eta^2)^2$ assures the correct behavior of the solution at the boundary points $\eta = 0$ and $\eta = 1$. The coefficients $A_k(z)$ are unknown functions of z to be determined subject to the boundary conditions

$$\begin{aligned} A_k'(0) &= A_k'''(0) = 0 \\ A_k'(0.5) &= A_k'''(0.5) = 0 \end{aligned} \tag{12}$$

These conditions result from the even behavior of the streamwise velocity v_ξ .

Friction factor for a packed bed

A friction factor for a packed bed may be defined as

$$f_B = \frac{6\varepsilon^3}{a} \left(\frac{-\Delta P_B}{L_B} \right) \frac{1}{\rho v_s^2} \tag{13}$$

The porosity dependence has been explicitly incorporated into this definition. For creeping flow, the product of the Reynolds number and the bed friction factor is a constant given by

$$\begin{aligned} f_B \text{Re}_B &= 72 \left(\frac{2\varepsilon}{ar_{Ad}} \right)^2 \left[1 + \frac{1}{2}(A/r_A)^2 \right] \int_0^1 \left(\frac{r_A}{r_w} \right)^4 \left\{ 1 + \sum_{k=1}^{NCP} A_k(z) \right. \\ &\quad \left. [2\phi_{k-1}(0) - \phi_{k-1}''(0)/2] \right\} dz \tag{14} \end{aligned}$$

This equation was derived by integrating the pressure gradient in the Navier-Stokes equations over a period at the centerline. The left side of equation 14 depends upon the macroscopic bed quantities while the right side depends upon the microscopic model parameters r_A and A/r_A only.

Method of Solution

Boundary collocation was used to determine the coefficients A_j , B_j of equation 9. Equation 9 identically satisfies the centerline conditions. It was forced to satisfy the remaining boundary conditions along the wall at a discrete number NCP of axial collocation points. These axial points were picked to be the zeros of the shifted Legendre or Tchebycheff polynomials. In addition to the wall boundary conditions given by equation 4(iii) and 4(iv), it was found necessary explicitly to force equation 9 to satisfy the no slip condition on the radial velocity v_r . Thus at each collocation point there are 3 boundary conditions to be satisfied. The number of approximating functions NCF are chosen so that the linear system of equations generated is determinant.

A comment should be made regarding the necessity of forcing v_r to equal zero at the wall. It was found that when this condition was not imposed on the solution, the v_r on the wall did not equal zero at the collocation points even though v_z did. This might seem suspicious since $\nabla\psi \equiv 0$ at $r_w(z)$. But this is only true when the ψ used in the gradient operation is the "correct" solution.

It does not apply to the approximating solution unless the approximation is forced to satisfy that equation. The wall direction was not correctly specified by the two wall boundary conditions alone.

The unknown coefficients $A_k(z)$ in the interior-collocation approximation for the stream function can be determined as follows. Equation 1 in the (η, z) coordinate system is applied to equation 11. (The E^4 operator in the (η, z) coordinate system is given in Appendix A). Interior collocation is then used at NCP points in the η coordinate. Since the η functional dependence is a priori postulated through the $\phi_{k-1}(\eta^2)$, this step reduces the partial differential equation to a set of coupled, fourth order, ordinary differential equations for the unknown A_k . This set of equations is solved on a finite-difference grid in the z coordinate by the method of Newman (1973). Legendre polynomials were used for the $\phi_{k-1}(\eta^2)$. The η collocation points were chosen to be the zeros of the shifted Legendre polynomials of order NCP-1

$$\eta_i = \sqrt{\frac{x_i + 1}{2}}$$

where x_i is the zero of the ordinary Legendre polynomial. The wall $\eta = 1$ was also used as a collocation point.

Further details of the calculational procedure are given by Fedkiw. All calculations were done on a CDC 7600 computer.

Results and Discussion

No numerical difficulty was encountered in solving the hydrodynamics in a PCT when the dimensionless wall oscillation amplitude was small (< 0.05). The two approaches outlined gave essentially the same velocity profiles. However, as the wall amplitude was increased, the boundary collocation solution became a progressively worse approximation. Increasing the number of collocation points did not help. The expansion for the correction function in the boundary-collocation solution at any position z is in terms of the weighted modified Bessel functions of the first kind. Unfortunately, these functions do not form a complete set. Thus as the correction function becomes more dominant (increasing amplitude) the approximating solution breaks down.

The interior collocation technique, on the other hand, encountered no problems. As the wall oscillation amplitude was increased in the calculations, the number of collocation functions NCP was increased to assure accuracy. It was found that for the range of parameters studied in this report, $NCP = 9$ insured sufficient accuracy of the solution. All results reported here use the interior-collocation solution to the hydrodynamics.

The interior collocation approximation for the stream function is solved in a generalized (η, z) coordinate system. This facilitates a straightforward calculation for the velocity field in any tube in the shape of a periodic, piecewise continuous body of revolution. Results are reported here for a parabolic and a sinusoidal PCT.

Figure 2 shows a comparison between the creeping flow axial velocity profile and that reported by Payatakes et al. for a tube Reynolds number equal to one. The profiles are compared at the minimum and maximum ($z = 0.5$) constriction diameters. The tube wall for these profiles is piecewise continuous, generated by two parabolas intersecting at $z = 0.5$ with their respective minima at $z = 0$ and $z = 1$. (See figure 1 of Payatakes et al.). The velocity here is scaled with respect to the average velocity in a tube of constant radius equal to the constriction radius. At the centerline the viscous flow profile is slightly larger than that of Payatakes et al. calculations. However, near the wall this trend is reversed. The integral of all the profiles is equal to a constant defined by the flowrate.

Figures 3 thru 6 show some typical creeping flow profiles in a sinusoidal PCT. The two dimensionless geometry groups r_A and A/r_A completely determine the solution behavior. These four figures illustrate the effect on the velocity profiles of manipulating one of these variables with the other held constant. The velocity profiles have been normalized with the average velocity at the average radius.

The effect on the axial and radial velocity profiles of varying the wall amplitude at a constant average radius is shown in figures 3 and 4. The radial velocity profile is plotted at $z = 0.25$. At this position v_r attains its maximum value. These figures indicate that at a constant radius the variation in the velocity profiles

across a half period becomes more dramatic as the oscillation amplitude increases.

Figure 5 and 6 illustrate the velocity profiles for a varying wall radius at a constant A/r_A . The effect of the tube geometry is again seen. The radial velocity increases with r_A since the velocity of the fluid in the radial direction is proportional to the slope of the wall. However, the variations in the axial velocity profiles across the half period become less pronounced with increasing r_A . This effect is due to the drag induced by the wall. As r_A increases the effect of the wall fluctuations become less important to the fluid in the central core of the tube.

The profiles of figures 3 thru 6 have been nondimensionalized with respect to the average axial velocity at the average tube radius. This normalization procedure illustrates the variation of the profiles from that at the average tube radius. If these profiles are multiplied by $\left(\frac{r_w(z)}{r_A}\right)^2$, the resulting profiles are then normalized by the average axial velocity at position z . Such a calculation shows that the parabolic axial velocity profile is approached as r_A becomes smaller. The radial velocity profile is then given by continuity. In the limit of $r_A \rightarrow 0$, the Hagen-Poiseuille case is recovered.

Figure 7 illustrates the bed friction factor, Reynolds number product of equation 14 as a function of r_A and A/r_A . The product $f_B Re_B$ depends upon the macroscopic bed parameters L_B , ϵ , and a . The microscopic PCT parameters r_A and A/r_A can be varied while holding these bed parameters constant. As A/r_A increases, the tubes

become more narrow at their constrictions. Because of the increased resistance this reduced flow area offers, the bed pressure drop increases with A/r_A . This effect decreases with larger r_A since the constriction size at any A/r_A increases with r_A .

The Blake-Kozeny equation as given in Bird et al. (1960) empirically recommends a value of 150 for the product $f_B Re_B$. Sørensen and Stewart (1974) have calculated the velocity profiles across a simple cubic packing of uniformly sized spheres. Their pressure-drop results yield a theoretical value of 158. Figure 7 shows that a range of parameters $(r_A, A/r_A)$ will give a $f_B Re_B$ near these two values. The A/r_A ratio which give $f_B Re_B$ a value near 150 seem to be concentrated near 0.33.

The straight tube capillary model gives the intercept value of 72 on figure 7. The usual argument given in explaining the discrepancy between this value and the empirically best fit value of 150 is a tortuosity and shape factor. The PCT model of a packed bed does not resort to these factors. However, another geometrical parameter (A/r_A) has been added.

Notation

A	dimensionless wall oscillation amplitude, A_d/ℓ
$A_k(z)$	interior collocation coefficient functions
A_j, B_j	boundary collocation coefficients
f_j	boundary collocation function defined by equation 7
f_B	bed friction factor defined by equation 13
L_B	length of packed bed, cm
ℓ	length of a PCT period, cm
NCP	number of collocation points
NCF	number of boundary collocation functions
P_B	pressure in bed
r	dimensionless radial coordinate, r_d/ℓ
r_A	dimensionless average PCT radius, r_{Ad}/ℓ
$r_w(z)$	dimensionless PCT wall radius, r_{wd}/ℓ
Re_B	bed Reynolds number, $6\rho v_s/\mu_a$
v_s	superficial bed approach velocity, cm/sec
$\langle v_{Ad} \rangle$	average velocity in a tube of constant radius r_{Ad} , cm/sec
v_r	dimensionless radial velocity, $v_{rd}/\langle v_{Ad} \rangle$
v_{zd}	dimensionless axial velocity, $v_{zd}/\langle v_{Ad} \rangle$
v_z	dimensionless streamwise velocity, $\sqrt{v_z^2 + v_r^2}$
z	dimensionless axial coordinate, z_d/ℓ

Greek

ϵ	bed porosity
ρ	density, gm/cm ³
η	$r/r_w(z)$

λ_j $2\pi j$, $j = 1, 2, \dots$

μ viscosity, gm/cm sec

ψ normalized dimensionless stream function $-2\psi_d^2 / \langle v_{Ad} \rangle r_A^2$

$\{\phi_k\}$ complete set of functions

Subscript

d dimensional quantity

Acknowledgment

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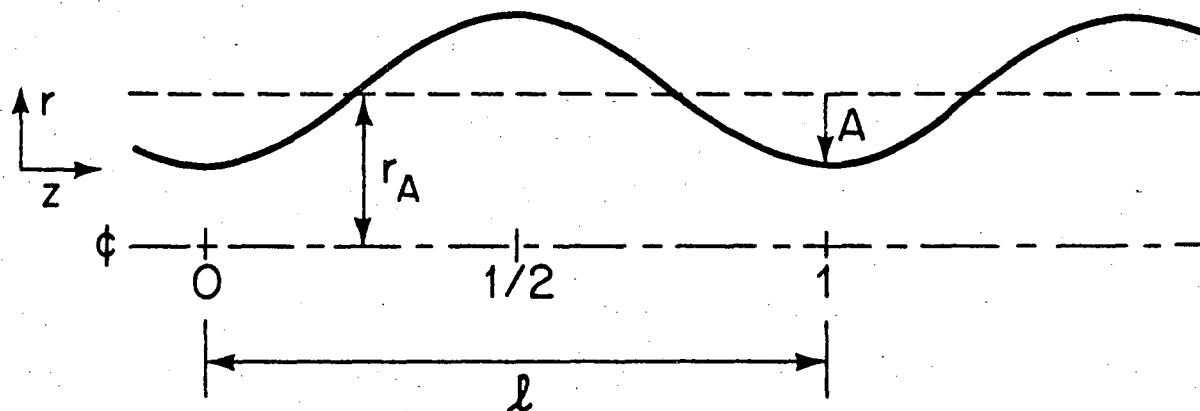
Appendix A

E^4 operator in (η, z) coordinate system

$$\begin{aligned}
 E^4 \psi = & \left\{ \left[1 + \eta^2 r_w'^2 \right] \frac{\partial^4}{\partial \eta^4} - 4\eta r_w r_w' \left[1 + \eta^2 r_w'^2 \right] \frac{\partial^4}{\partial z \partial \eta^3} \right. \\
 & + r_w^2 \left[2 + 6\eta^2 r_w'^2 \right] \frac{\partial^4}{\partial z^2 \partial \eta^2} - 4\eta r_w^3 r_w' \frac{\partial^4}{\partial z^3 \partial \eta} + r_w^4 \frac{\partial^4}{\partial z^4} + \\
 & \left[-\frac{2}{\eta} + 10\eta r_w'^2 + 12\eta^3 r_w'^4 - 2\eta r_w r_w'' - 6\eta^3 r_w'' r_w'^2 \right] \frac{\partial^3}{\partial \eta^3} + \\
 & r_w \left[-4r_w' - 24\eta^2 r_w'^3 + 12\eta^2 r_w r_w' r_w'' \right] \frac{\partial^3}{\partial z \partial \eta} + r_w^2 \left[12\eta r_w'^2 - 6\eta r_w r_w'' - \frac{2}{\eta} \right] \frac{\partial^3}{\partial \eta \partial z^2} \\
 & + r_w^2 \left[24\eta r_w' r_w'' - \frac{24\eta r_w'^3}{r_w} + \frac{4}{\eta r_w} r_w' - 4\eta r_w r_w'' \right] \frac{\partial^2}{\partial z \partial \eta} + \\
 & \left[-\frac{3}{\eta^3} - \frac{4}{\eta} + 24\eta r_w'^4 - 36\eta r_w r_w'^2 r_w'' + 8\eta r_w^2 r_w' r_w''' + 6\eta r_w^2 r_w''^2 + \frac{2}{\eta} r_w r_w'' \right. \\
 & \left. - \eta r_w^3 r_w''(iv) \right] \frac{\partial}{\partial \eta} \left. \right\} \psi = 0 .
 \end{aligned}$$

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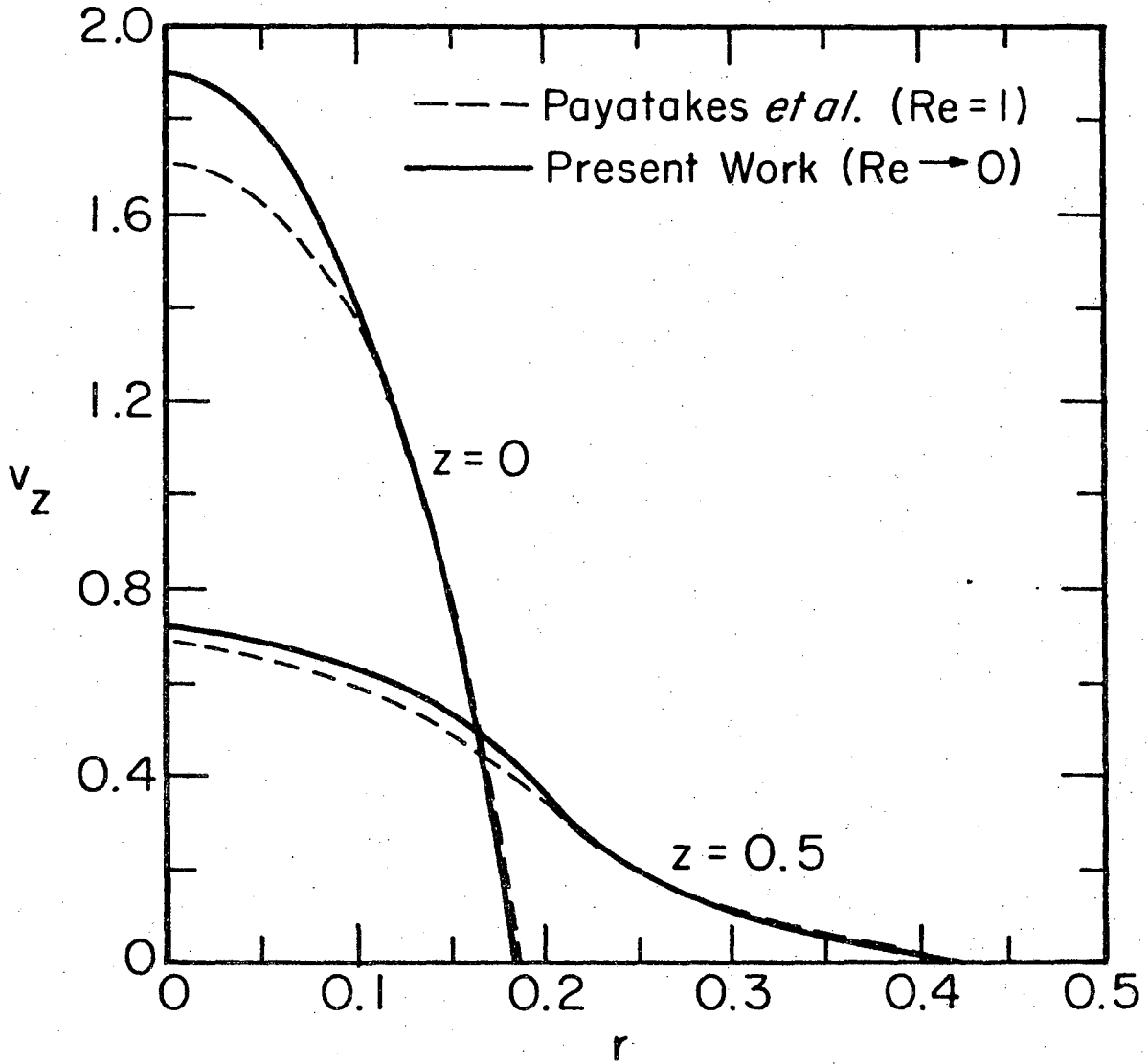
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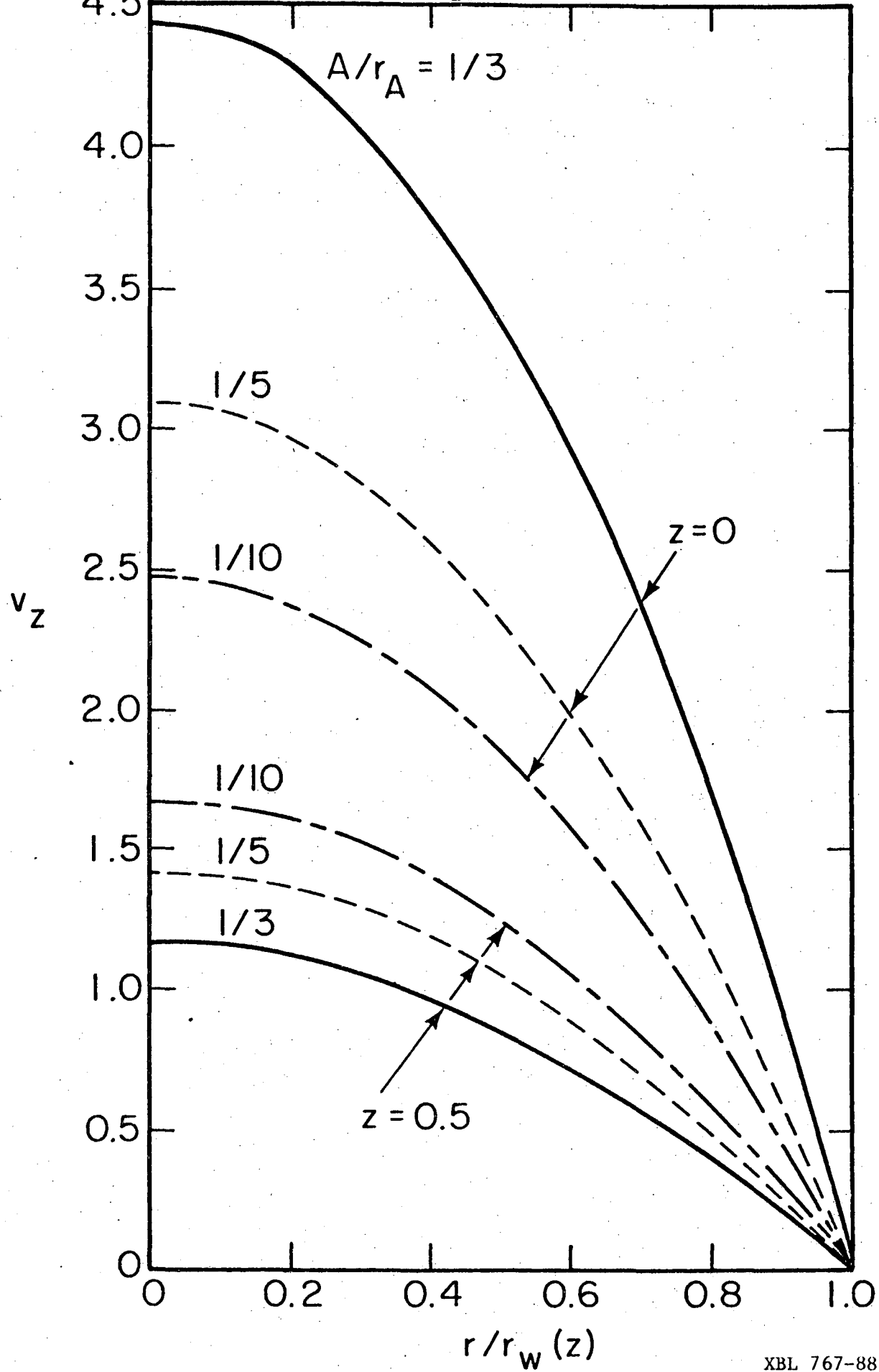
Figure 1. The wall of a PCT generated by $r_w(z) = r_A - A \cos(2\pi z)$.
 All lengths are dimensionless with respect to the period
 length l .

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Figure 2. Comparison of calculated axial velocity profiles with those of Payatakes et al. for a parabolic PCT.



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Figure 3. Effect of amplitude/radius ratio on axial velocity profiles for a sinusoidal PCT with $r_A = 0.1$.

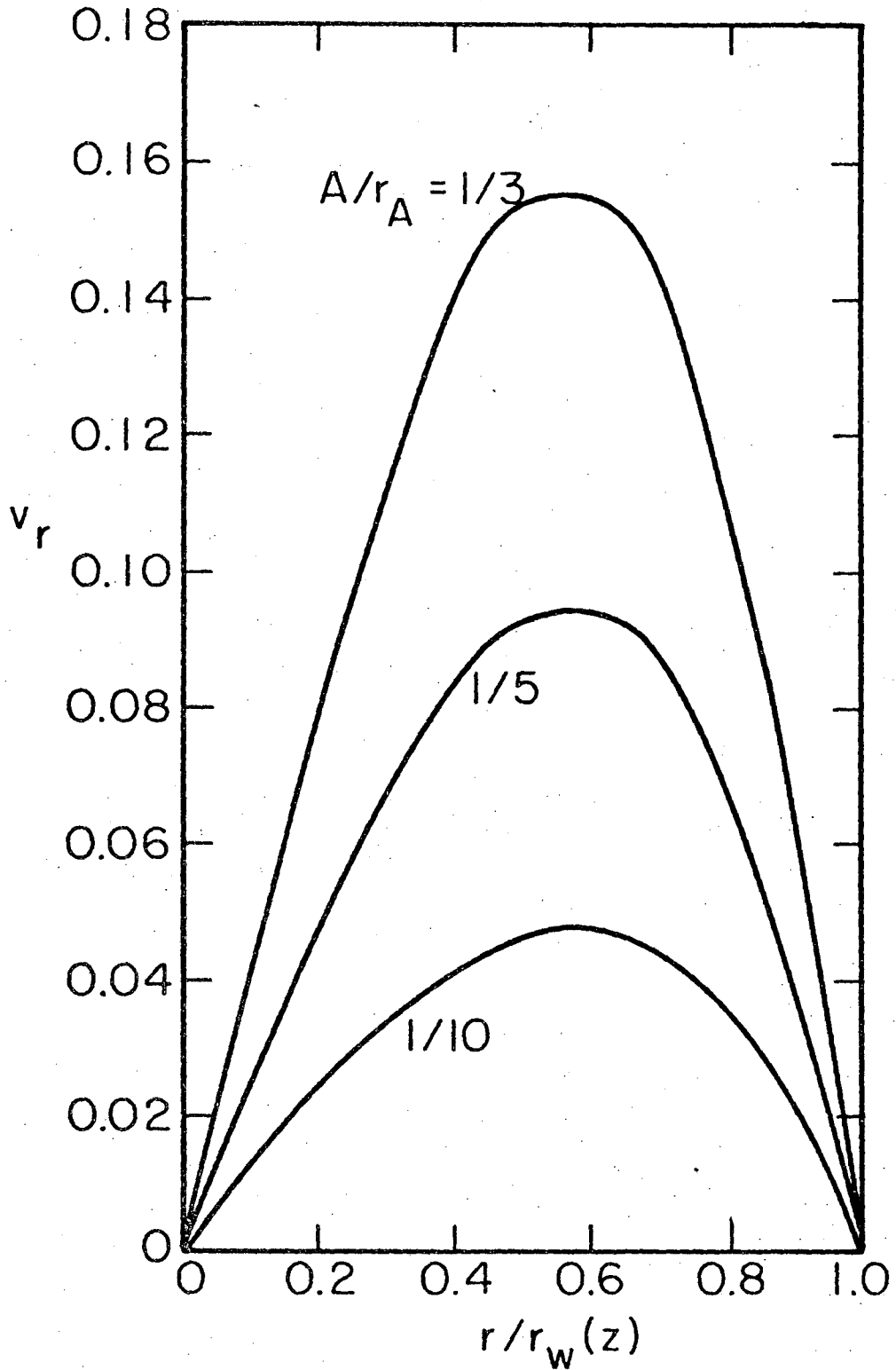
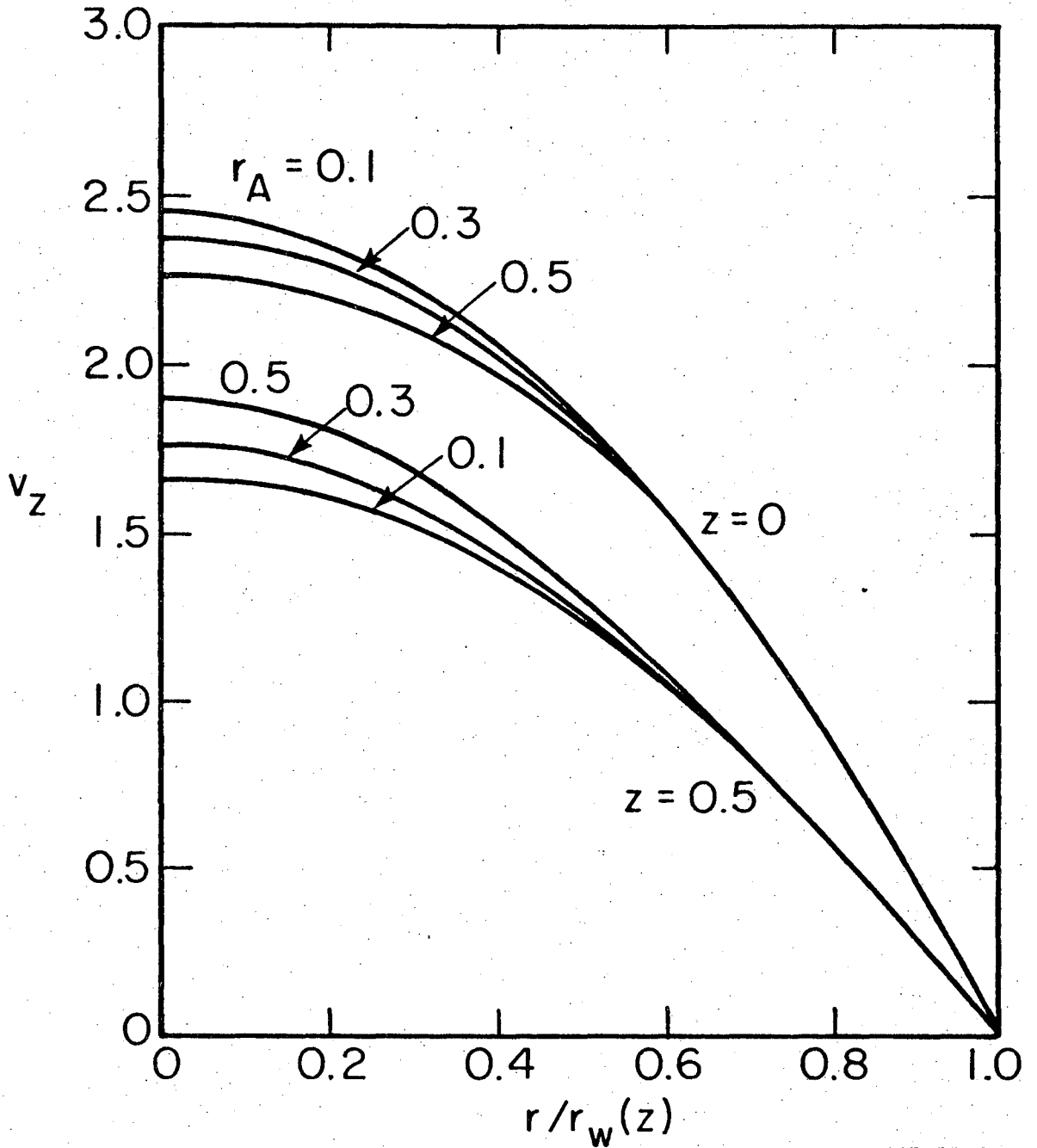
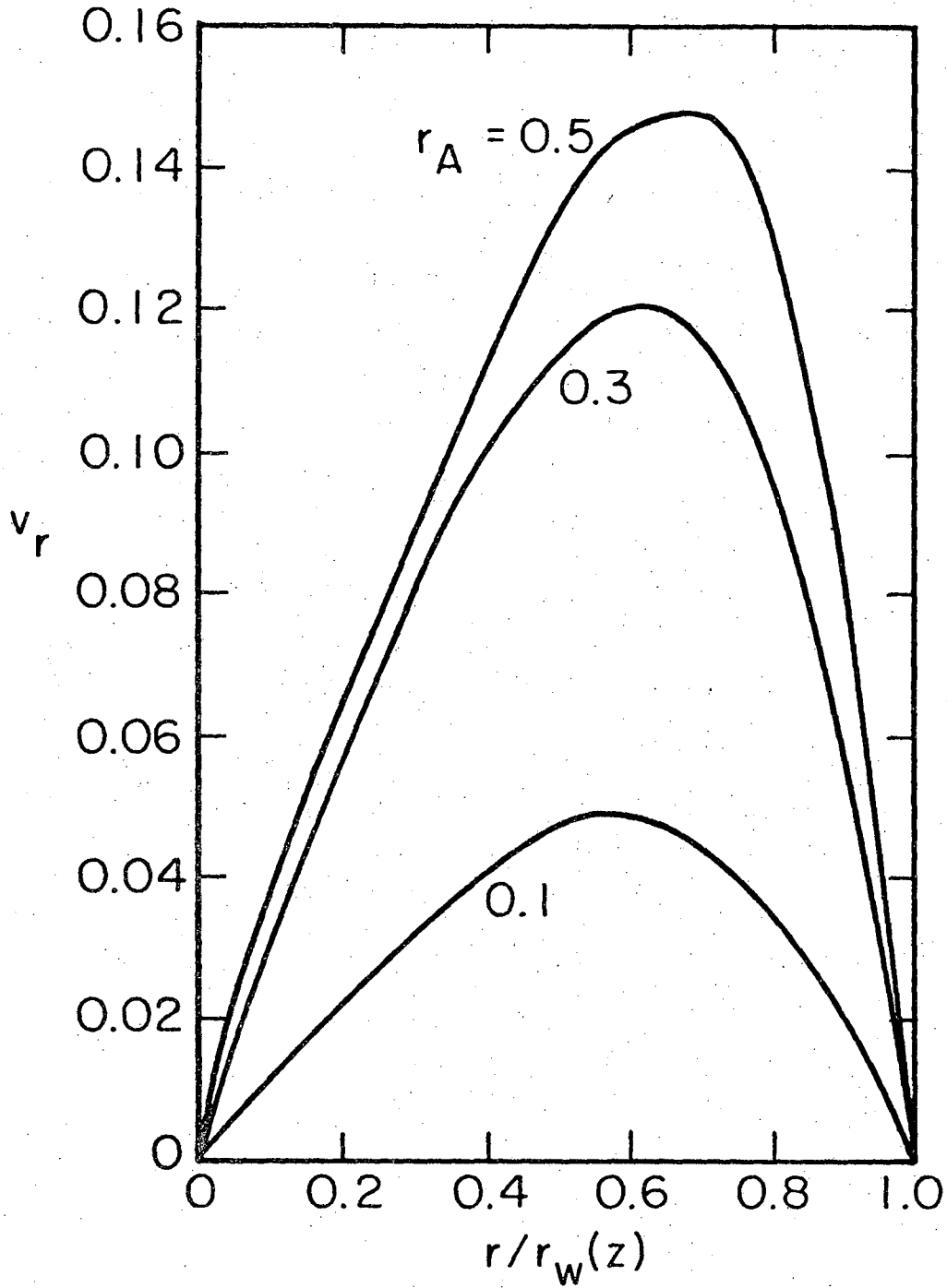


Figure 4. Effect of amplitude/radius ratio on radial velocity profiles in a sinusoidal PCT for $r_A = 0.1$ at $z = 0.25$.



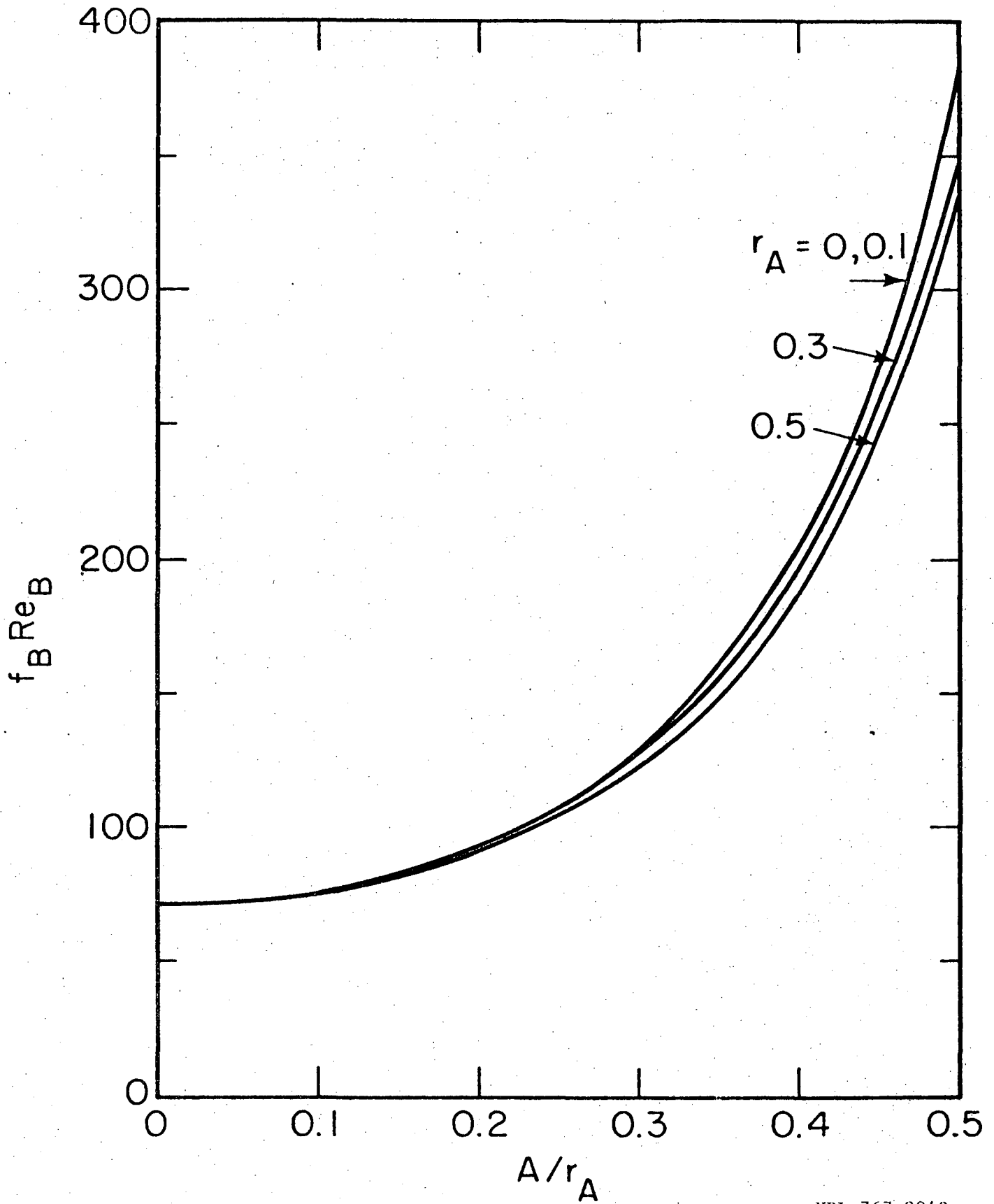
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Figure 5. Effect of average tube radius on axial velocity profiles in a sinusoidal PCT for $A/r_A = 0.1$.



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Figure 6. Effect of average tube radius on radial velocity profiles in a sinusoidal PCT for $\Lambda/r_\Lambda = 0.1$ at $z = 0.25$.



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Figure 7. Friction factor, Reynolds number product for a packed bed modeled as an array of sinusoidal PCT.

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