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ON THE ESTABLISHMENT OF DENSITY PROFILE FOR THE FLOW OF A TWO-FLUID SINGLE PHASE GAS MIXTURE

by Timothy W. Kao

Prepared under Grant No. NsG-586 *by*
CATHOLIC UNIVERSITY OF AMERICA
Washington, D. C.
for Lewis Research Center

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FOREWORD

The research described herein, which was conducted at the Catholic University of America, was performed under NASA Research Grant NsG-586 with Mr. Robert G. Ragsdale, Nuclear Reactor Division, NASA-Lewis Research Center, as Technical Manager.

ON THE ESTABLISHMENT OF DENSITY PROFILE FOR THE FLOW OF A TWO-FLUID SINGLE PHASE GAS MIXTURE

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Abstract. The establishment of density profile for a two-fluid single phase gas mixture under a body force from a uniformly mixed upstream condition is analysed. The flow is assumed to be two-dimensional and confined between two parallel walls. An inviscid hydrodynamical model is adopted. A perturbation procedure is used to obtain a closed from zeroth order solution. The interplay between Fickian and baro-diffusion is brought out. The problem bears on cavity type gaceous nuclear reactor propulsion device where the critical concentration of the nuclear fuel in a fuel-propellant mixture is important.

(1) Introduction

For many industrial purposes it is desirable to know the establishment of stratificatification for a two-fluid single phase fluid system in the presence of strong body forces. In particular, it is very often necessary to know the concentration of the heavier species at various points downstream of the inlet where the two fluids are uniformly mixed. This knowledge is needed, for example, in gaseous nuclear propulsion device where the heavier fluid is uranium, and the critical concentration for the onset of reaction is of paramount importance. In most problems of this nature the body force is usally a centrifugal force, and for high flow velocities the effect of viscosity is generally negligible. The dominant effect is one of mass diffusion.

In this paper an inviscid, incompressible, hydrodynamical theory is proposed. Strictly speaking the thermodynamics of the system has to be considered together with the mechanical equations in order to obtain a complete set of equations (see for example Landau and Lifshitz (1)). However, when the change of density of the fluid mixture taken as a whole is assumed to be proportional to the change in concentration of the heavier fluid, a purely mechanical consideration suffices and thermodynamics can be left out of the analysis. This of course results in a major simplification of the problem. A perturbation scheme is then used to solve the problem, which is here considered as a two-dimensional flow in a horizontal duct with a body force in the vertical direction.

2. The Governing Equations

The equation of continuity for the total mass of fluid is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 , \tag{1}$$

(1) L. D. Landau and E. M. Lifshitz, Fluid Mechanics. Addison-Wesley Publishing Co., Inc. Reading, Mass. pp 219-227.

where ρ is the total density of the fluid and $\vec{v}$ denotes the velocity. We note that velocity is here understood as the total momentum per unit mass of fluid, and the equations of motion are the Euler's equations

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \rho\vec{g}, \tag{2}$$

where p is the pressure, $\vec{g}$ is the body force and $\frac{D}{Dt} \equiv \left(\frac{\partial}{\partial t} + \vec{v}.\nabla\right)$ is the substantial derivative.

If we denote c to be the mass concentration of the heavier fluid, the equation of continity for that species is

$$\frac{Dc}{Dt} = -\nabla.\vec{i} \tag{3}$$

where $\vec{i}$ is the mass flux of that species.

The mass flux is made up of three parts

$$\vec{i} = -D\left[\nabla c + \left(\frac{\rho k_T}{T}\right)\nabla T + \left(\frac{\rho k_p}{p}\right)\nabla p\right], \tag{4}$$

where D is the diffusion coefficient or mass transfer coefficient

k_T is the thermal diffusion ratio

k_p is the barodiffusion ratio

and T is the absolute temperature.

k_T and k_p are determined by thermodynamic properties alone. For the purpose of this analysis it can be shown (see Landau and Lifshitz (1)) that k_p is negative.

In the present analysis we shall assume a uniform temperature distribution so that

$$\vec{i} = -D\left[\nabla c - \left(\frac{\rho k}{p}\right)\nabla p\right], \tag{5}$$

where $k \equiv -k_p$ is positive. From the above equation we can conclude at once that equilibrium is reached when the flux due to mass concentration is balanced by the pressure flux.

Substitution of (5) into (3) yields

$$\frac{Dc}{Dt} = \nabla\cdot(D\nabla c) - \nabla\cdot\left(\frac{\rho k D}{p}\nabla p\right). \tag{6}$$

(1), (2), and (6) are five equations for the six unknowns, c, ρ, p, $\vec{v}$. To complete the system we assume

$$(\rho - \rho^*) = \beta(c - c^*), \tag{7}$$

where ρ^* and c^* are reference quantities and ß is a constant of propotionality.

We shall now formulate our problem in terms of a duct flow. The flow is assumed to be steady two-dimensional and bounded by two parallel walls at y = 0 and y = L as shown in Figure 1. The body force $\vec{g}$ is taken to be in the negative y- direction. If we denote (u , v) to be the components of $\vec{v}$ in the (x, y) - directions, then for an incompressible flow the equation of continuity is

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad . \tag{8}$$

The equations of motion are

$$\rho \left(u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = - \frac{\partial p}{\partial x} , \tag{9}$$

$$\rho \left(u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = - \frac{\partial p}{\partial y} - \rho g , \tag{10}$$

and (6) becomes

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = \nabla . (D \nabla c) - \nabla . \left(\frac{\rho k D}{p} \nabla p \right) , \tag{11}$$

where $\nabla \equiv \vec{i} \frac{\partial}{\partial x} + \vec{j} \frac{\partial}{\partial y}$ and

$$(\rho - \rho^*) = \beta (c - c^*) . \tag{12}$$

Hence $$u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} = \nabla . (D \nabla \rho) - \beta \nabla . \left(\frac{\rho k D}{p} \nabla p \right) . \tag{13}$$

The boundary conditions are

ρ	= constant	for	$x = 0$,	$0 \leq y \leq L$,
$\lvert \rho \rvert$	$< \infty$	for	$x \to \infty$,	$0 \leq y \leq L$,
$\vec{i}$	= 0	for	$0 \leq x < \infty$,	$y = 0$,
$\vec{i}$	= 0	for	$0 \leq x < \infty$,	$y = L$.

3. Solution of the Boundary Value Problem and Discussion

The boundary value problem is now to be solved by a perturbation procedure. In general g may be assumed to be a function of x. Now D and k are known functions of ρ and p. We let $D = f_1(\rho, p)$, and $\left(\frac{\rho k D}{p} \right) = f_2(\rho, p)$.

We now assume a perturbation series of the form

$$u = u_0(y) + u_1 + u_2 + \dots$$
$$v = 0 + v_1 + v_2 + \dots$$
$$p = p_0(x,y) + p_1 + p_2 + \dots$$
$$\rho = \rho_0(x,y) + \rho_1 + \rho_2 + \dots$$

where terms of 1st and higher orders are $<<$ than the zeroth order quantities. It then follows that

$$f_1 = f_1(\rho_0, p_0) + \frac{\partial f_1}{\partial \rho}\rho_1 + \frac{\partial f_1}{\partial p}p_1 + \frac{1}{2!}\left(p_1\frac{\partial}{\partial p} + \rho_1\frac{\partial}{\partial \rho}\right)^2 f_1 + \dots$$
$$f_2 = f_2(\rho_0, p_0) + \frac{\partial f_2}{\partial \rho}\rho_1 + \frac{\partial f_2}{\partial p}p_1 + \frac{1}{2!}\left(p_1\frac{\partial}{\partial p} + \rho_1\frac{\partial}{\partial \rho}\right)^2 f_2 + \dots$$

Substitution of the above into the equations and collecting zeroth order terms we have

$$0 = -\frac{\partial p_0}{\partial x}, \tag{14}$$

$$0 = -\frac{\partial p_0}{\partial y} - \rho_0 g(x), \tag{15}$$

$$u_0\frac{\partial \rho_0}{\partial x} = \frac{\partial}{\partial x}\left(f_1(\rho_0,p_0)\frac{\partial \rho_0}{\partial x}\right) + \frac{\partial}{\partial y}\left(f_1(\rho_0,p_0)\frac{\partial \rho_0}{\partial y}\right) - \beta\frac{\partial}{\partial x}\left(f_2(\rho_0,p_0)\frac{\partial p_0}{\partial x}\right) - \beta\frac{\partial}{\partial y}\left(f_2(\rho_0,p_0)\frac{\partial p_0}{\partial y}\right). \tag{16}$$

Utilization of the 1st two we then have

$$u_0\frac{\partial \rho_0}{\partial x} = \frac{\partial}{\partial x}\left(f_1(\rho_0,p_0)\frac{\partial \rho_0}{\partial x}\right) + \frac{\partial}{\partial y}\left(f_1(\rho_0,p_0)\frac{\partial \rho_0}{\partial y}\right) + g\beta\frac{\partial}{\partial y}\left(f_2(\rho_0,p_0)\,\rho_0\right). \tag{17}$$

The system consisting of the above equation together with (14) and (15) is the non-linear zeroth order equations. Bearing in mind that f_1 and f_2 are really diffusion coefficients we could assume (as leading terms in an ordinary iterative procedure) f_1 and f_2 to be constants and denote f_1 by k_1, and f_2 by k_2. Hence we have

$$u_0 \frac{\partial \rho_0}{\partial x} = k_1 \left(\frac{\partial^2 \rho_0}{\partial x^2} + \frac{\partial^2 \rho_0}{\partial y^2} \right) + g\beta k_2 \frac{\partial \rho_0}{\partial y} ,$$

or

$$\left(\frac{\partial^2 \rho_0}{\partial x^2} + \frac{\partial^2 \rho_0}{\partial y^2} \right) - \frac{u_0}{k_1} \frac{\partial \rho_0}{\partial x} + \beta g \frac{k_2}{k_1} \frac{\partial \rho_0}{\partial y} = 0 . \tag{18}$$

The boundary conditions are now

$$\begin{array}{lll} \rho_0 = \text{constant} = \bar{\rho}_0 & \text{for} & x = 0, \quad 0 \le y \le L, \\ |\rho_0| < \infty & \text{for} & x \to \infty, \quad 0 \le y \le L, \\ \frac{\partial \rho_0}{\partial y} + \beta g \frac{k_2}{k_1} \rho_0 = 0 & \text{for} & 0 \le x < \infty, \quad y = 0, \\ \frac{\partial \rho_0}{\partial y} + \beta g \frac{k_2}{k_1} \rho_0 = 0 & \text{for} & 0 \le x < \infty, \quad y = L \end{array}$$

The velocity u_0 is determined by the inlet velocity distribution. For any given u_0 at the inlet and g equation (18) together with the above boundary can be readily solved by finite differences. For the important case when u_0 is constant $=A$ and g is constant an analytical solution is presented.

We first cast the equations into non-dimensional form by using L as the reference length, A the reference velocity and $\bar{\rho}_0$ as the reference density, we have using the same symbols to denote now the corresponding dimensionless quantities, the following:

$$\left(\frac{\partial^2 \rho_0}{\partial x^2} + \frac{\partial^2 \rho_0}{\partial y^2} \right) - \frac{1}{k_1} \frac{\partial \rho_0}{\partial x} + \beta \frac{k_2}{k_1} F^{-2} \frac{\partial \rho_0}{\partial y} = 0 ,$$

where $F^2 = A^2/Lg$ is a Froude number, and $k_1 = \frac{k_1}{LA}$, $k_2 = \frac{k_2 A}{L}$,

if we denote $\frac{1}{k_1}$ by α and $(\beta \frac{k_2}{k_1} F^{-2})$ by γ

we have

$$\frac{\partial^2 \rho_0}{\partial x^2} + \frac{\partial^2 \rho_0}{\partial y^2} - \alpha \frac{\partial \rho_0}{\partial x} + \gamma \frac{\partial \rho_0}{\partial y} = 0 , \tag{19}$$

$$\rho_0 = 1 , \quad \text{for} \quad x = 0 , \quad 0 \le y \le 1 ,$$

$$|\rho_0| < \infty , \quad \text{for} \quad x \to \infty , \quad 0 \le y \le 1 ,$$

$$\frac{\partial \rho_0}{\partial y} + \gamma \rho_0 = 0 , \quad \text{for} \quad 0 \le x < \infty , \quad y = 0 ,$$

$$\frac{\partial \rho_0}{\partial y} + \gamma \rho_0 = 0 , \quad \text{for} \quad 0 \le x < \infty , \quad y = 1 .$$

By separation of variables, the solution to the above problem is

$$\rho_0(x,y) = a\, e^{-\gamma y} + \sum_{n=0}^{\infty} a_n \varphi_n(y) \exp[-(\sqrt{\alpha^2 + \gamma^2/4 + n^2\pi^2} - \alpha)\frac{x}{2}] , \tag{20}$$

where $\varphi_n(y) = \exp(-\frac{\gamma y}{2}) (\sin n\pi y - \frac{2n\pi}{\gamma} \cos n\pi y)$ are eigen-functions of the Sturm-Liouville system from separation of variables and are orthogonal with respect to the weight function $e^{\gamma y}$ in the interval (0,1). a_n are the Fourier coefficients given by

$$a_n = [\int_0^1 \{ 1 - \frac{\gamma e^{-\gamma y}}{(1 - e^{-\gamma})} \} e^{\gamma y} \varphi_n(y)\, dy] / [\int_0^1 e^{\gamma y} \varphi_n^2(y)\, dy]$$

$$= n\pi \gamma^2 [(-1)^{n+1} e^{\gamma/2} + 1] / [(\frac{\gamma}{2})^2 + n^2\pi^2]^2 ,$$

and

$$a = \gamma / (1 - e^{-\gamma}) .$$

Note that eqn. (19) with its associated boundary conditions automatically ensures that $\int_0^1 \rho_0(x,y)\, dy = 1$ as it should be. This last result has been utilized to obtain a.

From the solution it is immediately clear that as $x \to \infty$, $\rho_0 \to (\gamma e^{-\gamma y})/(1 - e^{-\gamma})$. It is also seen that the important parameter of the problem is the dimensionless number γ. For $\gamma \to 0$, ρ_0 is constant throughout as to be expected. If γ is very large then the heavier gas sinks to the bottom. For some physically realistic value there would of course be a balance between baro-diffusion and mass diffusion and the asymptotic form of ρ_0 above indicates the equilibrium distribution. It has an exponential behavior as one would expect. The approach to the equilibrium position is also exponential. It is seen that the series converges rather rapidly for all $x > 0$.

Figures (2) and (3) are two typical cases (for fixed α , and γ) of density profiles as a function of depth for various values of distance from the inlet. The exponential profile is reached asymptotically for large x. Fig (4) shows for fixed α and γ the depth along the channel where an increase in density can be expected. For given values of α and γ, the above figures thus yields the information needed for determining the critical concentration for example.

Figures (5) shows the depth of where density increase can be expected for various values of γ. It shows that as γ increases, the depth of the region of increasing density decreases.

Figures (6) shows the distance downstream from the inlet as a function of γ for the density profile to reach 80 per cent of its asymptotic value. The graphs are plotted for constant values of α . It exhibits a maximum of γ approximately equal to 5. The curves goes to zero as $\gamma = 0$.

Figure (7) is a typical plot of the density as a function of depth with natural scales.

Appendix
Solution of the boundary value problem

By separtion of variables we assume

$$\rho_0(x,y) = X(x)\,Y(y)$$

Equation (19) and boundary condition become

$$\frac{d^2}{dx^2}X(x) - \alpha\frac{dX}{dx} - \lambda^2 X = 0, \qquad \text{(A1)}$$

$$|X(\infty)| < \infty,$$

$$\frac{d^2}{dy^2}Y(y) + \gamma\frac{dY}{dy} + \lambda^2 Y = 0, \qquad \text{(A2)}$$

$$\frac{dY}{dy} + \gamma Y = 0, \quad \text{at } y = 0, 1.$$

From (A1) we have, on using the condition at $x = \infty$,

$$X = A\,e^{-(\sqrt{\alpha^2+4\lambda^2}-\alpha)\frac{x}{2}},$$

and from (A2),we have

$$Y = e^{-\frac{\gamma y}{2}}[A_1 \sin\omega y + A_2 \cos\omega y], \qquad \text{(A3)}$$

where $\omega = \sqrt{\dfrac{4\lambda^2-\gamma^2}{4}}$

Substitution of (A3) into the boundary conditions following (A2) we obtain the secular equation

$$[\omega^2 + (\tfrac{\gamma}{2})^2]\ \sin\omega = 0,$$

$$\therefore \quad \sin\omega = 0$$

or

$$\omega = n\pi \,, \qquad n = 0, 1, 2, 3, \ldots$$

that is
$$\frac{4\lambda^2-\gamma^2}{4} = n^2\pi^2, \qquad \text{or} \qquad \lambda_n^2 = n^2\pi^2 + \frac{\gamma^2}{4}.$$

A particular solution, not an eigen solution, also comes from

$$\omega^2 = -\left(\frac{\gamma}{2}\right)^2$$

or
$$\frac{4\lambda^2-\gamma^2}{4} = -\frac{\gamma^2}{4}, \qquad \text{or} \quad \lambda = 0$$

For $\lambda = 0$, $Y = e^{-\gamma y}$, and $X = a$, a constant

For $\lambda_n^2 = n^2\pi^2 + \frac{\gamma^2}{4}$, $\sqrt{\alpha^2+4\lambda^2} > \alpha$, hence X satisfies the condition at $x = \infty$. Indeed $X \to 0$, as $x \to \infty$. The corresponding eigen functions are then

$$Y_n(y) = a_n e^{-\frac{\gamma}{2}y}\left[\sin n\pi y - \frac{2n\pi}{\gamma}\cos n\pi y\right].$$

We note that the eigen functions $Y_n(y)$ are orthogonel with respect to the weight function $e^{\gamma y}$ in the interval (0,1) and form a complete basis for expansion of L_2 - functions. Thus we write

$$\rho_0(x,y) = a e^{-\gamma y} + \sum_{n=0}^{\infty} a_n e^{-\frac{\gamma}{2}y}\left[\sin n\pi y - \frac{2n\pi}{\gamma}\cos n\pi y\right] e^{-\left(\sqrt{\alpha^2+\frac{\gamma^2}{4}+n^2\pi^2} - \alpha\right)\frac{x}{2}}.$$

At $x = 0$, $\rho_0(x,y) = 1$, at $x \to \infty$, $\rho_0(x,y) \to a e^{-\gamma y}$

and from the conservation of mass we have

$$1 = a\int_0^1 e^{-\gamma y}\,dy \qquad \therefore \quad a = \gamma/(1-e^{-\gamma}).$$

At $x = 0$, then

$$\left(1 - \frac{\gamma e^{-\gamma y}}{(1 - e^{-\gamma})}\right) = \sum_{n=0}^{\infty} a_n Y_n(y) ,$$

$$\therefore \quad a_n = \frac{\int_0^1 \left(1 - \frac{\gamma e^{-\gamma y}}{(1 - e^{-\gamma})}\right) e^{\gamma y} Y_n(y)\, dy}{\int_0^1 e^{\gamma y} Y_n^2(y)\, dy} .$$

The series converges by virture of the Sturm-Liouville Theorem.

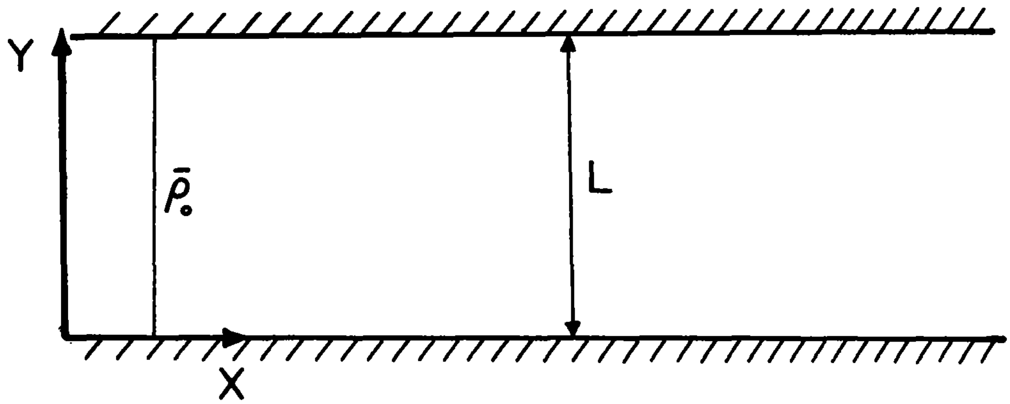

Figure 1. - Definition sketch.

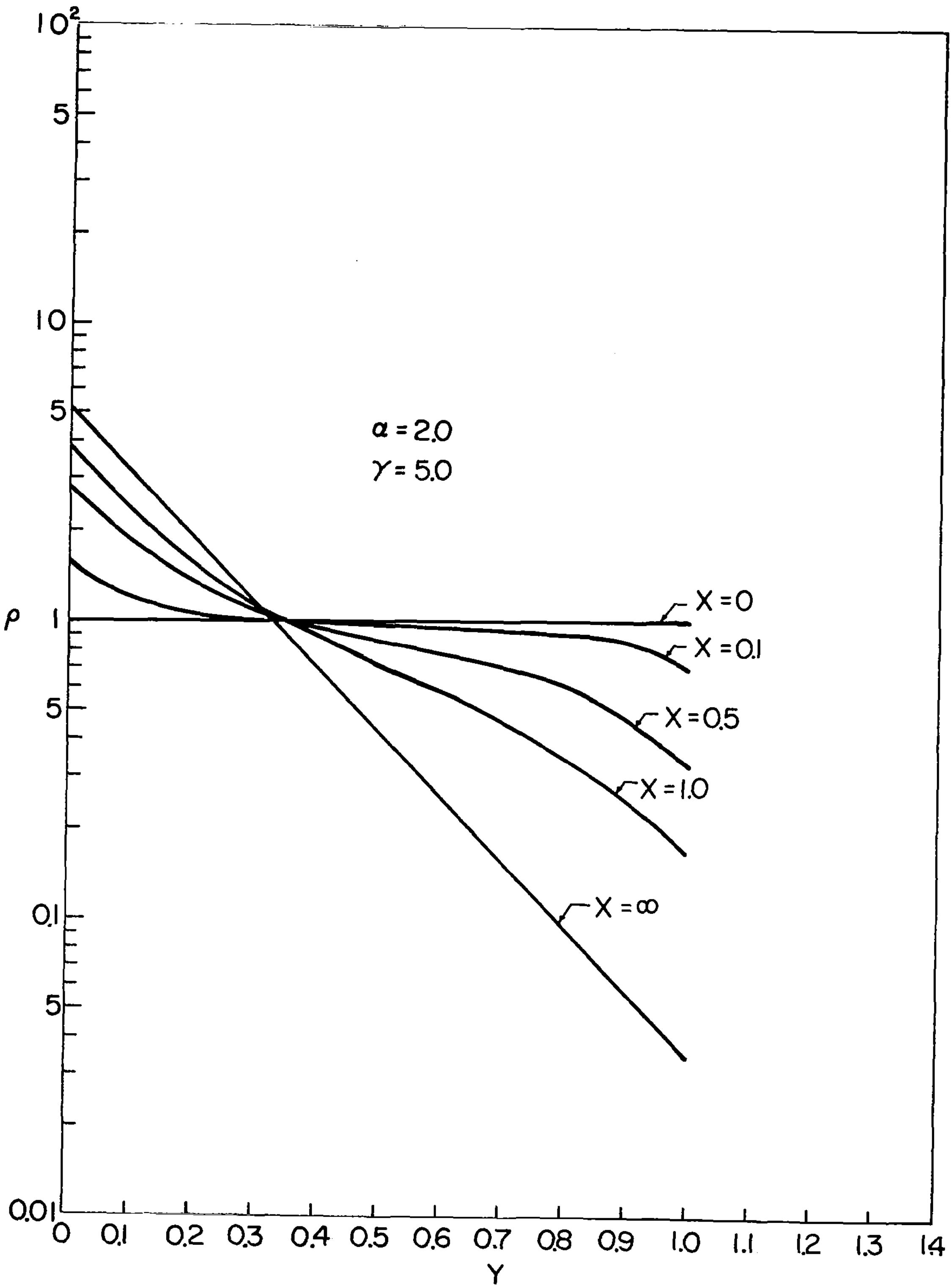

Figure 2. - Variation of density with depth for different distances downstream from the inlet. Case for $\gamma = 5$, $\alpha = 2$.

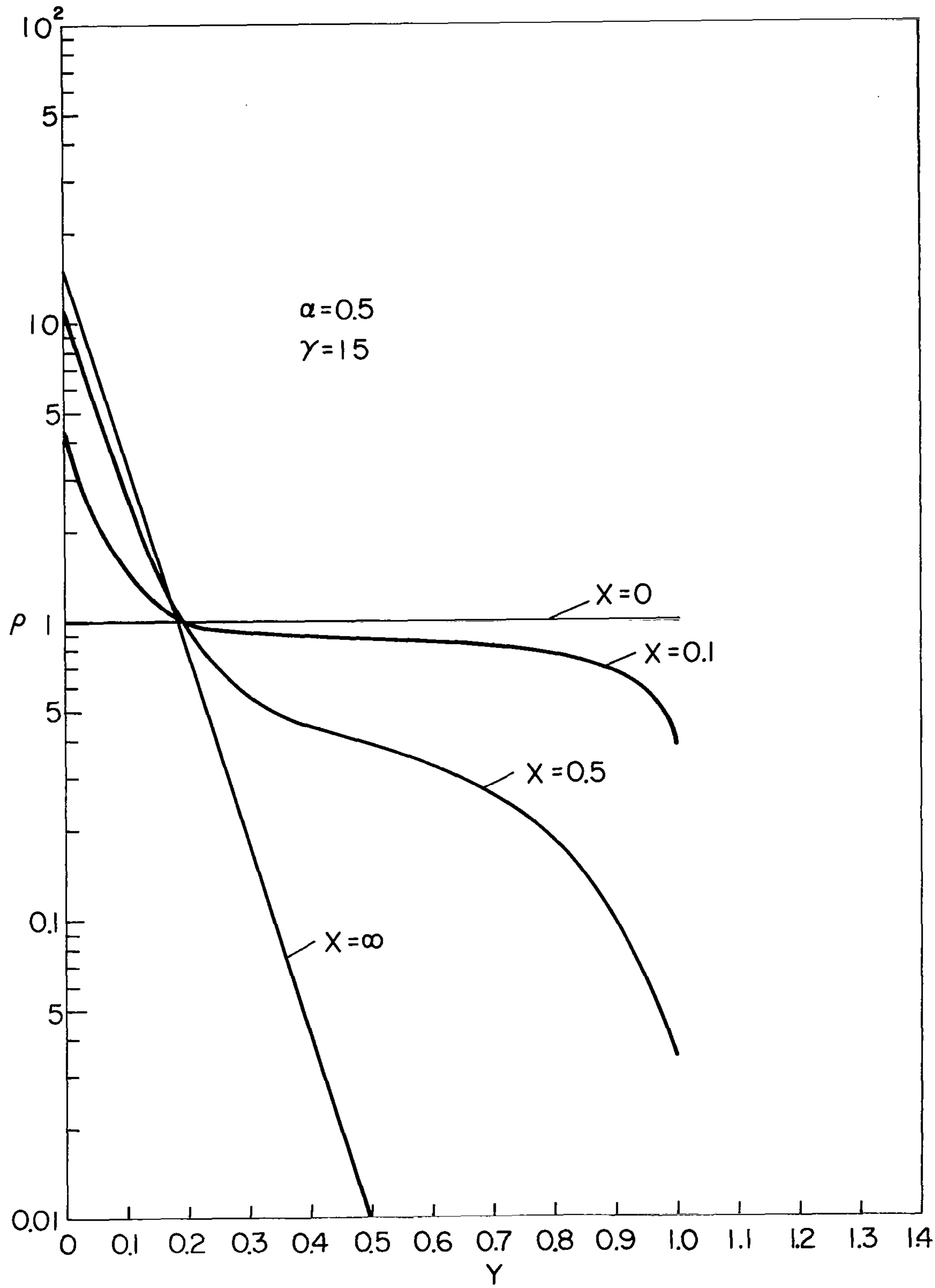

Figure 3. - Variation of density with depth for different distances downstream from the inlet. Case for $\gamma = 15$, $\alpha = 0.5$.

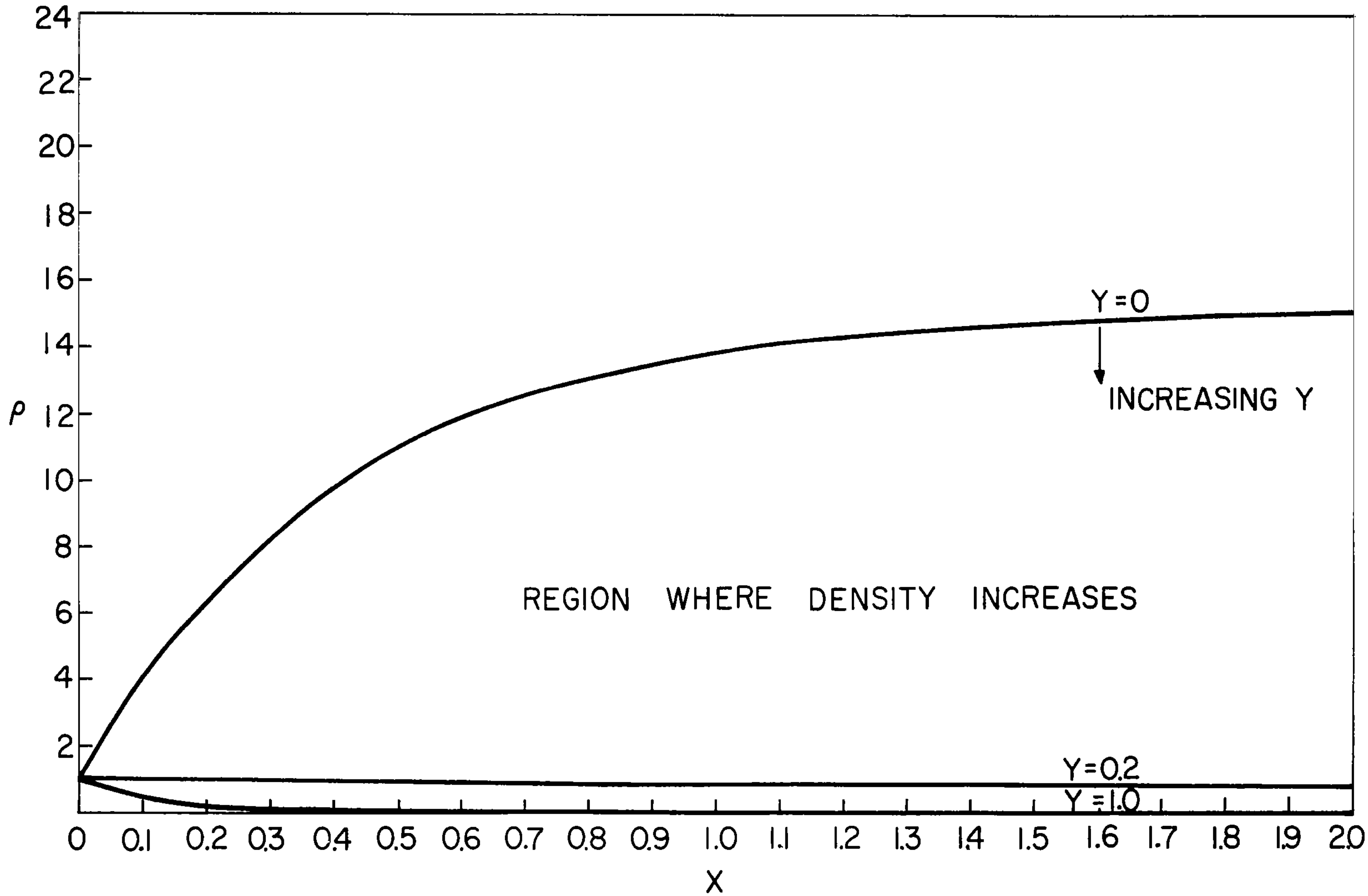

Figure 4. - Typical variation of density with distance downstream from inlet for various depths.

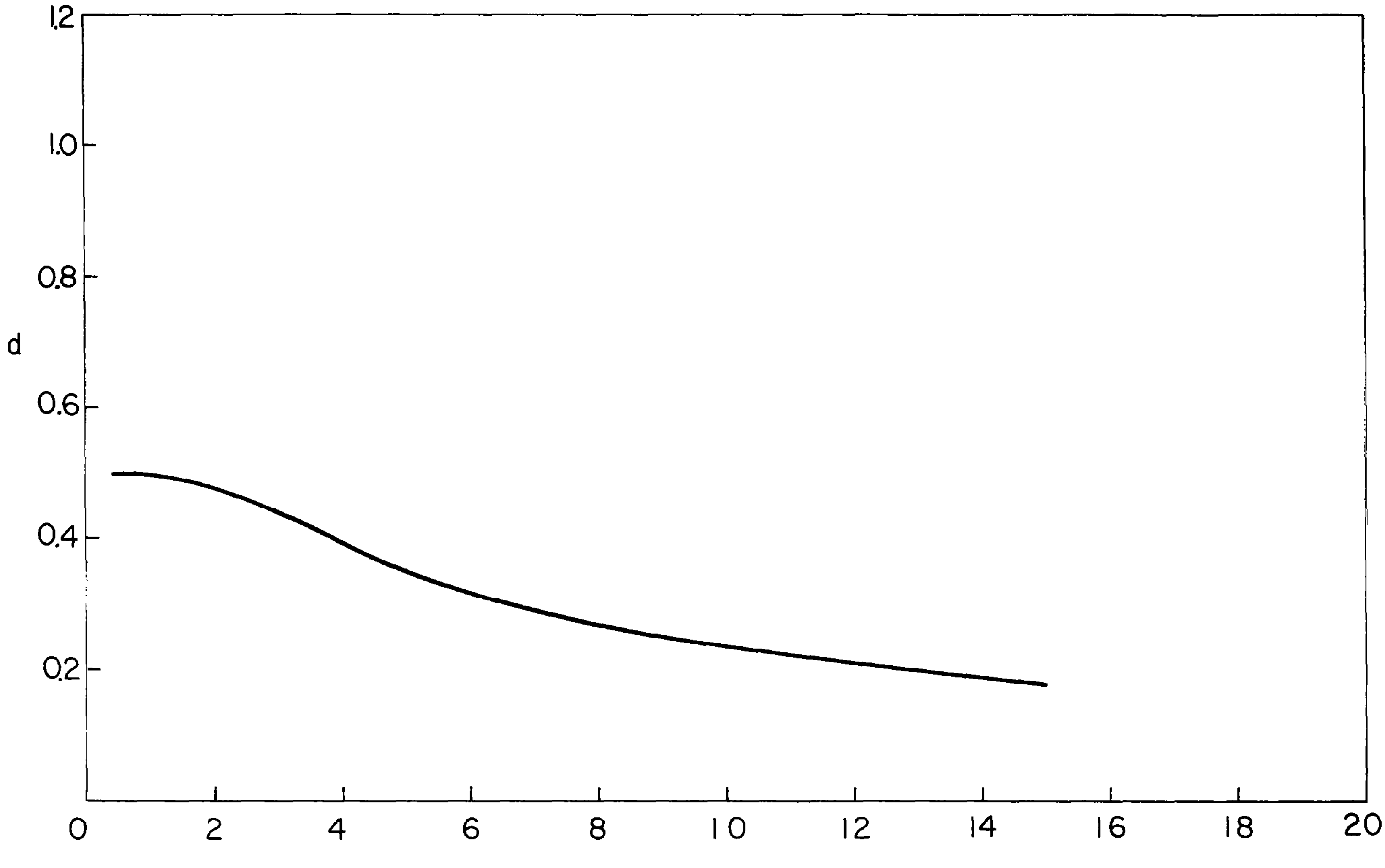

Figure 5. - Variation with γ of depth of zone where density increases.

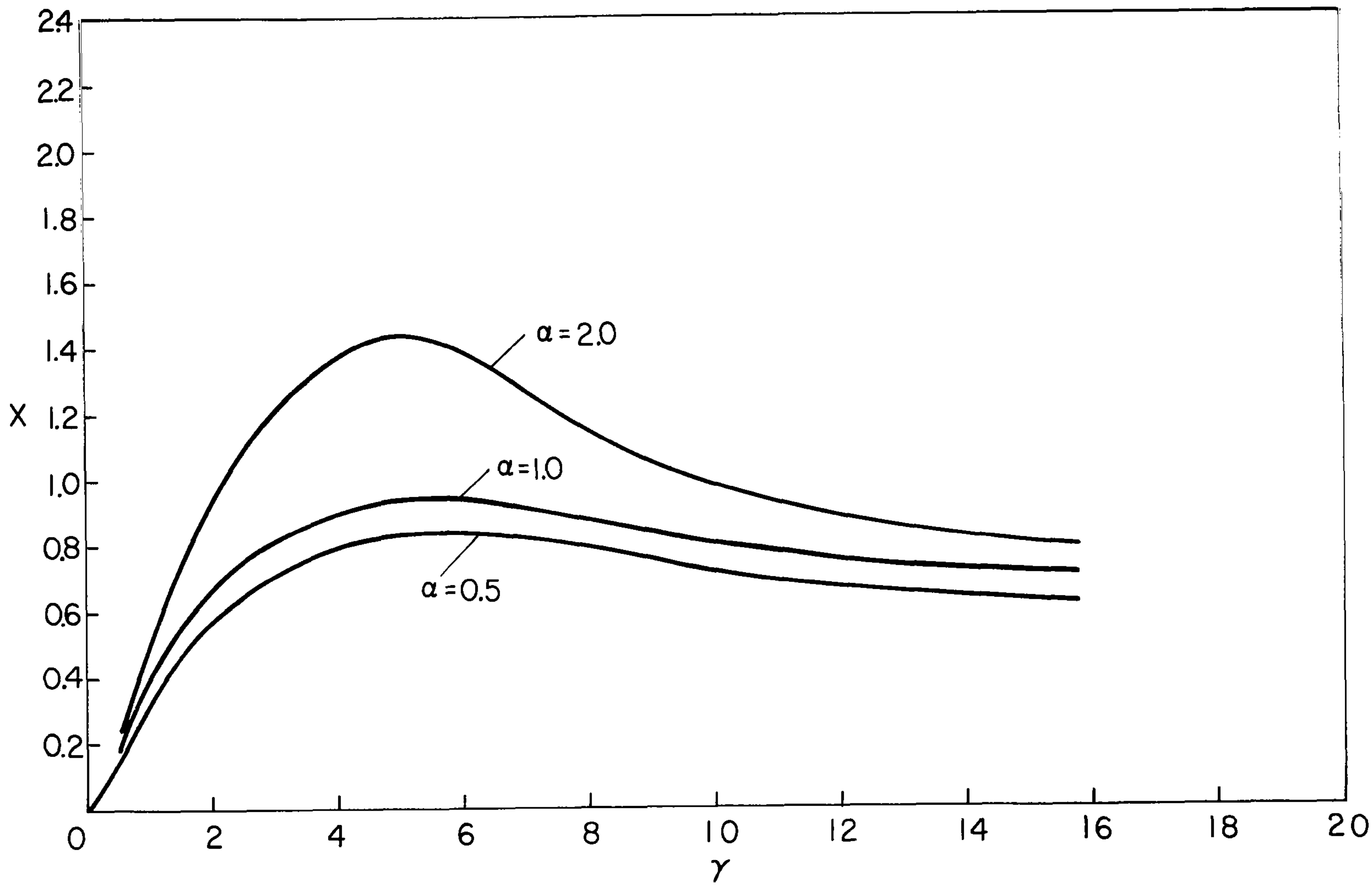

Figure 6. - Distances downstream, where 80 percent of equilibrium profile for $X = \infty$ is established, as a function of γ.

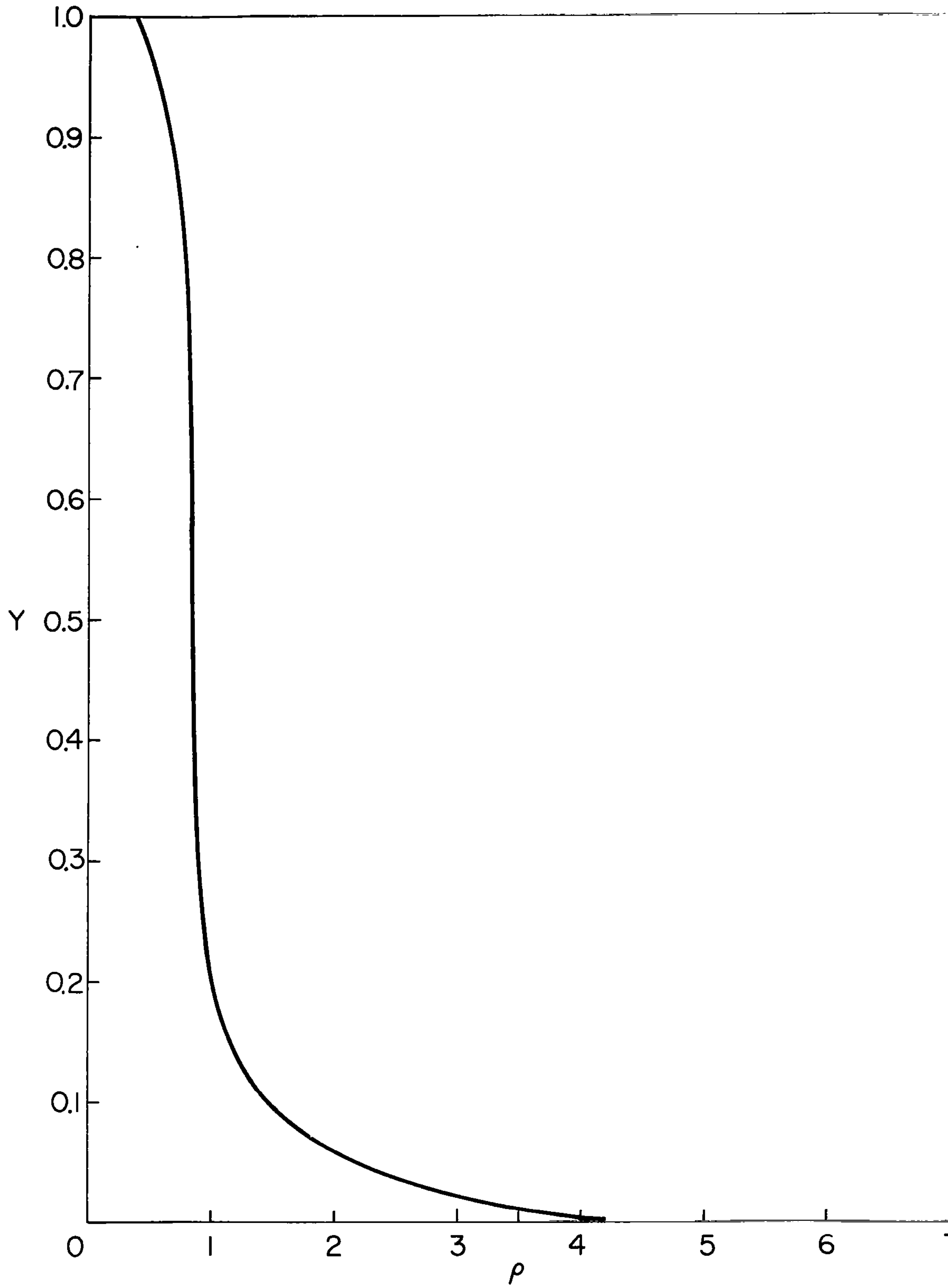

Figure 7. - Natural scale of typical plot of variation of density with depth.

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