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Steady natural convection flow over a semi-infinite vertical plate induced by diffusion and chemical reaction.

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STEADY NATURAL CONVECTION FLOW OVER A SEMI-INFINITE
VERTICAL PLATE INDUCED BY DIFFUSION AND CHEMICAL
REACTION

by

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ABSTRACT

An investigation is presented for steady natural convection flow over a semi-infinite vertical plate induced by diffusion and chemical reaction. The flow is assumed to be two-dimensional and laminar. For large Grashof numbers, the flow is reduced to a boundary-layer type, and this work is primarily concerned about a boundary-layer flow of binary systems with mass diffusion.

Perturbation-type similar solutions are obtained for the case of uniform concentration along the plate. The investigation is extended to second order perturbation terms. The similar coordinate length is contracted from infinity to unity by a suitable transformation and then Taylor series solutions are constructed. It has been observed that the first and second order perturbation solutions in concentration are found to be significantly smaller than the zeroth order solution.

Truncating the series after the 10th power, the zeroth order approximate solution is compared with the numerical solutions. These numerical solutions are obtained by the Runge-Kutta integration scheme in corporation with the Nachtsheim-Swigert technique (1965) to correct the initial

guesses at the surface boundary. The results for no reaction (i.e. zeroth order approximation) appear to be in a reasonable agreement for the small Schmidt numbers. But for high Schmidt numbers, the series solutions appear to be unstable.

An investigation upon the governing equations reveals that the similar solutions exist only for a certain type of problem consisting of distributed concentrations along the plate. The following three families of distributed surface concentrations whose functionalities are prescribed by the order of the reaction are studied:

1. For general nth order kinetics:

$$c_0 - c_\infty = N\, x^{\frac{1}{3-2n}}$$

2. For first order reaction kinetics:

$$c_0 - c_\infty = N\, x$$

3. For 3/2th order reaction-kinetics:

$$c_0 - c_\infty = N\, e^{4\lambda_1 C_1 x}$$

These families assume the similar solutions. For the problems 2 and 3, numerical results for negligible reaction

rate are compared with those of Sparrow and Gregg (1958).
The comparison shows excellent agreement.

DEDICATED TO:

LATE LUTFUR RAHMAN

my beloved father

ACKNOWLEDGEMENTS

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NOMENCLATURE

In the following list of symbols, dimensions are given in terms of mass (M), length (L), time (Θ) and temperature (T).

LATIN LETTERS:

C = non-dimensional species concentration.

C_p = specific heat of fluid at constant pressure,

$$L^2 T^{-1} \Theta^{-1}$$

D = chemical molecular diffusivity,

$$L^2 \Theta^{-1}$$

f = non-dimensional stream-function.

g = acceleration due to gravity,

$$L \Theta^{-2}$$

Grx = Grashof number = $\dfrac{g\beta^*(c_0 - c_\infty) x^3}{\nu^2}$

K = thermal conductivity of the fluid,

$$MLT^{-1} \Theta^{-3}$$

Le = Lewis number = α/D

Pr = Prandtl number = ν/α

Sc = Schmidt number = ν/D

T = absolute temperature of fluid, T

R = universal gas constant

$$ML^2 \Theta^{-2} T^{-1} \, (mole)^{-1}$$

u = velocity component in x - direction, $L\theta^{-1}$

v = velocity component in y - direction, $L\theta^{-1}$

x = vertical distance along the surface, L

y = horizontal distance from the surface, L

E = activation energy,

$$ML^2\theta^{-2}$$

$J^{\diamond}$ = mass flux

$$(\text{moles})\ L^{-2}\theta^{-1}$$

k = homogeneous chemical rate-constant

$$(\text{moles})^{1-n}L^{3n-3}\theta^{-1}$$

P = fluid pressure,

$$ML^{-1}\theta^{-2}$$

$\dot{Q}'''$ = volumetric heat-source rate.

$\dot{c}'''$ = r_A = chemical reaction-rate,

$$ML^{-3}\theta^{-1}$$

V = volume, L^3

$\underset{\sim}{V}$ = velocity vector, $L\theta^{-1}$

Z = similarity distance (dimensionless)

n = order of reaction

Re = Reynolds number.

Nu = Nusselt number.

GREEK LETTERS

$\alpha \quad = \quad \dfrac{k}{\rho \overline{C}_p}, \quad = \text{thermal diffusivity,} \quad L^2 \Theta^{-1}$

$\beta \quad = \quad \text{thermal coeficient of volumetric expansion,} \quad T^{-1}$

$\beta^* \quad = \quad \text{volumetric coefficient of expansion with concentration,}$

$$L^3 \, (\text{mole})^{-1}$$

$\phi \quad = \quad \text{non-dimensional temperature.}$

$\mu \quad = \quad \text{dynamic viscosity of fluid,}$

$$ML^{-1}\Theta^{-1} \qquad ,$$

$\nu \quad = \quad \dfrac{\mu}{\rho}, = \text{Kinematic viscosity of fluid } L^2 \Theta^{-1}$

$\rho \quad = \quad \text{fluid density,} \quad ML^{-3}$

$\psi \quad = \quad \text{Stream function, dimensions depend on the coordinate system.}$

$\eta \quad = \quad \text{Similarity variable} = \dfrac{y}{x}\left[\dfrac{Grx}{4}\right]^{1/4}$

$\epsilon \quad = \quad \text{Dimensionless reaction-numbers}$

$$= \frac{2k \, e^{n-3/2}}{\sqrt{g\beta^*}} \, x^{1/2}$$

$\underset{\sim}{\nabla} \quad = \quad \text{the "del" operator}$

$$= i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + k\frac{\partial}{\partial z} \quad ,$$

$\nabla^2 \quad = \quad \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$

SUBSCRIPTS

x = based on distance x

T = based on temperature level

C = based on species concentration level

O = at the surface

∞ = in the undisturbed fluid

CHAPTER I

INTRODUCTION

1.1   Concepts and definitions:

Boundary value problems involving the principles of heat and mass diffusion in a fluid medium, where the results are directly influenced by the presence of fluid motion may in general be termed convection processes. If the motion of the fluid is determined by boundary conditions specified externally to the system, such as forcing air through a passage in which an external pressure gradient is specified, the process is called forced convection. Otherwise, if the fluid velocities are caused by the effects of gravity force, i.e. by the interaction of a body force with variable density arising from heat or mass diffusion, then the process is called natural convection.

The phenomena of natural convection can be observed in the atmosphere, in bodies of water, adjacent to domestic heating radiators or over sun-heated fields and roads.

The basic equations which describe natural convection flows are similar to those of other fluid flows and diffusion processes, with the essential difference that, in natural

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convection, the motion of a fluid arises from buoyancy and not from an imposed motion or pressure gradient. The basic equations and their boundary layer approximations for natural convection flows are derived in the following chapter.

The characteristic numbers of natural convection which are commonly used are as follows:

Local Grashof number: $\quad Gr_x = \dfrac{g\beta^*(c_0 - c_\infty)x^3}{\nu^2}$

Schmidt number: $\quad Sc = \nu/D$

Prandtl number: $\quad Pr = \nu/\alpha$

Local Nusselt number: $\quad N_{ux} = \dfrac{J''(x)}{c_0 - c_\infty}\left(\dfrac{x}{D}\right)$

Local Reaction Rate number:

$$\epsilon(x) = \frac{2k(c_0 - c_\infty)^{n-3/2}}{\sqrt{g\beta^*}} x^{1/2}$$

where,

g = acceleration due to gravity

β^* = volumetric coefficient of expansion with concentration species

c_0 = species concentration at the plate surface

c_∞ = species concentration at the ambient fluid

x = co-ordinate length along the plate

ν = kinematic viscosity of the fluid

D = Chemical molecular diffusivity

α = thermal molecular diffusivity

$J''(x)$ = local mass flux

k = reaction-rate constant

n = order of reaction

The quantity $\quad Gr = \dfrac{g\beta^*(c_0 - c_\infty)L^3}{\nu^2}$

where L is a characteristic length of the plate, is called the Grashof number. This number is a measure of the vigor of the flow induced due to buoyancy-effects. It arises in the force-momentum balance as the ratio of the relative magnitudes of viscous force and the inertia force. The Grashof number of natural convection flow is analogous to the Reynolds number of forced flow, $\sqrt{Gr}$ corresponding to Re. The characteristic feature of this number is that stability and transition are defined in the limits of this number. The quantities $P_r = \nu/\alpha$ and $Sc = \nu/D$ are defined as the Prandtl and Schmidt numbers respectively. The former one occurs in the energy equation whereas the latter one occurs in the mass-diffusion equation. These two numbers are the indicators of the steepness of the gradients of temperature and concentration respectively in

the flow field. As for instance, for high Prandtl number fluids, the temperature gradient is much steeper than that for low Prandtl number fluids.

The local mass flow per unit area (mass flux) from the surface of the plate to the fluid may be calculated from Fick's first law of diffusion:

$$\underset{\sim}{J} = - D\underset{\sim}{\nabla}c,$$

which is the three-dimensional form of Fick's law. For a two dimensional case, if we assume that the mass flux component parallel to the surface is very small compared to that perpendicular to the surface, then the mass flux from the plate surface to the fluid may be written as

$$J''(x) = - D\left(\frac{\partial c}{\partial y}\right)_{y = 0}$$

It is customary to express mass transfer characteristics in terms of a "mass-transfer coefficient" h, defined as the mass transfer per unit area (i.e. mass flux) divided by the concentration difference causing the mass-transfer. Since the flux is often variable over the surface even for a uniform concentration difference, the mass transfer coefficient h varies over the surface. Therefore, one may speak of local values h_x or of average values h.

This local value is given by

$$h_x = \frac{J''(x)}{c_0 - c_\infty} = -\frac{D}{c_0 - c_\infty}\left(\frac{\partial c}{\partial y}\right)_{y=0}$$

Multiplying through by x/D, a dimensionless combination is found which is called the local Nusselt number (a mass transfer parameter):

$$Nux = \frac{h_x x}{D}$$

The average mass transfer coefficient h from $x = 0$ to L may be found from the following integral:

$$h = \frac{\text{average mass flux}}{\text{average concentration difference}}$$

$$= \frac{\left\{\frac{1}{L}\int_0^L J''(x)dx\right\}}{\left\{\frac{1}{L}\int_0^L (c_0 - c_\infty)dx\right\}}$$

Thus the average transport parameter is given by

$$N_{uL} = \frac{hL}{D},$$ which is a measure of mass flow per unit area from the surface of the plate to the fluid in dimensionless form.

The quantity

$$\frac{2k(c_0 - c_\infty)^{n-3/2} x^{1/2}}{\sqrt{g\beta^*}}$$

arises as an indication of the relative importance of the chemical reaction-rate in the mass diffusion equation and is called the reaction-rate number, details of which are discussed in Chapter IV.

1.2 <u>Historical Summary</u>

Investigation of natural convection flow began as early as 1881, when Lorenz calculated the heat transfer from a hot vertical plate in still air. He used the assumption that the velocity and temperature distributions at any point depend only on the distance from the plate. Schmidt and Beckmann in 1930 proved that this assumption was quite unsatisfactory. At about that time, Prandtl's laminar boundary-layer concepts were introduced to fluid mechanics. Schmidt and Beckmann were the first to apply the concepts of boundary-layer theory to natural convection flows. Their calculations for this problem indicated that the boundary-layer may be thin compared with the height of the vertical hot plate, and consequently, that the components of the gradients in velocity parallel to the surface of the plate would be relatively small. Hence they showed that the approximations of the boundary-layer theory were applicable to the formulation of natural convection problems.

An analysis of relative orders of magnitude, which is demonstrated by Gebhart (1971), yields the system of equations governing the distributions of velocity, and concentration applicable to flows which result in thin

convection layers. These convection layers are boundary-layers which arise in flows at high Grashof number. This number is indicative of the buoyancy force. (In forced convection flow the boundary-layer region results from flows at high Reynolds number.)

One classical problem of natural convection flow has been treated by Jakob in 1949, Bird et al in 1963 and Kays in 1966. The problem concerns the flow between two vertical parallel walls held at different temperatures and placed in a fluid of uniform density and viscosity. Heat transfer and the resulting buoyancy effect then cause the fluid near the hotter wall to rise and that near the colder wall to descend. Thus convection currents are set up in the fluid domain between the walls and the calculations infer that the temperature distribution is a linear function of the distance between the walls while the velocity profile shows a cubic variation. These results appear to conform well to the physical knowledge of the problem.

Another problem discussed by Bird et al in 1963 concerns a flat vertical plate held at temperature T_o and suspended in an infinite body of fluid, initially at rest with uniform density and viscosity. The temperature of the fluid

initially is T_1 where $T_1 << T_0$. Convection currents are essentially parallel to the plate and are set up by the buoyancy effect. Assuming that the flow is confined to a neighbourhood of the plate which is small in comparison with the plate length and that transverse velocity components are negligible, the steady state boundary-layer formulation yields a set of coupled non-linear ordinary differential equations for the flow field. The equations were not solved; rather the authors presented a dimensional analysis of these equations. This type of problem is best described and discussed in the work of Morgan and Warner (1956), also Ostrach (1953).

A problem of steady state natural convection induced by chemical diffusion from a vertical plate has been reported by Levich (1962). The plate, at zero concentration of a given chemical species A, but containing some catalytic substances, is placed in a fluid solution of A at con-centration $c_0 > 0$. When the plate comes into contact with the solution, an heterogeneous chemical reaction takes place on the plate, which disturbs the concentration of A near the surface. Changes in concentration imply density gradients which, in the presence of a gravitational field,

induce natural convection flow near the plate. Under the assumption that concentration gradients are significant only in a very thin layer immediately adjacent to the reaction surface, the author finds an approximate analytical solution for the concentration and velocity distributions, valid for high Schmidt numbers only.

A steady state two-dimensional boundary layer anlaysis (for temperature diffusion) of the effects of viscous dissipation in the case of external flows produced by a vertical surface in a fluid of uniform density and viscosity has been reported by Gebhart (1962). Similarity analysis of the relevant equations of motion and energy shows that the magnitude of the viscous dissipation effects is given by an x-dependent dissipation number defined by $\epsilon(x) = \dfrac{g\beta x}{c_p}$, where, β = volumetric coefficient of thermal expansion

c_p = specific heat at constant pressure.

For most practical cases with common fluids ϵ is very small of the order 10^{-6}, and on the basis of this fact, a perturbation analysis was carried out about this number. The resulting zero and first order approximations for temperature and zero order stream-function are integrated numerically for various Prandtl numbers. From the calculation it appears

that at the leading edge of the surface, the effect of dissipation on heat transfer is zero, whence the effect increases with increase of the body force and/or along the surface, becoming appreciable near the upper limit of the plate height. With the double boundary-layer concepts, Roy (1969) extended the above problem for high Prandtl number fluids and isothermal surfaces. A similar calculation, but for higher Prandtl numbers, was carried out by Stewartson and Jones (1957). Morgan and Warner (1956) have also considered several two-dimensional steady problems of heat transfer at high Prandtl numbers. The relevant equations of motion and temperature for forced and natural convection are transformed to the equations valid in the momentum boundary-layer using dimensional analysis. Their results are in good agreement with those of Ostrach (1953).

An analysis is presented for steady laminar natural convection from a vertical plate having a non-uniform temperature by Sparrow and Gregg (1958). They have considered two families of surface temperatures which permit the finding of similarity solutions of the boundary-layer equations. Numerical results are presented at $Pr = 0.7$ and 1.

Gebhart and Mollendorf (1969) considered the effects

of viscous dissipation in external steady natural convection flows over a vertical surface in an extensive medium at rest. They showed that a similarity solution exists for the boundary-layer equations when an exponential variation of surface temperature is assumed.

The distribution of a solute concentration in a layer of chemical solution subject to a drying process has been described by Meadley (1971). The author has considered a horizontal layer of a solid-in-liquid solution initially of uniform concentration and depth. The solvent is then forced to evaporate continuously from the free surface which causes a back-diffusion of the dissolved solids into the remaining liquid layer, and this results in a one dimensional unsteady distribution of solute concentration. This problem essentially describes the behaviour of the solute concentration in a liquid layer of continuously varying depth. Assuming this varying depth to be an analytic function of time, an approximate solution has been presented.

Combined thermal and species diffusion flows have been considered by some authors. A problem of this type, having simultaneous mass and heat diffusion from a wetted isothermal vertical surface in a non-saturated atmosphere, has been

reported by Somers (1956). He has assumed that the concentration of the diffusing species is very small. The coupled equations arising in this problem have been solved for uniform surface concentration and temperature by an analytical method similar to those used in classical boundary-layer theory.

Gill et al (1965) investigated these simultaneous buoyancy effects in gaseous binary diffusion. The enthalpy, thermal conductivity, viscosity and density have been allowed to vary with concentration and have been studied independently. A normal velocity condition is assumed to obtain at the surface. Numerical solutions are obtained with results which appear to be relatively significant.

Wilcox (1961) investigated the same problem by assuming the velocity, temperature and concentration distributions arbitrarily. Comparison has been made with results of Ostrach (1953).

Lowell and Adams (1967) have looked into the problem described by Gill et al (1965), from the similarity analysis viewpoint. The usual physical characteristics of the fluid are assumed constant. They have found that a similarity

solution for this problem is possible only for an isothermal surface. The usual velocity boundary condition and the effects of comparable concentration level are included in this study.

An asymptotic analysis of the same problem for $Sc \gg Pr$ has been made by Lightfoot (1968). He has assumed that the species diffusion buoyancy effect is very small compared to that caused by thermal diffusion. The resulting transport relation has not agreed with the general result of Wilcox (1961). Thus it seems that the interaction between heat and mass transfer in natural convection deserves some further analysis.

Pera and Gebhart (1972) have studied the process involved in heating of the earth by sunlight, where the resulting atmospheric thermal convection may be influenced by the presence of moisture evaporated from the ground. The authors have considered natural convection flows from a horizontal isothermal and semi-infinite surface given by the combined buoyancy effects of surface heating and diffusion of chemical species. Similarity anlalysis is used and the resulting differential equations are integrated with a fourth order Runge-Kutta Scheme, in combination with a linear interpolation to correct for unspecified boundary

conditions at the surface.

Natural convection flows adjacent to a vertical surface resulting from the simulteneous buoyancy effects of thermal and mass diffusion have been considered by Gebhart and Pera (1971). Their report shows that there is a similarity solution for combined buoyancy effects. The differential equations are solved by numerical computations for Pr = Sc. The effect of increasing the Prandtl number is to reduce the velocity level, with a consequent thinning of the thermal and species diffusion boundary-layer thicknesses. Stability analysis is also used with the combined buoyancy effects and neutral stability curves are shown in a stability plane for a flow of fluid having P_r = 6.7. It appears that increasing the species diffusion effects relative to thermal flux from the plate surface has a destabilizing influence on the flow near the leading edge.

Details of the principles of transport phenomena may be found by referring to Bird (1956) and that of chemical kinetics by referring to Aris (1965). Similarity and perturbation techniques are available in the references including the authors Hansen (1964) and VanDyke (1960).

1.3   Objectives

The foregoing discussion has presented a survey of principal past studies concerning natural convection flows over semi-infinite vertical plates immersed in an ambient fluid, where the flow is induced by both heat and chemical diffusion mechanisms and is governed by the usual steady state laminar boundary-layer assumptions.

An interesting extension of this problem, and one which, with the exception of Levich (1962), has been largely neglected to date, is the study of effects caused by the inclusion of general chemical reaction of order n. In particular, it is proposed here to study the steady state behaviour of the same binary system composed of a semi-infinite plate and ambient fluid, each initially at different concentrations of a given chemical species, but between which a homogeneous irreversible isothermal chemical reaction of order n is assumed to take place.

The basic equations of natural convection required for the formulation of this problem are discussed in Chapter II. A similarity analysis of these equations is then presented in Chapter III. The problem posed by retaining a uniform concentration of the chemical species along the plate

surface is studied in Chapter IV. The equations are

reduced, using perturbation expansions, to problems

in ordinary differential equations which are then solved

by means of both numerical and analytical techniques.

Following this, direct similarity solutions of the basic

equations are presented in Chapter V for the case of

distributed concentration along the plate.

The salient results and conclusions are discussed in

detail in Chapter VI.

CHAPTER II

BASIC EQUATIONS IN NATURAL CONVECTION

The basic equations of natural convection are those given by the principles of conservation of mass (fluid), conservation of momentum and conservation of mass (species) by diffusion. The equations are written in general form:

$$\frac{\partial \rho}{\partial \theta} + \underset{\sim}{\nabla} \cdot (\rho \underset{\sim}{v}) = 0 \tag{2.1}$$

$$\rho \left[\frac{\partial \underset{\sim}{v}}{\partial \theta} + (\underset{\sim}{v} \cdot \underset{\sim}{\nabla}) \underset{\sim}{v} \right] = \rho \underset{\sim}{g} - \underset{\sim}{\nabla} p + \mu \nabla^2 \underset{\sim}{v} + \frac{\mu}{3} \underset{\sim}{\nabla} (\underset{\sim}{\nabla} \cdot \underset{\sim}{v}) \tag{2.2}$$

$$\frac{\partial c}{\partial \theta} + (\underset{\sim}{v} \cdot \underset{\sim}{\nabla}) c = \underset{\sim}{\nabla} \cdot (D \underset{\sim}{\nabla} c) + \dot{c}''' \tag{2.3}$$

where,

$$\underset{\sim}{v} = \frac{\sum \rho_i \vec{v}_i}{\sum \rho_i} = \text{average velocity}$$

ρ_i = density of the ith species

$\vec{v}_i$ = velocity of the ith species

c = concentration of the ith species

$\rho = \sum \rho_i$ = total density of the mixture

θ = time

p = static pressure

$\underset{\sim}{\nabla} \cdot (\rho \underset{\sim}{v})$ = net rate of mass efflux per unit volume

$$\rho \left\{ \frac{\partial \underset{\sim}{v}}{\partial \Theta} + (\underset{\sim}{v} \cdot \underset{\sim}{\nabla})\underset{\sim}{v} \right\} = \text{mass of fluid mixture per unit volume times acceleration}$$

$$\rho \underset{\sim}{g} = \text{gravitational force on element of fluid per unit volume}$$

$$\underset{\sim}{\nabla}p = \text{pressure force on element of fluid per unit volume}$$

$$\mu[\nabla^2\underset{\sim}{v} + 1/3\underset{\sim}{\nabla}(\underset{\sim}{\nabla}\cdot\underset{\sim}{v})] = \text{viscous force on element per unit volume}$$

$$\frac{\partial c}{\partial \Theta} = \text{rate of accumulation per unit volume}$$

$$(\underset{\sim}{v}\cdot\underset{\sim}{\nabla})c = \text{rate of transport of chemical species by bulk flow per unit volume}$$

$$\underset{\sim}{\nabla}\cdot(D\underset{\sim}{\nabla}c) = \text{rate of transport of chemical species by molecular diffusion per unit volume}$$

$$\bar{c}''' = \text{rate of generation or loss of species mass by chemical reaction per unit volume.}$$

Here $\rho = \rho(c)$ is the density variation at a given point in the flow region. All remaining symbols are defined in the nomenclature.

Boussinesq Approximation:

Expanding $\rho = \rho(c)$ about c_∞ by Taylor series expansion, keeping the pressure fixed, we have

$$\rho = \rho_\infty + (c - c_\infty)\left(\frac{\partial \rho}{\partial c}\right)_{c=c_\infty} + 0\left\{(c-c_\infty)^2\right\}$$

where ρ_∞ = density of the ambient fluid at a point away from the plate,

and c_∞ = concentration of the species at the ambient fluid. If the concentration changes from c_∞ are small such that second and lower order terms may be neglected in this expansion, then we have

$$\rho = \rho_\infty - \rho_\infty \beta^*(c-c_\infty)$$
$$= \rho_\infty\left\{1 - \beta^*(c-c_\infty)\right\}$$

where $\beta^* = -\frac{1}{\rho_\infty}\left(\frac{\partial \rho}{\partial c}\right)_{c=c_\infty}$ is defined

as mass coefficient of the volumetric expansion.

Thus, for steady flow, the continuity equation becomes

$$\nabla \cdot (\rho \underline{v}) = 0.$$

Then using $\rho = \rho_\infty\left\{1 - \beta^*(c-c_\infty)\right\}$, we have

$$\nabla \cdot [\rho_\infty\left\{1 - \beta^*(c-c_\infty)\right\}]\underline{v} = 0$$

which implies that $\rho(\nabla \cdot \underline{v}) - \rho_\infty \beta^*(\underline{v}\cdot\nabla c) = 0$

and hence $\nabla \cdot \underset{\sim}{V} = 0$ is a good approximation

provided that β^{*} is sufficiently small.

The quantity in the momentum equation is the actual

local static pressure, which may be decomposed in the

following way:

$$P = P_h + P_m$$

where P_h = hydrostatic pressure in the remote medium at rest.

P_m = pressure due to motion which is usually small
compared to P_h.

With this definition, the difference between the body

force $\rho \underset{\sim}{g}$ and the gradient of pressure ∇p in the momentum

equation is

$$\rho \underset{\sim}{g} - \nabla p = \rho \underset{\sim}{g} - \nabla P_h - \nabla P_m$$

For the body force arising from gravity acting in the

negative x direction,

$$\nabla P_h = \underset{\sim}{i} \frac{\partial P_h}{\partial x} = -\underset{\sim}{i} \rho_{\infty} g$$

where $\underset{\sim}{i}$ is the unit vector in the x-direction (c.f. Fig. 1).

Thus,

$$\rho \underset{\sim}{g} - \nabla p = - \underset{\sim}{i} g \rho_{\infty} \left\{ 1 - \beta^{*}(c - c_{\infty}) \right\} + \underset{\sim}{i} \rho_{\infty} g - \nabla P_m$$

$$= \underset{\sim}{i} g \rho_{\infty} \beta^{*}(c - c_{\infty}) - \nabla P_m$$

and the momentum equation for steady motion becomes, with $\underset{\sim}{\nabla} \cdot \underset{\sim}{V} = 0$,

$$\rho_\infty \left\{ 1 - \beta_0^*(c-c_\infty) \right\} \left\{ (\underset{\sim}{V} \cdot \underset{\sim}{\nabla})\underset{\sim}{V} \right\} = \mu \nabla^2 \underset{\sim}{V} + \underset{\sim}{i} g \rho_\infty \beta^*(c-c_\infty) - \underset{\sim}{\nabla} p_m$$

Thus for $\beta^*(c-c_\infty) \ll 1$,

$$(\underset{\sim}{V} \cdot \underset{\sim}{\nabla})\underset{\sim}{V} = \nu \nabla^2 \underset{\sim}{V} + \underset{\sim}{i} g \beta^*(c-c_\infty) - \frac{\underset{\sim}{\nabla} p_m}{\rho_\infty}$$

Thus the equations of <u>continuity</u>, <u>momentum</u> and <u>mass</u> for steady, laminar motion can be written as

<u>Continuity</u>: $\underset{\sim}{\nabla} \cdot \underset{\sim}{V} = 0$ (2.4)

<u>Momentum</u>: $(\underset{\sim}{V} \cdot \underset{\sim}{\nabla})\underset{\sim}{V} = \nu \nabla^2 \underset{\sim}{V} + \underset{\sim}{i} g \beta^*(c-c_\infty) - \frac{1}{\rho_\infty} \underset{\sim}{\nabla} p_m$ (2.5)

<u>Mass</u>: $(\underset{\sim}{V} \cdot \underset{\sim}{\nabla})c = D\nabla^2 c + \dot{c}'''$ (2.6)

The equations (2.4), (2.5) and (2.6) result from the Boussinesq approximation and apply in the case of constant viscosity μ and diffusion coefficient D.

ORDER ANALYSIS

Consider a vertical surface of height L at a uniform concentration C_0, in an extensive uniform medium at concentration C_∞. Let a characteristic length, velocity, pressure and concentration be given by L, U_c, $\rho_\infty U_c^2$ and $c_0 - c_\infty$ respectively.

Introducing the following dimensionless quantities

$$x' = \frac{x}{L}$$

$$y' = \frac{y}{L}$$

$$\underline{V} = (u,v)$$

$$u' = \frac{u}{U_c}$$

$$v' = \frac{v}{U_c}$$

$$C = \frac{c-c_\infty}{c_0-c_\infty}$$

$$P'_m = \frac{P_m}{\rho_\infty U_c^2}$$

$$(2.7)$$

into equations (2.4), (2.5) and (2.6) yields the following dimensionless equations:

Continuity: $\quad \dfrac{\partial u'}{\partial x'} + \dfrac{\partial v'}{\partial y'} = 0$ $\qquad\qquad$ (2.8)

Momentum:

$$u'\frac{\partial u'}{\partial x'} + v'\frac{\partial u'}{\partial y'} = \frac{g\beta^*L(c_0-c_\infty)}{U_c^2}c - \frac{\partial p_m'}{\partial x'}$$

$$+ \frac{\nu}{U_cL}\left(\frac{\partial^2 u'}{\partial x'^2} + \frac{\partial^2 u'}{\partial y'^2}\right) \qquad (2.9)$$

$$u'\frac{\partial v'}{\partial x'} + v'\frac{\partial v'}{\partial y'} = -\frac{\partial p_m'}{\partial y'} + \frac{\nu}{U_cL}\left(\frac{\partial^2 v'}{\partial x'^2} + \frac{\partial^2 v'}{\partial y'^2}\right) \quad (2.10)$$

Mass:

$$u'\frac{\partial c}{\partial x'} + v'\frac{\partial c}{\partial y'} = \frac{D}{LU_c}\left(\frac{\partial^2 c}{\partial x'^2} + \frac{\partial^2 c}{\partial y'^2}\right) + \frac{Lc'''}{U_c(c_0-c_\infty)} \quad (2.11)$$

Considering that $\dfrac{g\beta^*(c_0-c_\infty)L}{U_c^2} = O(1)$,

it follows that $\dfrac{U_cL}{\nu} = \sqrt{\dfrac{g\beta^*(c_0-c_\infty)L^3}{\nu^2}} = \sqrt{Gr}$.

Thus the dimensionless parameters which arise in natural convection are

Gr = Grashof number = $\dfrac{g\beta^*L^3(c_0-c_\infty)}{\nu^2}$

Sc = Schmidt number = ν/D

The quantity $\text{Gr} = \dfrac{g\beta^{*}L^{3}(c_{0}-c_{\infty})}{\nu^{2}}$ is usually called the Grashof number, which indicates a measure of the flow induced. The Grashof number is analogous to the Reynolds number of forced flow, $\text{Re} = \dfrac{U_{\infty}L}{\nu}$, with $\sqrt{\text{Gr}}$ corresponding to Re.

It was almost 30 years after the discovery of the boundary-layer concepts by Prandtl for forced flows, that Schmidt and Beckmann (1930) proved experimentally, for a flow around a heated vertical plate in air, that the boundary region is thin compared with the height of the surface. As a result, the components of gradients parallel to the surface are relatively small. Thus one is encouraged to apply the boundary-layer concept and assumptions to the general equations of the present problem.

Following the usual technique, c.f. Curle and Davies (1968), we assume that

$$
\left.
\begin{aligned}
u' &= 0(1) \\
x' &= 0(1) \\
y' &= 0(\delta, \delta_{c}) \\
v' &= 0(\delta) \\
c &= 0(1)
\end{aligned}
\right\} \qquad (2.12)
$$

where, δ is the thickness of a momentum boundary layer,

δ_c is the thickness of a concentration boundary layer,

and δ, $\delta_c \ll 1$.

Equations (2.8, (2.9), (2.10) and (2.11) are written as follows, with respective orders indicated below each term:

$$\frac{\partial u'}{\partial x'} + \frac{\partial v'}{\partial y'} = 0 \tag{2.13}$$

$\quad\quad 1 \quad\quad\quad 1$

$$u'\frac{\partial u'}{\partial x'} + v'\frac{\partial u'}{\partial y'} = c + \frac{1}{\sqrt{Gr}}\left[\frac{\partial^2 u'}{\partial x'^2} + \frac{\partial^2 u'}{\partial y'^2}\right] - \frac{\partial P_m'}{\partial x'} \tag{2.14}$$

$\quad 1 \quad 1 \quad\quad \delta \quad 1/\delta \quad\quad 1 \quad\quad\quad\quad 1 \quad\quad 1/\delta^2$

$$u'\frac{\partial v'}{\partial x'} + v'\frac{\partial v'}{\partial y'} = \frac{1}{\sqrt{Gr}}\left[\frac{\partial^2 v'}{\partial x'^2} + \frac{\partial^2 v'}{\partial y'^2}\right] - \frac{\partial P_m'}{\partial y'} \tag{2.15}$$

$\quad 1 \quad \delta \quad\quad \delta \quad 1 \quad\quad\quad\quad \delta \quad\quad 1/\delta$

$$u'\frac{\partial c}{\partial x'} + v'\frac{\partial c}{\partial y'} = \frac{1}{Sc\sqrt{Gr}}\left[\frac{\partial^2 c}{\partial x'^2} + \frac{\partial^2 c}{\partial y'^2}\right] + \frac{L\,\dot{c}'''}{U_c(c_0 - c_\infty)}$$

$$\tag{2.16}$$

$\quad 1 \quad 1 \quad\quad \delta \quad 1/\delta_c \quad\quad\quad\quad 1 \quad\quad 1/\delta_c^2$

From (2.14), it follows that, for $\delta \ll 1$,

$$\frac{\partial^2 u}{\partial x^2} \ll \frac{\partial^2 u}{\partial y^2} \; .$$

Further, if the Grashof number is large, and we assume that in the convection region near the surface, the viscous force is of the same order as the force due to convection of momentum as well as the buoyancy force, then we must have

$$\delta^2 \sqrt{Gr} = O(1)$$

$$\delta = O\left[\frac{1}{\sqrt[4]{Gr}}\right]$$

From (2.15), it is clear that all the terms are $O(\delta)$ so that

$$\frac{\partial P_m'}{\partial y'} \to 0 \qquad \text{as} \quad \delta \to 0$$

and (2.15) is equivalent to $P_m' = P_m'(x)$.

Assuming that from (2.16), we have for $\delta_c \ll 1$, $\dfrac{\partial^2 c}{\partial x'^2} \ll \dfrac{\partial^2 c}{\partial y'^2}$

and further if we assume that for sufficiently large Grashof number, $O(\delta) = O(\delta_c)$, then

$$\delta_c^2 \left[Sc \sqrt{Gr} \right] = O(1),$$

whence, $\quad \delta_C = 0 \left[\dfrac{1}{\sqrt{Sc} \quad \sqrt[4]{Gr}} \right]$.

Consideration of these results leads to the set of basic equations which are valid within a convection-layer and which have the following form:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2.17}$$

$$u\,\frac{\partial u}{\partial x} + v\,\frac{\partial u}{\partial y} = g\beta^{*}(c-c_{\infty}) + \nu\,\frac{\partial^{2} u}{\partial y^{2}} - \frac{1}{\rho_{\infty}}\frac{dp_{m}}{dx} \tag{2.18}$$

$$u\,\frac{\partial c}{\partial x} + v\,\frac{\partial c}{\partial y} = D\,\frac{\partial^{2} c}{\partial y^{2}} + \dot{c}\,''' \tag{2.19}$$

CHAPTER III

FORMULATION OF THE PROBLEM

3.1   General Statement of the Problem

We consider steady two-dimensional laminar viscous flow

over a semi-infinite vertical plate immersed in an ambient

fluid, where a homogeneous isothermal irreversible chemical

reaction of n th order is assumed to occur in the fluid,

between the chemical constituents of plate and fluid. The

following assumptions are made:

1.   The fluid is Newtonian.

2.   Two-dimensional laminar steady flow is considered.

3.   The physical properties associated with the problem
     such as viscosity, diffusivity etc. are assumed
     constant.

4.   The Boussinesq approximation is taken into con-
     sideration for buoyancy effects, which implies
     small density changes in the gravitational field.

5.   The Reaction number is assumed small.

6.   Static pressure gradients arising from the con-
     vection currents are neglected; that is, inertial
     forces in the convective flow field are assumed to
     be in balance with buoyancy and viscous forces,
     and there is no externally applied pressure gradient.

A change in chemical composition of the fluid near the

surface of the plate is considered to produce lighter fluid

there, which rises as the buoyancy force overcomes gravity resulting in an upward movement of the fluid particles (c.f. fig. 1 and 2). If a heavier fluid were produced the reverse effect would be observed but the mathematical problem would be essentially the same. The chemical species is first transferred from the plate to the ambient fluid by diffusion and then carried away by induced convection currents. A distinguishing feature of this problem is that when a chemical reaction occurs in the bulk of the fluid, the diffusing species may be depleted, whereas in problems without chemical reaction, no such effect is possible. The basic equations which govern this process derive from the following principles:

1. Conservation of mass (fluid).

2. Conservation of momentum.

3. Conservation of mass (species) - (Fick's second law of diffusion).

4. Appropriate law of chemical reaction.

The equations that are used to describe this type of flow problem have already been discussed in Chapter II and have been derived with the aid of the usual boundary-layer assumptions. These are equations(2.17) to(2.19) of Chapter II and they have incorporated the assumptions (1) to (5).

They may now be used with the appropriate chemical reaction law, for which the reaction-rate term $\dot{c}'''$ arising in the equations is described in the appendix and takes the form $\dot{c}''' = -k[c - c_\infty]^n$, where k is the reaction-rate and n is the order of reaction. Assumption (5) relates to the magnitude of k and will be discussed later. Now invoking the last assumption (6) $\frac{dp_m}{dx} \to 0$, equations (2.17) to (2.19) reduce finally to:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{3.1}$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2} + g\beta^* c \tag{3.2}$$

$$u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = D\frac{\partial^2 c}{\partial y^2} - kc^n \tag{3.3}$$

where $C = c - c_\infty$.

The relevant boundary conditions are:

at $y = 0$, $\quad u = v = 0$, $\quad \forall x$ (no slip condition)

at $y \to \infty$, $\quad u = v = 0$, $\quad \forall x$ (uniformity at ∞)

$\qquad\qquad\qquad\qquad c \to 0$, $\quad \forall x$ (uniformity at ∞) $\qquad$ (3.4)

Further, $C = c_0(x)$ is prescribed at the plate surface $y = 0$. $\qquad\qquad$ (3.5)

*Here $c_0(x)$ is a given function of x representing the concentration distribution prescribed along the plate.

For the purpose of formulating the general mathematical problem, the prescribed function $c_0(x)$ is considered to be arbitrary. In reality, however, the nature of this function may be subject to severe limitations which arise from the chemical kinetics involved in setting up steady-state conditions for a given species and ambient fluid.

Introducing the stream function $\psi(x,y)$ defined by

$$\left. \begin{aligned} u &= \frac{\partial \psi}{\partial y}, \\ v &= -\frac{\partial \psi}{\partial x}, \end{aligned} \right\} \tag{3.6}$$

equations (3.1) to (3.5) reduce to

$$\psi_y \psi_{yx} - \psi_x \psi_{yy} = \nu \psi_{yyy} + g\beta^* c \tag{3.7}$$

$$\psi_y c_x - \psi_x c_y = D c_{yy} - k c^n \tag{3.8}$$

with boundary conditions

$$y = 0: \quad \left. \begin{aligned} \psi_y &= \psi_x = 0 \\ c &= c_0(x) \end{aligned} \right\} \tag{3.9}$$

$$y \to \infty: \quad \left. \begin{aligned} \psi_y &= \psi_x = 0 \\ c &= 0 \end{aligned} \right\} \tag{3.10}$$

We shall now investigate the possibility of similarity solutions for this set of equations (c.f Hansen (1964)).

3.2   <u>Similarity analysis of Basic Equations</u>

Consider the following one-parameter transformation group.

$$
\left.
\begin{aligned}
\bar{x} &= a^m x \\
\bar{y} &= a^{n_1} y \\
\bar{\psi} &= a^p \psi \\
\bar{c} &= a^q c
\end{aligned}
\right\}
\tag{3.11}
$$

where a is a parameter and the exponents m, n_1, p and q are constants.   Then we have the following quantities:

$$
\left.
\begin{aligned}
\psi_y &= a^{-p+n_1} \ \bar{\psi}_{\bar{y}} \\[4pt]
\psi_{yy} &= a^{-p+2n_1} \ \bar{\psi}_{\bar{y}\bar{y}} \\[4pt]
\psi_{yyy} &= a^{-p+3n_1} \ \bar{\psi}_{\bar{y}\bar{y}\bar{y}} \\[4pt]
\psi_x &= a^{-p+m} \ \bar{\psi}_{\bar{x}} \\[4pt]
\psi_{yx} &= a^{-p+m+n_1} \ \bar{\psi}_{\bar{y}\bar{x}} \\[4pt]
c_x &= a^{-q+m} \ \bar{c}_{\bar{x}} \\[4pt]
c_y &= a^{-q+n_1} \ \bar{c}_{\bar{y}} \\[4pt]
c_{yy} &= a^{-q+2n_1} \ \bar{c}_{\bar{y}\bar{y}}
\end{aligned}
\right\}
\tag{3.12}
$$

Substituting (3.12) into (3.7) and (3.8), after simplification we have,

$$\overline{\Psi}_{\overline{y}}\,\overline{\Psi}_{\overline{y}\overline{x}} - \overline{\Psi}_{\overline{x}}\,\overline{\Psi}_{\overline{y}\overline{y}} = \nu a^{p-m+n_1}\,\overline{\Psi}_{\overline{y}\overline{y}\overline{y}} + a^{-q+2p-2n_1-m}\,g\beta^{*}c \qquad (3.13)$$

$$\overline{\Psi}_{\overline{y}}\,\overline{c}_{\overline{x}} - \overline{\Psi}_{\overline{x}}\overline{c}_{\overline{y}} = Da^{n_1-m+p}\,\overline{c}_{\overline{y}\overline{y}} - ka^{-nq+p+q-n_1-m}\,\overline{c}^{\,n} \qquad (3.14)$$

If (3.13) and (3.14) are invariant under the transformation group (3.11), then one must have,

$$\left. \begin{array}{l} p = m - n_1 \\[2mm] q = n - 4n_1 \\[2mm] \dfrac{m}{n_1} = \dfrac{6-4n}{1-n} \end{array} \right\} \qquad (3.15)$$

Now consider the following group of the independent variables:

$$\overline{x}^{\alpha}\,\overline{y}^{\beta} = a^{\alpha m + \beta n_1}\,(x^{\alpha}y^{\beta})$$

This group will be invariant if $\quad \alpha = -\beta/\gamma$

where $\quad \gamma = \dfrac{m}{n_1} = \dfrac{6-4n}{1-n}$ $\qquad\qquad$ (3.16)

Thus we have the following possible similarity variables:

$$\eta(x,y) = k_1 e^{-k_2\left(yx^{-1/\gamma}\right)^{\beta}} \tag{3.17}$$

$$\eta(x,y) = k_2\left(yx^{-1/\gamma}\right)^{\beta} \tag{3.18}$$

where k_1, k_2 and β are arbitrary constants.

Next consider the complete group with respect to the stream function $\psi(x,y)$.

$$\bar{x}^{\mu_1}\bar{y}^{\mu_2}\bar{\psi}^{\mu_3} = a^{\mu_1 m + \mu_2 n_1 + \mu_2 p}\left(x^{\mu_1}y^{\mu_2}\psi^{\mu_3}\right)$$

This group will be invariant if $\quad \mu_3 = -\dfrac{\mu_2 + \gamma\mu_1}{\gamma - 1}$

Without loss of generality, choosing $\mu_2 = 0$, $\mu_1 = 1$, one can write the transformation of the stream function $\psi(x,y)$ as follows:

$$\psi(x,y) = \lambda_1 x^{\frac{\gamma - 1}{\gamma}} f_1(\eta) \tag{3.19}$$

where λ_1 is an arbitrary constant and $f_1(\eta)$ is a function of η alone.

Similarly, we can write the transformation of the concentration-distribtuion as follows:

$$c(x,y) = \lambda_2 x^{\frac{\gamma - 4}{\gamma}} f_2(\eta) \tag{3.20}$$

where λ_2 is an arbitrary constant, and $f_2(\eta)$ is another function of η alone.

These general transformation groups (3.17), (3.18), (3.19) and (3.20) are found to be valid except for the following orders of reaction: $n = 1$, 3/2 and 5/3.

Using relations (3.17), (3.19) and (3.20), the boundary conditions (3.9) and (3.10) imply the following:

at $\eta = 0$:

$$\left. \begin{array}{l} f_1(0) = 0 \\ f_2(0) = 0 \end{array} \right\} \qquad (3.21)$$

at $\eta = K_1$:

$$\left. \begin{array}{l} f_1(K_1) = 0 \\ f_1'(K_1) = 0 \\ f_2(K_1) = \dfrac{1}{\lambda_2}\left[x^{\frac{4-\gamma}{\gamma}} c_0(x)\right] \end{array} \right\} (3.22)$$

Also using relations (3.18), (3.19) and (3.20), the boundary conditions (3.9) and (3.10) would require that

at $\eta = 0$:

$$\left. \begin{array}{l} f_1(0) = 0 \\ f_1'(0) = 0 \\ f_2(0) = \dfrac{1}{2}\left[x^{\frac{4-\gamma}{\gamma}} c_0(x)\right] \end{array} \right\} (3.23)$$

and at $\eta = \infty$:

$$\left. \begin{array}{l} f_1(\infty) = 0 \\ f_2(\infty) = 0 \end{array} \right\} \qquad (3.24)$$

Thus for $\beta \neq 1$, with the transformations (3.17), (3.19) and (3.20), the following ordinary differential equations result:

$$\lambda_1 K_2 \,\beta \left(\frac{\gamma-2}{\gamma}\right)\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}^{\frac{1+\beta}{\beta}} \cdot (\eta f_1')^2$$

$$+ \lambda_1(\beta-1)\left(\frac{\gamma-1}{\gamma}\right)\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}^{1/\beta} \eta f_1 f_1'$$

$$- \lambda_1 K_2 \beta \left(\frac{\gamma-1}{\gamma}\right)\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}^{\frac{1+\beta}{\beta}} \left\{\eta f_1 f_1' + \eta^2 f_1 f_1''\right\}$$

$$= -\nu\left[(\beta-1)(\beta-2)\,\eta f_1' - 3K_2\beta(\beta-1)\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}\left\{\eta f_1 + \eta^2 f_1\right\}\right.$$

$$\left. + K_2^2\,\beta^2\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}^2 \left\{\eta f_1' + 3\eta^2 f_1'' + \eta^3 f_1'''\right\}\right]$$

$$+ \frac{g\beta^* \lambda_2}{\lambda_1 K_2 \beta}\left\{- \frac{\ln(\eta/K_1)}{K_2}\right\}^{\frac{3-\beta}{\beta}} f_2 \qquad\qquad (3.25)$$

$$\lambda_1 \lambda_2 K_2^\beta \left\{ -\frac{\ln(\eta/K_1)}{K_2} \right\}^{\frac{\beta-1}{\beta}} \left\{ \frac{\gamma-1}{\gamma} \eta f_1 f_2' - \left(\frac{\gamma-4}{\gamma}\right) \eta f_1' f_2 \right\}$$

$$= - D\lambda_2^\beta K_2 \left[(\beta-1) \left\{ -\frac{\ln(\eta/K_1)}{K_2} \right\}^{\frac{\beta-2}{\beta}} \eta f_2' \right.$$

$$\left. - K_2^\beta \left\{ -\frac{\ln(\eta/K_1)}{K_2} \right\}^{\frac{2\beta-2}{\beta}} \left\{ \eta f_2' + \eta^2 f_2'' \right\} \right]$$

$$- k \lambda_2^n f_2^n \qquad (3.26)$$

For $\beta = 1$, equations (3.25) and (3.26) reduce to the following simpler forms:

$$f_1' + 3\eta^2 f_1'' + \eta^3 f_1''' - f_2$$

$$+ \left[\frac{\gamma-2}{\gamma} (\eta f_1')^2 - \frac{\gamma-1}{\gamma} \left\{ \eta f_1 f_1' + \eta^2 f_1 f_1'' \right\} \right] = 0 \qquad (3.27)$$

$$\frac{1}{Sc} \left[\eta f_2' + \eta^2 f_2'' \right] + \frac{\gamma-4}{\gamma} \eta f_1' f_2$$

$$- \frac{\gamma-1}{\gamma} \eta f_1 f_2' - \frac{k \lambda_2^{n-3/2}}{\sqrt{g\beta^*}} f_2^n = 0 \qquad (3.28)$$

The boundary conditions for equations (3.25), (3.26), or (3.27) and (3.28) are given by (3.21) and (3.22). Again for $\beta \neq 1$, with the transformations (3.18), (3.19) and (3.20), the following ordinary differential equations result:

$$\nu_E \beta^2 f_1''' = 2\beta(2-n)\eta^{\frac{1-\beta}{\beta}} f_1'^2 - (\beta-1)(5-3n)\eta^{\frac{1-2\beta}{\beta}} f_1 f_1'$$

$$- \beta(5-3n)\eta^{\frac{1-\beta}{\beta}} f_1 f_1''$$

$$- \nu_E \left[(\beta-1)(\beta-2)\eta^{-2}f_1' + 3\beta(\beta-1)\eta^{-1}f_1'' \right]$$

$$- g\beta^* M \eta^{\frac{3(1-\beta)}{\beta}} f_2 \qquad (3.29)$$

$$D_E \beta f_2'' = \eta^{\frac{1-\beta}{\beta}} \left[2f_1' f_2 + (3n-5)f_1 f_2' \right]$$

$$- D_E(\beta-1)\eta^{-1} f_2' + k\, G \eta^{2\frac{(1-\beta)}{\beta}} f_2^n \qquad (3.30)$$

where

$$E = \frac{K_2^{1/\beta}(6-4n)}{\lambda_1}$$

$$M = \frac{\lambda_2(6-4n)}{\beta \lambda_1^2 K_2^{2/\beta}}$$

$$G = \frac{\lambda_2^{n-1}(6-4n)}{\beta \lambda_1 K_2^{1/\beta}}$$

For $\beta = 1$, equations (3.29) and (3.30) reduce to the following simpler forms:

$$f_1''' + f_2 + \frac{\gamma-1}{\gamma} f_1 f_1'' - \frac{\gamma-2}{\gamma} f_1'^2 = 0 \qquad (3.31)$$

$$\frac{1}{Sc} f_2'' + \frac{\gamma-1}{\gamma} f_1 f_2' - \frac{\gamma-4}{\gamma} f_1' f_2 - \frac{k \lambda_2^{n-1}}{\nu K_2^2} f_2^n = 0 \qquad (3.32)$$

The boundary conditions for (3.29) and (3.30) or for (3.31) and (3.32) are given by (3.23) and (3.24).

Examination of the boundary conditions (3.22) and (3.23) reveals that similarity analysis based on the transformation group (3.11) is not meaningful when

(a) $C_{j0}(x)$ = Constant (uniform concentration along the plate)

(b) $C_0(x) = F(x)$ (the most general condition
where F is an arbitrary function
of x alone)

However, a tractible problem is obtained provided that

$$C_0(x) = N x^{\frac{\gamma - 4}{\gamma}}$$ (3.33)

where N is some given constant.

It appears from these results that a formal simplification of the problem using similarity analysis (with the simplest transformation group (3.11)), that is, a precise definition of the problem in terms of ordinary differential equations, is possible only if the initial concentration is described along the plate according to (3.33). This would be useful in the case where the prescribed distribution approximates a simple power law where form depends on the particular order of reaction of the system. In practice, depending on the particular chemical constituents chosen, it may or may not be possible to achieve and maintain in steady-state a concentration distribution along the plate in accordance with (3.33), such as to permit useful application of this approach. The mathematical treatment is valid, however, and some theoretical inferences may be of considerable academic interest.

CHAPTER IV

UNIFORM CONCENTRATION AT THE PLATE

We consider that a vertical plate composed of species A has been immersed in a fluid at rest with uniform density and viscosity. We will assume that the concentration of A in the solution at the plate surface is maintained (by some suitable external means) at a uniform concentration c_0. Concentration differences between the plate and the ambient fluid will induce convection-diffusional flow and we assume that steady-state conditions have been attained.

During this process, the species A and the fluid B will react chemically with each other. The primary objective in this study is to show the effect of this reaction upon the mass transfer and the natural convection flow which ensues.

4.1   <u>The Perturbation Method</u>

The differential equations which describe the steady-state behaviour of the system described above and which incorporate the assumptions listed in Chapter III can be written as

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad , \tag{4.1}$$

$$u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2} + g\beta^*(c - c_\infty) \quad , \tag{4.2}$$

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2} + \dot{c}''' \quad . \tag{4.3}$$

The appropriate boundary conditions are:

at $y = 0$: $\left. \begin{array}{l} u = v = 0 \\ \\ c = c_0 \end{array} \right\}$ (4.4)

at $y \rightarrow \infty$: $\left. \begin{array}{l} u = v = 0 \\ \\ c = c_\infty \end{array} \right\}$ (4.5)

A stream function $\psi(x,y)$ is introduced to satisfy the continuity equation (4.1). Also, as described in the appendix, $\dot{c}'''$ may be replaced with the appropriate reaction

rate function, and the governing equations become

$$u = \frac{\partial \psi}{\partial y} ,$$

$$v = -\frac{\partial \psi}{\partial x} . \quad\quad\quad (4.6)$$

$$\psi_y \psi_{yx} - \psi_x \psi_{yy} = \nu \psi_{yyy} + g\beta^*(c - c_\infty), \quad\quad (4.7)$$

$$\psi_y c_x - \psi_x c_y = D c_{yy} - k(c - c_\infty)^n, \quad\quad (4.8)$$

with boundary conditions

$$y = 0: \quad\quad \psi_y = \psi_x = 0,$$

$$c = c_0 , \quad\quad\quad (4.9)$$

$$y \to \infty \quad\quad \psi_y = \psi_x = 0,$$

$$c = c_\infty . \quad\quad\quad (4.10)$$

Introducing the transformations

$$C = \frac{c - c_\infty}{c_0 - c_\infty} , \quad\quad\quad (4.11)$$

$$\eta(x,y) = \frac{y}{x} \left\{ \frac{G_{rx}}{4} \right\}^{1/4} , \quad\quad\quad (4.12)$$

$$\psi(x,y) = 4\nu\left\{\frac{G_{rx}}{4}\right\}^{1/4} f(\eta) , \qquad (4.13)$$

where
$$Gr_x = \frac{g\beta^* x^3(c_0 - c_\infty)}{\nu^2} \qquad (4.14)$$

which may be called the local Grashof number, equations (4.7) and (4.8) reduce to

$$\frac{d^3f}{d\eta^3} + c + 3f\frac{d^2f}{d\eta^2} - 2\left(\frac{df}{d\eta}\right)^2 = 0 \qquad (4.15)$$

and
$$\frac{1}{Sc}\frac{d^2c}{d\eta^2} + 3f\frac{dc}{d\eta} - \epsilon(x)\, c^n = 0 , \qquad (4.16)$$

where
$$\epsilon(x) = \frac{2k(c_0 - c_\infty)^{n-3/2}}{\sqrt{g\beta^*}}\, x^{1/2} \qquad (4.17)$$

and $Sc = \nu/D$, which is called the Schmidt number.

Use of the transformations (4.11), (4.12) and (4.13) reveals that the partial differential equations (4.7) and (4.8) nearly reduce to ordinary differential equations in the variable η excepting for one coefficient $\epsilon(x)$ which remains dependent on x. This coefficient may be termed the local reaction-rate number and may be considered arbitrarily small depending on the slowness of the reaction. Hence

for $\epsilon = 0$, the similarity analysis is complete and
equations (4.15) and (4.16) may be assumed to admit a
solution $C = C_0(\eta)$ and $f = f_0(\eta)$. In the case
$\epsilon \neq 0$, if the reaction-rate is such that

$$\frac{k^2(c_0 - c_\infty)^{2n-3}}{g\beta^*} = O(\xi)$$

for some $\xi > 0$, a solution may be possible by perturbation-
expansion about $\epsilon(x)$ of order ξ, provided attention is
confined to the region downstream of the leading edge
given by $0 < x \leqslant \xi$

We therefore rewrite the transforms as follows:

$$C(x,y) = C(\eta,\epsilon) \qquad (4.19)$$

$$\psi(x,y) = 4\nu\left\{\frac{Gr_x}{4}\right\}^{1/4} f(\eta,\epsilon) \qquad (4.20)$$

where

$$\eta(x,y) = \frac{y}{x}\left\{\frac{Gr_x}{4}\right\}^{1/4} \qquad (4.21)$$

and $\quad \epsilon(x) = \frac{2k(c_0 - c_\infty)^{n-3/2)}}{\sqrt{g\beta^*}} x^{1/2} \qquad (4.22)$

Thus we have the following derivatives:

$$\psi_y = 4\nu \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{1/2} x^{1/2} f_\eta \qquad (4.23)$$

$$\psi_{yy} = 4\nu \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{3/4} x^{1/4} f_{\eta\eta} \qquad (4.24)$$

$$\psi_{yyy} = 4\nu \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\} f_{\eta\eta\eta} \qquad (4.25)$$

$$\psi_x = 3\nu \left\{ \frac{g\beta(c_0 - c_\infty)}{4\nu^2} \right\}^{1/4} x^{-1/4} f$$

$$- \nu y \, x^{-1/2} \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\} f_\eta$$

$$+ \frac{4\nu k (c_0 - c_\infty)^{n-5/2}}{\sqrt{g\beta^*}} \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{1/4} f_\epsilon \quad (4.26)$$

$$\psi_{yx} = 2\nu x^{-1/2} \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{1/2} f_\eta$$

$$- \nu y \, x^{-3/4} \left\{ \frac{g\beta(c_0 - c_\infty)}{4^2} \right\}^{3/4} f_{\eta\eta}$$

$$+ \frac{4\nu k (c_0 - c_\infty)^{n-1}}{\sqrt{4\nu^2}} f_{\eta\epsilon} \qquad (4.27)$$

$$c_x = -\frac{1}{4} y\, x^{-5/4} \left\{ \frac{g\beta^*(c_0' - c_\infty)}{4\nu^2} \right\}^{1/4} c_\eta$$

$$+ \frac{k(c_0 - c_\infty)^{n-3/2}}{\sqrt{g\beta^*}} x^{-1/2} c_\epsilon \qquad (4.28)$$

$$c_y = x^{-1/4} \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{1/4} c_\eta \qquad (4.29)$$

$$c_{yy} = \left\{ \frac{g\beta^*(c_0 - c_\infty)}{4\nu^2} \right\}^{1/2} x^{-1/2} c_{\eta\eta} \qquad (4.30)$$

Introducing these derivatives into equations (4.7) and (4.8) results in

$$f_{\eta\eta\eta} + c + 3ff_{\eta\eta} - 2f_\eta^2 + 2\epsilon \left\{ f_\epsilon f_{\eta\eta} - f_\eta f_{\eta\epsilon} \right\} = 0 \qquad (4.31)$$

and

$$\frac{c_{\eta\eta}}{Sc} + 3fc_\eta + \epsilon \left\{ 2f_\epsilon c_\eta - 2f_\eta c_\epsilon - c^n \right\} = 0 \qquad (4.32),$$

and the following perturbation scheme about ϵ may be employed:

$$f(\eta, \epsilon) = f_0(\eta) + \epsilon f_1(\eta) + \epsilon^2 f_2(\eta) + \cdots \qquad (4.33)$$

$$c(\eta, \epsilon) = c_0(\eta) + \epsilon c_1(\eta) + \epsilon^2 c_2(\eta) + \cdots \qquad (4.34)$$

Substituting (4.33) and (4.34) into (4.31) and (4.32)
results in the following sets of ordinary differential
equations for each order of ϵ:

The zeroth-order approximation:

$$f_0''' + c_0 + 3f_0 f_0'' - 2f_0'^2 = 0 \tag{4.35}$$

$$c_0'' + 3Scf_0 c_0' = 0 \tag{4.36}$$

The first-order approximation:

$$f_1''' + c_1 + 5f_1 f_0'' + 3f_0 f_1'' - 6f_0' f_1' = 0 \tag{4.37}$$

$$c_1 + Sc\left\{5f_1 c_0' + 3f_0 c_1' - 2c_1 f_0' - c_0^n\right\} = 0 \tag{4.38}$$

The second-order approximation:

$$f_2''' + c_2 + 3f_0 f_2'' + 7f_0'' f_2 - 8f_0' f_2' = 4f_1'^2 - 5f_1 f_1'' \tag{4.39}$$

$$\frac{c_2''}{Sc} + 3f_0 c_2' - 4f_0' c_2 + 7f_2 c_0' = 2f_1' c_1 + n c_1 c_0^{n-1} - 5f_1 c_1' \tag{4.40}$$

The third-order approximation:

$$f_3''' + c_3 + 3f_0 f_3'' + 9f_0'' f_3 - 10f_0' f_3'$$
$$= 10f_1' f_2' - 5f_1 f_2'' - 7f_1'' f_2 \tag{4.41}$$

$$\frac{c_3''}{Sc} + 3f_0c_3' + 5f_1c_2' + 7f_2c_1' + 9f_3c_0'$$

$$- 6f_0'c_3 - 4f_1'c_2 - 2f_2'c_1 \qquad \Big)$$

$$= nc_2c_0^{n-1} + \frac{n(n-1)}{2!} c_1^2 c_0^{n-2} \qquad (4.42)$$

The mth approximation:

$$f_m''' + c_m + \sum_{r=0}^{m} (2r + 3) f_r f_{m-r}''$$

$$- 2 \sum_{r=0}^{m} (m - r + 1) f_r' f_{m-r}' = 0 \qquad (4.43)$$

$$\frac{c_m''}{Sc} + \sum_{r=0}^{m} (2r + 3)f_r c_{m-r}' - 2 \sum_{r=0}^{m} (m-r)f_r' c_{m-r}$$

$$= \text{Coefficient of } \epsilon^{m-1} \text{ in the expansion of}$$

$$\Big\{ c_0 + \epsilon c_1 + \ldots + \epsilon^{m-1} c_{m-1} \Big\}^n \qquad (4.44)$$

The boundary conditions may be written as

$$\left. \begin{array}{ll} f_r(0) & = \ 0 \\[4pt] f_r'(0) & = \ 0 \\[4pt] c_0(0) & = \ 1 \\[4pt] c_{r+1}(0) = 0 \end{array} \right\} \quad \eta = 0 \qquad (4.45)$$

$$f'_r(\infty) = c_r(\infty) = 0 \qquad \eta \to \infty$$

$$(4.46)$$

$$r = 0, 1, 2, 3, \ldots m.$$

Here the prime denotes differentiation with respect to η.

The zeroth-order approximations describe the stream function and the concentration distribution without chemical reaction, whereas the higher order approximations describe these distributions when chemical reaction is present in the system.

$$(1-Z) \, G_0'' - G_0' + 3Sc \, F_0 \, G_0' = 0 \qquad (4.54)$$

and the initial conditions

$$
\left.
\begin{array}{rcl}
F_0(0) & = & 0 \\[4pt]
F_0'(0) & = & 0 \\[4pt]
F_0''(0) & = & A \\[4pt]
G_0(0) & = & 1 \\[4pt]
G_0'(0) & = & B
\end{array}
\right\} \qquad \text{at} \quad Z = 0 \qquad (4.55)
$$

A and B are constants representing the extra (but unknown) required initial conditions, which may be evaluated such that the asymptotic boundary conditions

$$
\begin{array}{l}
F_0' \longrightarrow 0 \\[8pt]
G_0 \longrightarrow 0
\end{array}
\qquad (4.56)
$$

are satisfied as $Z \longrightarrow 1$.

The Taylor series about $Z = 0$ have been constructed up to the order Z^{11} as follows,

$$
\begin{aligned}
F_0(Z) = A \, \frac{Z^2}{2!} \; + \; \frac{(3A-1)}{3!} \, Z^3 + (11 \, A - B - 6) \, \frac{Z^4}{4!} \\[10pt]
+ \, (A^2 + 50A - 10B - 35) \, \frac{Z^5}{5!} \\[10pt]
+ \, (15A^2 + 274A - 85B - 225) \, \frac{Z^6}{6!}
\end{aligned}
$$

$$+ (17A^2 + 1764A - 735B - 1624 + 3ScAB + 5AB)\ \frac{z^7}{7!}$$

$$+ (-13A^3 + 1960A^2 + 13068A - 6774B - 13132 + 84ScAB$$

$$+ 140AB - 3ScB)\ \frac{z^8}{8!}$$

$$+ (-468A^3 + 22467A^2 + 109584A - 6764B_2 - 118124$$

$$+ 1638ScAB + 2730AB - 108ScB - 3ScB^2 - 5B^2)\ \frac{z^9}{9!}$$

$$+ (-10210A^3 + 324435A^2 + 958076A - 718530B - 1151700$$

$$+ 28350\,ScAB + 31250AB - 2610ScB - 135ScB^2 + 775B^2$$

$$- 111\,ScBA^2 - 90Sc^2A^2B - 262\,A^2B)\ \frac{z^{10}}{10!} + 0(z^{11}) \quad (4.57)$$

$$G_0 = 1 + BZ + \frac{BZ^2}{2!} + (2B)\frac{z^3}{3!} + (6B - 3ScAB)\ \frac{z^4}{4!}$$

$$+ (24B - 30ScAB + 3ScB)\ \frac{z^5}{5!}$$

$$+ (120B - 255ScAB + 45ScB + 3ScB^2)\ \frac{z^6}{6!}$$

$$+ (720B - 2205ScAB + 525ScB + 63ScB^2 - 3ScBA^2$$

$$+ 90Sc^2A^2B)\ \frac{z^7}{7!}$$

$$+ (5040B - 20307ScAB + 5880ScB + 966ScB^2 - 84ScBA^2$$

$$+ 2520Sc^2A^2B - 315Sc^2AB)\ \frac{z^8}{8!}$$

$$+ (40320B - 201852ScAB + 67347ScB + 13608ScB^2$$

$$- 1638ScBa^2 - 15ScAB^2 + 49140Sc^2A^2B - 11340Sc^2AB$$

$$- 513Sc^2B^2A + 315Sc^2B) \frac{z^9}{9!}$$

$$+ (362880B - 2170340ScAB + 807975ScB + 189834ScB^2$$

$$- 28340ScBA^2 - 675ScAB^2 + 39ScA^3B + 850500ScA^2B$$

$$- 273420Sc^2AB - 23085Sc^2B^2A + 14175Sc^2B + 756Sc^2A^3B$$

$$- 7560Sc^3A^3B + 1143Sc^2B^2) \frac{z^{10}}{10!} + O(z^{11}) \qquad (4.58)$$

Here A and B are obtained by applying the conditions
(4.56), (4.57) and (4.58).

The following numerical values of A and B have been
obtained for the indicated values of the Schmidt numbers Sc.

Sc	A	$-B$
0.01	1.7370415	0.346431
0.72	1.4745512	1.3404531
1.0	1.2300844	2.21663
2.0	0.643657	4.11492

Table I: Series solution up to z^{10}

Sc	A	−B
0.01	0.587793	0.368832
0.72	0.570367	0.440012
1.00	0.562434	0.472388
2.00	0.529362	0.607107

Table 2:   Series solution up to z^8

Sc	A	−B
0.01	0.4902845	0.4086164
0.72	0.485261	0.443084
1.00	0.4830848	0.458013
2.00	0.4742812	0.518398

Table 3:   Series solution up to z^6

It should be noted that these values are to be interpreted as having validity for the approximating Taylor expansions, only in a neighbourhood of $z = 0$ ($\eta = 0$) and not for the full range $0 \leqslant z \leqslant 1$ ($0 \leqslant \eta \leqslant \infty$).

Solution of the first-order approximation:

Let $\quad f_1(\eta) = F_1(z)$

$$c_1'(\eta) = G_1(z) \tag{4.59}$$

where $\quad z = 1 - e^{-\eta}$

Introducing (4.59) into equations (4.37) and (4.38) one obtains the following differential equations with their initial and asymptotic boundary conditions:

$$(1-z)^3 F_1''' - 3(1-z)^2 F_1'' + (1-z)F_1' + G_1$$

$$+ 5 F_1 \left\{ (1-z)^2 F_0'' - (1-z)F_0' \right\}$$

$$+ 3F_0 \left\{ (1-z)^2 F_1'' - (1-z)F_1' \right\} - 6(1-z)^2 F_0' F_1' = 0 \tag{4.60}$$

$$(1-z)^2 G_1'' - (1-z)G_1' + Sc \left\{ 5(1-z)G_0' F_1 \right.$$

$$\left. + 3(1-z) F_0 G_1' - 2(1-z)F_0' G_1 - G_0^n \right\} = 0 \tag{4.61}$$

The initial conditions are:

$$\left. \begin{array}{l} F_1'(0) = 0 \\ F_1''(0) = 0 \\ F_1(0) = A_1 \\ G_1(0) = 0 \\ G_1'(0) = B_1 \end{array} \right\} \qquad \text{at} \quad z = 0 \tag{4.62}$$

The asymptotic conditions are:

$$F_1'(1) \longrightarrow 0$$
$$G_1(1) \longrightarrow 0 \qquad\qquad\qquad (4.63)$$

as $z \longrightarrow 1$.

Here, A_1 and B_1 are the unknown initial conditions at the surface of the plate.

The Taylor series about $z = 0$ have been constructed up to the order z^6 as follows:

$$F_1(z) = \frac{A_1 z^2}{2!} + (3A_1) \frac{z^3}{3!} + (11A_1 - B_1) \frac{z^4}{4!}$$
$$+ (50A_1 - 10B_1 + 12AA_1 - Sc) \frac{z^5}{5!} + 0(z^6) \qquad (4.64)$$

$$G_1(z) = B_1 z + (B_1 + Sc) \frac{z^2}{2!} + \left\{ 2B_1 + Sc(3 + nB) \right\} \frac{z^3}{3!}$$

$$+ [6 B_1 + Sc \left\{ n(n-1)B^2 + 6nB + AB_1 - 5BA_1 + 11 \right\}] \frac{z^4}{4!}$$

$$+ [24B_1 + Sc \left\{ n(n-1)(n-2)B^3 + 10n(n-1)B^2 \right.$$

$$+ 35nB + 10AB_1 - 50A_1 B - 3B_1 \}$$

$$+ 3Sc^2(2A-3)] \frac{z^5}{5!} + 0(z^6) \qquad (4.65)$$

Solution of the Second-order approximation:

Let
$$f_2(\eta) = F_2(z)$$
$$c_2(\eta) = G_2(z)$$
where $z = 1 - e^{-\eta}$ \qquad (4.66)

By using (4.66), equations (4.39) and (4.40) can be transformed to the following differential equations with their initial and asymptotic boundary conditions:

$$(1-z)^3 F_2''' - 3(1-z)^2 F_2'' + (1-z)F_2' + G_2$$
$$+ 3 F_0 \left\{ (1-z)^2 F_2'' - (1-z)F_2' \right\}$$
$$- 8(1-z)^2 F_0' F_2' + 7F_2 \left\{ (1-z)^2 F_0'' - (1-z)F_0' \right\}$$
$$= 4(1-z)^2 F_1'^2 - 5F_1 \left\{ (1-z)^2 F_1'' - (1-z)F_1' \right\} \qquad (4.67)$$

$$\frac{1}{Sc} \left\{ (1-z)^2 G_2'' - (1-z)G_2' \right\} + 3F_0(1-z)G_2'$$
$$- 4(1-z)F_0' G_2 + 7(1-z)F_2 G_0'$$
$$= 2(1-z)G_1 F_1' - 5(1-z)F_1 G_1' + nG_1 G_0^{n-1} \qquad (4.68)$$

The initial conditions are:

$$F_2(0) = 0$$
$$F_2'(0) = 0$$
$$F_2''(0) = A_2$$
$$G_2(0) = 0$$
$$G_2'(0) = B_2$$

$$\text{at } z = 0 \qquad (4.69)$$

The asymptotic conditions are:

$$F_2'(1) \longrightarrow 0$$
$$G_2(1) \longrightarrow 0$$
(4.70)

$$\text{as} \quad Z \longrightarrow 1$$

Here A_2 and B_2 are the assumed initial conditions at the surface of the plate.

The Taylor series about $Z = 0$ have been constructed as follows:

$$F_2(Z) = A_2 \frac{z^2}{2!} + (3 A_2) \frac{z^3}{3!} + (11A_2 - B_2) \frac{z^4}{4!}$$

$$\left\{ (50 + 6A)A_2 - 10B_1 + 3A_1^2 \right\} \frac{z^5}{5!} + 0(z^6) \qquad (4.71)$$

$$G_2(Z) = B_2 Z + B_2 \frac{z^2}{2:} + \left\{ 2B_2 + nSc\, B_1 \right\} \frac{z^3}{3!}$$

$$[6B_2 + 5nScB_1 + Sc \left\{ 5AB_2 - 7BA_2 \right.$$

$$\left. + A_1 B_1 + 2n(n-1)BB_1 \right\}] \frac{z^4}{4!} + 0(z^5) \qquad (4.72)$$

The unknown quantities A_1, B_1 and A_2, B_2 are all determined by using the conditions (4.63) and (4.70) in terms of Sc, n, A and B. The values of A_1, B_1, and A_2, B_2 are given by,

$$A_1 = \left[Sc \left\{ 2036 + 1190\, B\, n + 210n\,(n-1)B^2 \right. \right.$$

$$\left. \left. + 14n(n-1)(n-2)B^3 \right\} + 3Sc^2(23A - 41) \right]$$

$$\Big/ \left\{ 1050\ Sc\ B - (154 + 12A)(274 + Sc(15A - 3)) \right\} \tag{4.73}$$

$$B_1 = \frac{(154 + 12A)A_1 - Sc}{14} \tag{4.74}$$

$$A_2 = \frac{14B_2 - 3A_1^2}{154 + 6A} \tag{4.75}$$

$$B_2 = Sc \left[21BA_1^2 + (154 + 6A) \left\{ 9nB_1 + A_1B_1 \right. \right.$$

$$\left. \left. + 2n(n-1)BB_1 \right\} \right] \Big/ \left[98ScB \right.$$

$$\left. - (50 + 5Sc\ A)(154 + 6A) \right] \tag{4.76}$$

4.3   <u>Numerical Solution</u>

Equations (4.35), (4.36), (4.37), and (4.38) with their appropriate boundary conditions (4.45) and (4.46) have been integrated numerically for various Schmidt numbers and reaction orders using a Runge-Kutta integration program in conjunction with the Nacht Sheim-Swigert technique (1965) to correct for assumed starting values of the initial conditions at the surface. The results, therefore, will be restricted to the first-order approximation in the basic perturbation expansions.

The general forms of the equations to be treated are:

$$f'''(\eta) = F(f'', f', g', f, g, \eta) \qquad (4.77)$$

$$g''(\eta) = G(f'', f', g', f, g, \eta) \qquad (4.78)$$

with initial and asymptotic boundary conditions.

$$\eta = 0, \qquad \begin{aligned} f(0) &= f'(0) = 0 \\ g(0) &= 1 \end{aligned} \Bigg\} \qquad (4.79)$$

and

$$\eta \longrightarrow \infty \qquad \begin{aligned} f'(\infty) &\longrightarrow 0 \\ g(\infty) &\longrightarrow 0 \end{aligned} \Bigg\} \qquad (4.80)$$

With two asymptotic boundary conditions it is necessary to assume starting values for two additional initial conditions i.e. let

$$A = f''(0) \tag{4.81}$$

$$B = g'(0) \tag{4.82}$$

and it is required that

as $\lim_{\eta \to \infty} f'(A,B,\eta) = f'_\infty(A,B) = 0$ \hfill (4.83)

$$\lim_{\eta \to \infty} g(A,B,\eta) = g_\infty(A,B) = 0 \tag{4.84}$$

Suppose that A_1 and B_1 are trial values for A and B such that

$$A = A_1 + h$$

$$B = B_1 + k$$

Where h and k are small, and thus we have by (4.83) and (4.84) that

$$f'_\infty(A_1 + h, B_1 + k) = 0 \tag{4.85}$$

$$g_\infty(A_1 + h, B_1 + k) = 0 \tag{4.86}$$

Also to satisfy the asymptotic boundary conditions, we assume that the gradients of (4.85) and (4.86) must be zero at infinity.

Thus we have

$$f_{\infty}''(A_1 + h, B_1 + k) = 0 \qquad\qquad (4.87)$$

$$g_{\infty}'(A_1 + h, B_1 + k) = 0 \qquad\qquad (4.88)$$

By applying Taylor series expansions for small h and k to the equations (4.85) to (4.88) and truncating the higher order terms including $O(h^2)$ and $O(k^2)$ we have the following four equations for two unknowns h and k.

$$f_{\infty}'(A,B) + h\,\frac{\partial f_{\infty}'}{\partial A} + k\,\frac{\partial f_{\infty}'}{\partial B} = 0 \qquad\qquad (4.89)$$

$$g_{\infty}(A,B) + h\,\frac{\partial g_{\infty}}{\partial A} + k\,\frac{\partial g_{\infty}}{\partial B} = 0 \qquad\qquad (4.90)$$

$$f_{\infty}''(A,B) + h\,\frac{\partial f_{\infty}''}{\partial A} + k\,\frac{\partial f_{\infty}''}{\partial B} = 0 \qquad\qquad (4.91)$$

$$g_{\infty}'(A,B) + h\,\frac{\partial g_{\infty}'}{\partial A} + k\,\frac{\partial g_{\infty}'}{\partial B} = 0 \qquad\qquad (4.92)$$

(Using the current values of A and B instead of A_1 and B_1)
The values of h and k are extracted with the aid of a least-square method and these values are given by the following matrix equation.

$$\begin{bmatrix} \left(\dfrac{\partial f'_\infty}{\partial A}\right)^2 + \left(\dfrac{\partial g_\infty}{\partial A}\right)^2 + \left(\dfrac{\partial f''_\infty}{\partial A}\right)^2 + \left(\dfrac{\partial g'_\infty}{\partial A}\right)^2 & \dfrac{\partial f'_\infty}{\partial A}\dfrac{\partial f'_\infty}{\partial B} + \dfrac{\partial g_\infty}{\partial A}\dfrac{\partial g_\infty}{\partial B} + \dfrac{\partial f''_\infty}{\partial A}\dfrac{\partial f''_\infty}{\partial B} + \dfrac{\partial g'_\infty}{\partial A}\dfrac{\partial g'_\infty}{\partial B} \\[3mm] \dfrac{\partial f'_\infty}{\partial A}\dfrac{\partial f'_\infty}{\partial B} + \dfrac{\partial g_\infty}{\partial A}\dfrac{\partial g_\infty}{\partial B} + \dfrac{\partial f''_\infty}{\partial A}\dfrac{\partial f''_\infty}{\partial B} + \dfrac{\partial g'_\infty}{\partial A}\dfrac{\partial g'_\infty}{\partial B} & \left(\dfrac{\partial f'_\infty}{\partial B}\right)^2 + \left(\dfrac{\partial g_\infty}{\partial B}\right)^2 + \left(\dfrac{\partial f''_\infty}{\partial B}\right)^2 + \left(\dfrac{\partial g'_\infty}{\partial B}\right)^2 \end{bmatrix}\begin{bmatrix} h \\ k \end{bmatrix}$$

$$= \begin{bmatrix} f'_\infty \dfrac{\partial f'_\infty}{\partial A} + g_\infty \dfrac{\partial g_\infty}{\partial A} + f''_\infty \dfrac{\partial f''_\infty}{\partial A} + g'_\infty \dfrac{\partial g'_\infty}{\partial A} \\[4mm] f'_\infty \dfrac{\partial f'_\infty}{\partial B} + g_\infty \dfrac{\partial g_\infty}{\partial B} + f''_\infty \dfrac{\partial f''_\infty}{\partial B} + g'_\infty \dfrac{\partial g'_\infty}{\partial B} \end{bmatrix} \qquad (4.93)$$

The least-square error is given by

$$E = f'^2_\infty + g^2_\infty + f''^2_\infty + g'^2_\infty \qquad (4.94)$$

The partial derivatives that appear in the solutions of h and k can be obtained by integrating the perturbed differential equations with their appropriate initial conditions.

The perturbed differential equations for the A-derivatives with the initial conditions are: (from eq. (4.77))

$$\frac{\partial f'''}{\partial A} = \frac{\partial F}{\partial f''}\frac{\partial f''}{\partial A} + \frac{\partial F}{\partial f'}\frac{\partial f'}{\partial A} + \frac{\partial F}{\partial g'}\frac{\partial g'}{\partial A} + \frac{\partial F}{\partial f}\frac{\partial f}{\partial A} + \frac{\partial F}{\partial g}\frac{\partial g}{\partial A} \qquad (4.95)$$

$$\frac{\partial g''}{\partial A} = \frac{\partial G}{\partial f''}\frac{\partial f''}{\partial A} + \frac{\partial G}{\partial f'}\frac{\partial f'}{\partial A} + \frac{\partial G}{\partial g'}\frac{\partial g'}{\partial A} + \frac{\partial G}{\partial f}\frac{\partial f}{\partial A} + \frac{\partial G}{\partial g}\frac{\partial g}{\partial A} \qquad (4.96)$$

$$\eta = 0: \quad \frac{\partial f}{\partial A} = \frac{\partial f'}{\partial A} = \frac{\partial g}{\partial A} = \frac{\partial g'}{\partial A} = 0$$

$$\frac{\partial f''}{\partial A} = 1 \tag{4.97}$$

The perturbed differential equations for B-derivatives with the initial conditions are: (from equation(4.78))

$$\frac{\partial f'''}{\partial B} = \frac{\partial F}{\partial f''}\frac{\partial f''}{\partial B} + \frac{\partial F}{\partial f'}\frac{\partial f'}{\partial B} + \frac{\partial F}{\partial g'}\frac{\partial g'}{\partial B} + \frac{\partial F}{\partial f}\frac{\partial f}{\partial B} + \frac{\partial F}{\partial g}\frac{\partial g}{\partial B} \tag{4.98}$$

$$\frac{\partial g''}{\partial B} = \frac{\partial G}{\partial f''}\frac{\partial f''}{\partial B} + \frac{\partial G}{\partial f'}\frac{\partial f'}{\partial B} + \frac{\partial G}{\partial g'}\frac{\partial g'}{\partial B} + \frac{\partial G}{\partial f}\frac{\partial f}{\partial B} + \frac{\partial G}{\partial g}\frac{\partial g}{\partial B} \tag{4.99}$$

$$\eta = 0: \quad \frac{\partial f}{\partial B} = \frac{\partial f'}{\partial B} = \frac{\partial g}{\partial B} = \frac{\partial f''}{\partial B} = 0$$

$$\frac{\partial g'}{\partial B} = 1 \tag{4.100}$$

Thus to correct the trial values of A_1 and B_1, the original equations (4.77) to (4.82) plus the perturbed equations (4.95) to (4.100) with their appropriate initial conditions should be integrated simultaneously up to a certain suitable point, where the trial values of A_1 and B_1 are corrected.

After two or three iterations at the same point, where the least-square errors appear to be steady, the integration-

range is extended and the integration is repeated up to that extended point. This iteration process will continue and the integration range may be increased until we arrive at the solution we desire, where the least square error assumes a minimum, smaller than a pre-assigned value.

The principal results of the calculations for Sc = 0.01 and for the second order reactions are listed in Tables 4 and 5.

It should be noted that the asymptotic behaviour of these results is probably characterized by exponential decay. For example, one can see this from eq. (4.47) which, as $\eta \to \infty$, takes the form

$$f_0''' + 3 f_0 f_0'' = 0, \quad \text{for} \quad f_0 \to \text{constant},$$

indicating the exponential dependence on η.

The conclusions and the interpretations of the results are discussed in Chapter VI.

η	c_0	c_0'	c_1	c_1'
0	1.00000	−0.08365	0.00000	−0.03161
1	0.91644	−0.08335	−0.02689	−0.02244
2	0.83375	−0.08181	−0.04541	−0.01484
3	0.75324	−0.07902	−0.05705	−0.00868
4	0.67604	−0.07525	−0.06322	−0.00386
5	0.60297	−0.07080	−0.06516	−0.00022
6	0.53457	−0.06594	−0.06399	+0.00239
7	0.47115	−0.06089	−0.06066	+0.00416
8	0.41279	−0.05582	−0.05589	+0.00526
9	0.34956	−0.05088	−0.05030	0.00585
10	0.31096	−0.04614	−0.04432	0.00606
11	0.26707	−0.04168	−0.03827	0.00599
12	0.22749	−0.03753	−0.03240	0.00574
13	0.19189	−0.03371	−0.02683	0.00537
14	0.15995	−0.03022	−0.02167	0.00494
15	0.13134	−0.02705	−0.01696	0.00447
16	0.10575	−0.02418	−0.01272	0.00401
17	0.08288	−0.02160	−0.00893	0.00355
18	0.06245	−0.01929	−0.00559	0.00312
19	0.04421	−0.01722	−0.00267	0.00273
20	0.02793	−0.01536	−0.00012	0.00236
21	0.01341	−0.01371	−	−
22	0.00045	−0.01223	−	−

Table 4: Results of Numerical solutions of concentrations with their gradients for $Sc = 0.01$ and $n = 2$.

	f_0'	f_0''	f_1'	f_1''
0	0.00000	0.98302	0.00000	-0.01282
1	0.53484	0.17050	-0.00993	-0.00622
2	0.54730	-0.06764	-0.01449	-0.00365
3	0.47118	-0.07544	-0.01722	-0.00166
4	0.40050	-0.06596	-0.01790	+0.00018
5	0.33887	-0.05749	-0.01709	+0.00131
6	0.28515	-0.05009	-0.01543	0.00193
7	0.23839	-0.04356	-0.01335	0.00219
8	0.19778	-0.03777	-0.01112	0.00223
9	0.16262	-0.03264	-0.00893	0.00212
10	0.13231	-0.02807	-0.00689	0.00192
11	0.10629	-0.02401	-0.00509	0.00167
12	0.08412	-0.02040	-0.00355	0.00140
13	0.06535	-0.01718	-0.00228	0.00112
14	0.04963	-0.01431	-0.00129	0.00086
15	0.03662	-0.01175	-0.00056	0.00060
16	0.02602	-0.00947	-0.00007	0.00037
17	0.01757	-0.00744	+0.00020	0.00017
18	0.01105	-0.00563	0.00027	-0.00001
19	0.00624	-0.00401	0.00018	-0.00017
20	0.00296	-0.00257	-0.00006	-0.00031
21	0.00105	-0.00128	–	–
22	0.00035	-0.00013	–	–

Table 5: Results of Numerical solutions of Velocity distributions and their gradients for $Sc = 0.01$

$n = 2$

4.4 <u>Effect upon mass-transfer</u>

The local and average mass fluxes from the surface of the plate are presented in this section. The dimensionless mass flux parameter known as the Nusselt number is calculated in terms of the solutions of the differential equations.

Thus the local mass-transfer parameter is given by,

$$Nu_x = \frac{J''(x)}{c_0 - c_\infty} \frac{x}{D}$$

$$= -\left[\frac{Gr_x}{4}\right]^{1/4} c'(0)$$

$$= -\left[\frac{Gr_x}{4}\right]^{1/4} c_0'(0)\left[1 + \epsilon(x)\frac{c_1'(0)}{c_0'(0)} + \epsilon^2(x)\frac{c_2'(0)}{c_0'(0)} + \cdots\right]$$

$$(4.101)$$

And the average mass transfer parameter for a plate of height L is given by

$$Nu_L = -\int_0^L \frac{1}{x}\left[\frac{Grx}{4}\right]^{1/4} c_0'(0)\left[1 + \epsilon(x)\frac{c_1'(0)}{c_0'(0)} + \epsilon^2(x)\frac{c_2'(0)}{c_0'(0)} + \cdots\right] dx$$

$$= -\frac{4}{3} c_0'(0)\left[\frac{Gr_L}{4}\right]^{1/4}\left[1 + \frac{3}{5}\epsilon(L)\frac{c_1'(0)}{c_0'(0)} + \frac{3}{7}\epsilon^2(L)\frac{c_2'(0)}{c_0'(0)} + \cdots\right]$$

$$(4.102)$$

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where $\quad Gr_L = \dfrac{g\beta^*(c_0 - c_\infty) L^3}{\nu^2}$, $\quad \epsilon(L) = \dfrac{2k(c_0 - c_\infty)^{n-3/2}}{\sqrt{g\beta^*}} L^{1/2}$

From the relations (4.101) and (4.102), it has been observed that the mass transfer is a function of concentration gradient at the surface of the plate. This concentration-gratient is again dependent upon the Schmidt number and the reaction-kinetics. Solving the governing equations by numerical and analytical procedure, the numerical values of this con-centration-gratient are evaluated for different Schmidt numbers and for different reaction orders. From the mass transfer parameter, it is observed that the transport is nil at the leading edge of the plate, and it becomes prominent at the upper limit of the plate height.

CHAPTER V

DISTRIBUTED CONCENTRATION ALONG THE PLATE FOR VARIOUS

REACTION-KINETICS

This Chapter consists of similarity solutions which may be found when the initial concentration along the surface of the plate is assumed to obey some algebraic law with respect to the order of chemical reaction. In the previous chapter, we have presented an analysis giving rise to perturbation-type similarity solutions.

5.1 Basic Equations for various orders of Reaction-Rate

Case (I): For general nth order-chemical reaction.

Consider the following transformation:

Similarity variable: $\eta(x,y) = y \cdot b(x)$ (5.1)

Stream function: $\psi(x,y) = \nu\, a(x)\, f(\eta)$ (5.2)

dimensionless concentration: $C(x,y) = \dfrac{c - c_\infty}{c_0 - c_\infty}$ (5.3)

and $e(x) = c_0 - c_\infty$ (5.4)

Introducing these transformations into equations (4.7) and (4.8), one obtains the following ordinary differential equations:

$$f''' + \frac{g\beta^{*}e}{ab^3\nu^2}\,c + \frac{a_x}{b}\,ff'' - \left(\frac{ab_x}{b^2} + \frac{a_x}{b}\right)f'^2 = 0 \quad (5.5)$$

$$\frac{c''}{Sc} + \frac{a_x}{b}\,fc' - \frac{a}{b}\frac{e_x}{e}\,f'c - \frac{k\,e^{n-1}}{\nu b^2}\,c^n = 0 \qquad (5.6)$$

provided,

$$\frac{a_x}{b} = c_1 \tag{5.7}$$

$$\frac{ab_x}{b^2} = c_2 \tag{5.8}$$

$$\frac{ae_x}{be} = c_3 \tag{5.9}$$

$$\frac{g\beta^{*}e}{ab^3\nu^2} = c_4 \tag{5.10}$$

$$\frac{k\,e^{n-1}}{\nu_{\Gamma}^2} = F(\eta) \tag{5.11}$$

where c_1, c_2, c_3, c_4 are constants and F is an arbitrary function of η alone, and sub x means differentiation with respect to x.

The relations (5.7) to (5.11) reveal that the transformations (5.1) to (5.4) must be of the following forms:

$$\eta(x,y) = \frac{y}{x}\left[\frac{Gr_x}{5-3n}\right]^{1/4}$$ (5.12)

$$\psi(x,y) = \nu(5-3n)\left[\frac{Gr_x}{5-3n}\right]^{1/4} f(\eta)$$ (5.13)

$$c(x,y) = \frac{c - c_\infty}{c_0 - c_\infty}$$ (5.14)

and $c_0 - c_\infty$ = initial distribution function

$$= N x^{\frac{1}{3-2n}}$$ (5.15)

where Gr_x = local Grashof numbers

$$= \frac{g\beta^* x^3 (c_0 - c_\infty)}{\nu^2}$$ (5.16)

and N is a dimensional quantity.

The equations (5.5) and (5.6) become:

$$f''' + C + (5-3n)ff'' - (4-2n)f'^2 = 0$$ (5.17)

$$\frac{c''}{Sc} + (5-3n)fc' - \frac{5-3n}{3-2n}f'c - pc^n = 0$$ (5.18)

where $p = \dfrac{k N^{n-1}}{\sqrt{\dfrac{Ng\beta^*}{5-3n}}}$, a dimensionless rate number.

The boundary conditions are:

$$f(0) = 0$$
$$\left. \begin{aligned} f(0) &= 0 \\ f'(0) &= 0 \\ c(0) &= 1 \end{aligned} \right\} \qquad \eta = 0 \qquad\qquad (5.19)$$

$$\eta \to \infty \qquad \left. \begin{aligned} f'(\infty) &= 0 \\ c(\infty) &= 0 \end{aligned} \right\} \qquad\qquad (5.20)$$

It has been observed that the initial distribution (5.15) can produce valid ordinary differential equations (5.17) and (5.18) except for $n = 1$, 3/2 and 5/3. From physical considerations, the analysis for the case $n = 5/3$ is of little importance, because a reaction with this order is very rare. The following analysis is made only for $n = 1$ and 3/2.

Case II: <u>For the first order chemical reaction.</u>

Assume the following transformations.

Similarity variable: $\eta(x,y) = \dfrac{y}{x} \left[\dfrac{Grx}{c_1} \right]^{1/4}$ (5.21)

Stream function: $\psi(x,y) = \nu c_1 \left[\dfrac{Grx}{c_1} \right]^{1/4} f(\eta)$ (5.22)

Concentration:
$$C(x,y) = \frac{c - c_\infty}{c_0 - c_\infty} \qquad (5.23)$$

and $c_0 - c_\infty = Nx$ $\qquad (5.24)$

The equations become,

$$f''' + C + C_1(ff'' - f'^2) = 0 \qquad (5.25)$$

$$\frac{C''}{Sc} + C_1(fC' - f'C) - qC = 0 \qquad (5.26)$$

where $\quad q = \dfrac{kC_1}{g\beta^* N}$

The boundary conditions are given by (5.19) and (5.20).

Case III: **For the 3/2th order chemical reaction.**

In this case, assume the following transformations:

Similarity variable:

$$\eta(x,y) = \left(\frac{Ng\beta^*}{\nu^2}\right)^{1/3} y \, e^{\left(\frac{Ng\beta^*}{\nu^2}\right) C_1 x} \qquad (5.27)$$

Stream function:

$$\psi(x,y) = \nu \, e \left(\frac{Ng\beta^*}{\nu^2}\right)^{1/3} C_1 x \, f(\eta) \qquad (5.28)$$

Dimensionless concentration:

$$C(x,y) = \frac{c - c_\infty}{c_0 - c_\infty} \tag{5.29}$$

and $c_0 - c_\infty = N \ e^4 \left[\dfrac{Ng\beta}{2} \right]^{1/3} c_1 x$ (5.30)

The equations become

$$f''' + C + C_1(ff'' - 2f'^2) = 0 \tag{5.31}$$

$$\frac{C''}{Sc} + C_1(fC' - 4f'C) - rC^{3/2} = 0 \tag{5.32}$$

where $r = \dfrac{k \ N^{1/2}}{\nu \left\{ \dfrac{Ng\beta^*}{\nu 2} \right\}^{2/3}}$

The boundary conditions are given by (5.19) and (5.20).

5.2   Series Solutions.

The series solutions of the equations in the Case I with their relevant boundary conditions are given by,

$$F(z) = A \cdot \frac{z^2}{2!} + \left(\frac{3A-1}{}\right)\frac{z^3}{3!} + \left(\frac{11A-B-6}{}\right)\frac{z^4}{4!}$$

$$+ [50A + (3-n)A^2 - 10B - 35 - pSc] \frac{z^5}{5!} + O(z^6) \qquad (5.33)$$

$$G(z) = 1 + Bz + (B + pSc)\frac{z^2}{2!}$$

$$+ \left[2B + 3pSc + Sc\left\{\frac{5-3n}{3-2n}A + pnB\right\}\right]\frac{z^3}{3!}$$

$$+ \left[6B + 11pSc + 5Sc\left(\frac{5-3n}{3-2n}A + pnB\right)\right.$$

$$+ Sc\left\{\frac{5-3n}{3-2n}(A + 2AB - 1) - (5-3n)AB\right.$$

$$\left.\left. + pn(n-1)B^3 - pn(B + pSc)\right\}\right]\frac{z^4}{4!} + O(z^5) \qquad (5.34)$$

where

$$\left.\begin{array}{l} f(\eta) = F(z) \\ C(\eta) = G(z) \\ z = 1 - e^{-\eta} \\ A = F''(0) \\ B = G'(0) \end{array}\right\} \qquad (5.35)$$

The series solutions of the equations in the Case II, with $c_1 = 1$ are given by

$$F(Z) = A\frac{z^2}{2!} + (3A-1)\frac{z^3}{3!} + (11A-B-6)\frac{z^4}{4!}$$

$$+ (A^2 + 50A - 10B - 35 - qSc)\frac{z^5}{5!} + 0(z^6) \qquad (5.36)$$

$$G(Z) = 1 + BZ + (B + qSc)\frac{z^2}{2!}$$

$$+ \left\{ 2B + 3qSc + Sc(A + qB) \right\}\frac{z^3}{3!}$$

$$+ \left[6B + Sc\left\{ A + AB - 1 - q(B + qSc) \right. \right.$$

$$\left. \left. + 5(A + qB) + 11q \right\} \right]\frac{z^4}{4!} + 0(z^5) \qquad (5.37)$$

Similarly, series solutions in the Case III with $c_1 = 1$ are given by

$$F(Z) = A\frac{z^2}{2!} + (3A-1)\frac{z^3}{3!} + (11A-B-6)\frac{z^4}{4!}$$

$$+ (3A^2 + 50A - 10B - 35 - rSc)\frac{z^5}{5!} + 0(z^6) \qquad (5.38)$$

$$G(Z) = 1 + BZ + (B + rSc)\frac{z^2}{2!}$$

$$+ \left\{ 2B + 3rSc + Sc\left(4A + 3r\frac{B}{2}\right)\right\}\frac{z^3}{3!}$$

$$+ \left[6B + 11rSc + 5Sc\left(4A + \frac{3rB}{2}\right)\right.$$

$$+ Sc\left\{ 4(A + 2AB - 1) - AB + \frac{3rB^2}{4}\right.$$

$$\left.\left.- \frac{3r}{2}(B + rSc)\right\}\right]\frac{z^4}{4!} + 0(z^5) \tag{5.39}$$

The values of A and B in all the three cases are found by approximate solutions of the equations

$$\left.\begin{array}{l} F'(A,B) = 0 \\ G(A,B) = 0 \end{array}\right\} \quad \text{as } Z \longrightarrow 1 \tag{5.40}$$

The roots of A and B are obtained by the use of Newton-Raphson methods for small Schmidt numbers. The following numerical values of A and B for Sc = 0.72 and for reaction number unity have been obtained for the indicated values of the order of reaction.

n	A	−B
1	0.3775115	0.939694
3/2	0.3824861	0.905062
2	0.3900558	0.821376

Table 6:   Numerical values of A and B for various order

of reaction.

5.3   Numerical Solution:

The differential equations (5.17), (5.18), (5.25), (5.26), (5.31) and (5.32) are all integrated numerically with their relevant boundary conditions. These equations are integrated by using a Runge-Kutta method with Nachtsheim-Swigert technique (1965) to correct the first choices of the initial values. Results of the numerical solutions of the concentration and the velocity distributions are discussed for various flow parameters in Chapter VI. Finally, Table 7 gives the results of the numerical solutions of velocity and concentration distributions with their gradients for Sc = 0.01, n = 0. The conclusions and the interpretations of the results are discussed in the following Chapter.

η	f'	f''	c	c'
0	0.00000	0.77841	1.00000	-0.18036
0.5	0.27191	0.33106	0.91130	-0.17403
1.0	0.36024	0.05359	0.82624	-0.16600
1.5	0.35293	-0.06157	0.74540	-0.15730
2.0	0.31360	-0.08941	0.66897	-0.14839
2.5	0.26821	-0.08782	0.59700	-0.13947
3.0	0.22721	-0.07980	0.52948	-0.13062
3.5	0.18850	-0.07106	0.46635	-0.12189
4.0	0.15509	-0.06262	0.40756	-0.11331
4.5	0.12580	-0.05464	0.35301	-0.10491
5.0	0.10036	-0.04717	0.30261	-0.09672
5.5	0.07853	-0.04022	0.25625	-0.08874
6.0	0.06004	-0.03381	0.21383	-0.08098
6.5	0.04463	-0.02792	0.17523	-0.07345
7.0	0.03203	-0.02257	0.14033	-0.06615
7.5	0.02198	-0.01773	0.10903	-0.05908
8.0	0.01421	-0.01341	0.08121	-0.05224
8.5	0.00847	-0.00959	0.05675	-0.04561
9.0	0.00453	-0.00626	0.03555	-0.03921
9.5	0.00213	-0.00341	0.01750	-0.03301
10.0	0.00103	-0.00102	0.00251	-0.02701

Table 7:   Results of Numerical Solutions of velocity and

Concentration distributions with their gradients

for Sc = 0.01

n = 0

P = 1
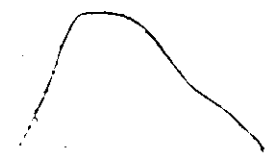
5.4 Effect upon Mass transfer

The local mass fluxes from the surface of the plate are calculated as follows:

Local mass transfer parameter for the case I is given by

$$Nu_x = \frac{J''(x)}{c_0 - c_\infty} \cdot \frac{x}{D} = - c'(0) \left[\frac{Ng\beta^*}{\nu^2 (5-3n)} \right]^{1/4} x^{\frac{5-3n}{6-4n}}$$

(5.41)

Similarly, we can have the local mass transfer parameters for the cases II and III respectively as follows:

$$Nu_x = - c'(0) \left[\frac{Grx}{c_1} \right]^{1/4}$$

(5.42)

$$Nu_x = - c'(0) \left[\frac{Ng\beta \, x^3}{\nu^2} \right]^{1/3} \exp \left[c_1 \left\{ \frac{Ng\beta^* x^3}{\nu^2} \right\}^{1/3} \right]$$

(5.43)

The relations (5.41) to (5.43) are all dependent upon the Schmidt numbers and the order of reactions. The following table 8 shows the mass transfer parameter $c'(0)$ for different values of the Schmidt numbers and for the reaction order $n = 0$ and the reaction number unity for the relation (5.41).

Sc	$-c'(0)$
0.01	0.18036753
0.72	1.3369751
1.00	1.5467215
10.00	4.565486
100.00	14.990554
1000.00	45.008224

Table 8:   Mass transfer parameters for different Schmidt numbers.

Mass transfer parameters $c'(0)$ for the relations (5.42) and (5.43) are given in Table 10, for the reaction rate number of 0.01.

RESULTS AND CONCLUSIONS

6.1   Discussion of Results

Preliminary Remarks

The reaction rate number

$$\epsilon(x) = \frac{2k(c_0 - c_\infty)^{n-3/2}}{\sqrt{g\beta^*}} x^{1/2} \tag{6.1}$$

is small for most chemical species with slow reaction rate. For example, chemicals such as sodium chloride, or potassium chloride with dilute acids and sugar with dilute acids can be categorized in this class of species. This number plays an important role for the problem described in Chapter IV. Thus to establish the numerical order for $\epsilon(x)$ in the case of uniform concentration at the plate, we may present the following discussion.

The basic perturbation expansion is

$$c(\eta, \epsilon) = c_0(\eta) + \epsilon(x) c_1(\eta) + \epsilon^2(x)c_2(\eta) + \ldots \tag{6.2}$$

Suppose that $\left|\dfrac{c_2}{c_1}\right| < K$, where K is a numerically known

upper bound for all η in calculations. (The graph of $\left|\dfrac{c_2}{c_1}\right|$

as a function of η for $Sc = 0.01$ and $n = 1$ from the truncated

series solution up to z^8 is shown in Fig. (21)). Assuming

that $\lim\limits_{\eta \to \infty} \left|\dfrac{c_2}{c_1}\right| = 0$, and that (6.2) is a convergent series,

let $\left|\dfrac{\epsilon^2(x)c_2(\eta)}{\epsilon(x)c_1(\eta)}\right| \leqslant 0.1 \%$ say, for $0 < \eta < \infty$, (6.3)

so that an estimate of the error in using the truncated

solution,

$$C = c_0(\eta) + \epsilon(x)\, c_1(\eta) \tag{6.4}$$

is of order 0.1% or

$$\left|\epsilon(x)\right| \leq 0.001 \left|\dfrac{c_1}{c_2}\right| \tag{6.5}$$

Since $\left|\dfrac{c_1}{c_2}\right|$ has the lower bound $\dfrac{1}{K}$, we therefore require that

$$\left|\epsilon(x)\right| \leq \dfrac{0.001}{K} . \tag{6.6}$$

Let $\dfrac{0.001}{K} \equiv \xi$, so that $0 < \left|\epsilon(x)\right| \leq \xi$, and $\epsilon(x)$ is of

order ξ.

Then

$$|\epsilon(x)| = \frac{2k(c_0-c_\infty)^{n-3/2}}{\sqrt{g\beta^*}} \cdot |x^{1/2}| \leqslant \xi \qquad (6.7$$

implies

$$0 < x \leqslant \left[\frac{g\beta^*}{4k^2(c_0-c_\infty)^{2n-3}}\right] \xi^2 \qquad (6.8)$$

If we define the non-dimensional plate coordinate

$$x' = \left[\frac{4k^2(c_0-c_\infty)^{2n-3}}{g\beta^*}\right] \cdot x, \qquad (6.9)$$

then we require that

$$0 < x' \leqslant \xi^2, \text{ where } \xi = \frac{0.001}{K}$$

and K is the upper bound of $\left|\dfrac{c_2}{c_1}\right|$ for $0 < \eta < P$,

given that $P = P(Sc, n)$ is numerically known as the practical range of η in the calculations when $c \longrightarrow 0$ asymptotically.

As we know that the similarity variable η is given by

$$\eta = \frac{y}{x}\left[\frac{Grx}{4}\right]^{1/4}, \text{ dimensionless co-ordinates } x'$$

and y' can now be defined as

$$x' = \left[\frac{4k^2(c_0-c_\infty)^{2n-3}}{g\beta^*} \right] x \qquad (6.10)$$

$$y' = \left[\frac{k^{1/2}(c_0-c_\infty)^{\frac{n-1}{2}}}{\nu^{1/2}} \right] y \qquad (6.11)$$

where $\quad \gamma = y'(x')^{-1/4} \qquad (6.11)$

Thus, for the calculated solutions, the domain of validity along the plate length is given by $\quad 0 < x \leqslant \xi^2. \qquad (6.12)$

With this choice of x' and y', the nondimensional velocity component parallel to the body force may be defined by

$$\left[\frac{u}{\frac{g\beta^*}{k(c_0-c_\infty)^{2n-2}}} \right]' \equiv u' \equiv \left\{ f_0'(\gamma) + (x')^{1/2} f_1'(\gamma) \right\} (x')^{1/2}$$

$$(6.13)$$

Also the local mass transfer parameter Nu_x, can be calculated as follows:

$$\left[\frac{Nu_x}{\frac{g\beta^*}{4\,\nu^{1/2}k^{3/2}(c_0-c_\infty)^{\frac{3n-5}{2}}}} \right] = N'u_x = -\left\{ c_0'(0) + (x')^{1/2} c_1'(0) \right\}(x'^{3/4})$$

$$(6.14)$$

From the distributed initial concentration theory, we know that the concentration at the plate must be a function of the plate length prescribed by the order of reaction, of the form

$$c_0(x) = N x^{\frac{1}{3-2n}} + c_\infty \tag{6.15}$$

which can be written as,

$$c_0(x') = N a^{\frac{1}{3-2n}} (x')^{\frac{1}{3-2n}} + c_\infty \tag{6.16}$$

where

$$a = \frac{g \beta}{4k^2(c_0 - c_\infty)^{2n-3}} \tag{6.17}$$

The domain of validity of the calculations for the uniform concentration problem is known to be $0 < x' \ll \xi^2$.

It would now be of interest to compare results between the two types of problems, i.e. between the case of an initial concentration distributed along the plate and that of a uniform initial concentration, for fixed values of n and Sc. In order for this comparison to be meaningful, however, it would be necessary that the distributed concentration $c_0(x')$ has a magnitude over the range $0 < x \ll \xi^2$ which is in some way based on the chosen uniform value c_0.

For example, one could use an averaging process for the distributed concentration at the plate which is averaged to the uniform concentration value chosen for comparison, requiring that

$$\frac{1}{\xi^2} \int_0^{\xi^2} c_0(x')dx' = c_0. \qquad (6.18)$$

Using the expression for $c_0(x')$ from above, and performing the integration, one obtains

$$(c_0 - c_\infty) = N a^{\frac{1}{3-2n}} \left\{ \frac{3-2n}{4-2n} \right\} \xi^{\frac{1}{3-2n}} \qquad (6.19)$$

$$(n \neq 2)$$

Thus using the value of a, we have,

$$1 = N \left\{ \frac{3-2n}{4-2n} \right\} \left[\frac{g\beta^*}{4k^2} \right]^{\frac{1}{3-2n}} \xi^{\frac{2}{3-2n}} \qquad (6.20)$$

$$(n \neq 2)$$

We know from the distributed theory that the reaction rate parameter is given by,

$$p = \frac{k N^{n-1}}{\sqrt{\frac{Ng\beta^*}{5-3n}}} \qquad (6.21)$$

which can be rewritten as

$$
N \left[\frac{g\beta^*}{4k^2} \right]^{\frac{1}{3-2n}} = \left[\frac{5-3n}{4} \right]^{\frac{1}{3-2n}} p^{-\left\{ \frac{2}{3-2n} \right\}} \tag{6.22}
$$

Thus the relation between p and ξ which is required for meaningful comparison is given by the combination of (6.20) and (6.22).

$$
p = \left(\frac{3-2n}{4-2n} \right)^{\frac{3-2n}{2}} \left(\frac{5-3n}{4} \right)^{1/2} \xi , \tag{6.23}
$$
$$(n \neq 2)$$

e.g. when $n = 0$,

$$
p = \frac{3\sqrt{15}}{16} \xi = 0.73 \, \xi . \tag{6.24}
$$

Hence for an averaged comparison and for given ξ, i.e. for given Sc, n for some uniform concentration problem, p must be chosen according to (6.23). Accordingly, functional distribution of concentration $c_0(x')$ with respect to the uniform concentration c_0 at the plate is given by the following relation:

$$\frac{c_0(x')-c_\infty}{c_0 - c_\infty} = \left[\left(\frac{5-3n}{4}\right)^{\frac{1}{3-2n}} - p^{\frac{2}{3-2n}}\right] x'^{\frac{1}{3-2n}}, \quad (6.25)$$

and when $n = 0$,

$$\frac{c_0(x') - c_\infty}{c_0 - c_\infty} = \left[\left(\frac{5}{4}\right)^{1/3} p^{-2/3}\right](x')^{1/3} . \quad (6.26)$$

The graphical representation of the distributed concentration is shown in Fig. 28, compared with the uniform case according to (6.26).

In getting the boundary-layer thickness, the following criteria are used.

Let y'_b = maximum value of y' corresponding to a velocity value u'_b,

and u'_m = maximum velocity value over the flow region.

Then if $\left|\dfrac{u'_b}{u'_m}\right| = 0.01$, we say that

Y'_b is the boundary-layer thickness for that particular profile.

Results For Uniform Concentration at the Plate

In the following, we discuss the results obtained previously by numerical and analytical procedures.

Fig. 1 sketches the physical plane of the velocity field and Fig. 2 sketches the velocity and concentration distributions in the physical plane.

Solutions of the zeroth order approximation (without the reaction-rate term) in concentration by Taylor series expansion are displayed graphically in Fig. 3. These solutions are obtained for small Schmidt number, e.g. $Sc = 0.01$. Here Z represents the contracted co-ordinate length

$$Z = 1 - e^{-\eta} \quad \text{where } \eta = \frac{y}{x} \left[\frac{Grx}{4} \right]^{1/4}$$

a similarity variable of the problem. This figure shows the gradual improvement in the solution by the addition of terms. Comparison between the zeroth, first and second-order terms in the perturbation expansion is shown in Fig. 4, for Schmidt number $Sc = 0.01$, and the reaction order $n = 1$. It may be observed that the perturbation function c_1 is $O(10^{-2})$ and c_2 is $O(10^{-4})$ indicating their smallness of magnitude relative to c_0.

The numerical solutions for the concentration distribution C, in terms of the zeroth and first order functions (c_0 and c_1), are presented in Figs. 5,6 and 7, for the Schmidt numbers Sc = 0.01, 100, 10,000 respectively and for the fixed reaction-order n = 2. The numerical procedure adopted here has been described in Chapter IV. It has been numerically found that the estimations of the values of $\epsilon(x)$ for these values of Schmidt numbers and the reaction order are as follows:

$$O(\xi) = \epsilon(x) \leqslant 7 \times 10^{-1} \qquad \text{for} \qquad Sc = 0.01$$
$$n' = 2$$

$$\epsilon(x) \leqslant 7 \times 10^{-2} \qquad \text{for} \qquad Sc = 100$$
$$n = 2$$

$$\epsilon(x) \leqslant 8 \times 10^{-3} \qquad \text{for} \qquad Sc = 10,000$$
$$n = 2$$

when the error bound in the solution is allowed to   10% in each case.

The dimensionless concentration profiles C as a function of   the dimensionless coordinate y′ (perpendicular to the vertical plate) are depicted in Fig. 8, for Sc = 0.01 and n = 2 and for various dimensionless stations x′ on the plate. It may be observed that when x′ increases,

the concentration distributions expand and consequently
one may expect the boundary-layer thickness (y'_b) to
increase accordingly. This illustrates the physical
situation of boundary-layer growth.

As we know, the movement of a chemical species from
a high concentration region to a low concentration region
can be observed with the naked eye, when, for example a
small crystal of potassium permanganate $(KMnO_4)$ is dropped
into a beaker of water. The $KMnO_4$ begins to dissolve in
the water and we observe that there is a dark purple
concentrated solution of $KMnO_4$ very near to the crystal.
The progress of the diffusion can best be followed by
observing the growth of the purple region, the dark purple
where the $KMnO_4$ concentration is high and the light purple
where it is low.

The situation described above, for a simple experiment,
can be observed for the present problem in Fig. 9, which is
a consequence of the numerical solutions obtained for a
case of uniform concentration along the plate. (Fig. 8).
The picture displayed in Fig. 9 demonstrates the way in
which concentration varies away from its maximum value at
the surface of the vertical plate. The family of

concentration curves is determined by a scaling technique
in which the line density varies along the orthogonal
curves in proportion to the actual concentration distribution.
Fig. 10 and Fig. 11 show the concentration distributions
for Sc = 100, 10,000 and for n = 2 for various stations
at the dimensionless plate length (x').

The results shown in Figs. 12 and 13 demonstrate
the concentration variations within a thin region for high
Schmidt number fluids, namely, for Sc = 100, 10,000 and
for n = 2. By comparison of these concentration pictures
with that of Fig. 9, it may be observed that for high
Schmidt number fluids i.e. for species with low diffusivities,
mass transfer occurs in a very thin region near the plate.
This is a physical result which has been readily deduced
from the mathematical calculations.

The dimensionless velocity distributions at various
distances x' along the plate and the consequent boundary-
layer growth are shown in Fig. 14. It is observed that
very near to the leading edge of the plate, the boundary-
layer thickness appears insignificant, but grows rapidly
a small distance away from the leading edge, as expected.

Fig. 15 graphs the boundary-layer thicknesses y_b' as a function of the plate coordinate x' for Sc = 100, 10,000 and for n = 2. This figure indicates the maximum boundary-layer thickness according to the arbitrary definition given on page 94 and shows the rapid growth of the layer within which the effective flow occurs.

The effect of chemical reaction rate on the concen-tration profile may be observed in Fig. 16. The constant concentration curve C = 0.8 of Fig. 9 appears to flatten out, expanding the indicated diffusion domain by as much as 50% as the rate of reaction increases tenfold.

Thus from this it appears that increasing the reaction rate, while keeping all other parameters fixed, tends to encourage the solute mass transport away from the plate, an effect which may be expected in practice.

Figs. 17 and 18 demonstrate a similar behaviour for the constant concentration curves C = 0.6 and C = 0.4.

A comparison of the numerical and series solutions for Sc = 0.01 and k = 0 (without reaction) is presented in

Fig. 19. The series solution for concentration up to order z^{10} is compared with the numerical solution for the same case, showing a maximum discrepancy at $z = 0.8$ of 10 % in the series solution relative to the numerical calculation.

Fig. 20 shows the instability in the series solution for concentration in terms of the zeroth order approximation up to z^{10} for high Schmidt numbers thus indicating that the series solution is meaningful only for small Schmidt numbers of the order $0(10^{-2})$.

Fig. 21 shows a typical graph of $\left| \dfrac{c_2}{c_1} \right|$ as a function of η, taken from the series solution for the concentration distribution and from which it appears that the upper bound of $\left| \dfrac{c_2}{c_1} \right|$, discussed previously, seems to occur about $\eta = 1$.

Fig. 22 shows the effect of order of reaction n, as it varies from $n = 0, 1, 2$ at fixed $Sc = 0.01$ on the concentration distribution at the station $x' = 0.5$. From these results it is evident that an increase in the order n of reaction over $[0,2]$ (effectively increasing the sensitivity of the species depletion rate with change in concentration) tends to expand the diffusion-convection

layer away from the plate by a factor from two to three times, with a general decrease in concentration gradients. Hence one may expect a larger, while less distinct, diffusion-layer for larger orders, n.

Fig. 23 shows similar effects of varying n on the velocity profiles at the same station, emphasizing the expansion of the actual convection-layer in concert with the diffusion-layer when n is increased.

Fig. 24 shows the effect of reaction order and Schmidt number on the mass transfer at the plate. The graphs are plotted to display the mass transfer parameter Nux as a function of Schmidt number for varying n.

The results show that for $0 \leqslant Sc \leqslant 10^{4}$ and $0 \leqslant n \leqslant 2$, at the point $x' = 10^{-4}$, the initial mass transfer of the species from the plate Nux is close to a linear increasing function of Sc with slope of order 10^{-6}, while there appears to be only a marginal decrease with increasing n.

Gebhart investigated the viscous dissipation effects in natural convection about semi-infinite flat vertical surfaces (isothermal) in 1962. He started with the usual equations for conservation of mass, momentum and energy.

Though the mathematical formulation of the problem of uniform concentration along the plate is similar up to zeroth order terms to that of Gebhart's (1962), the essential difference occurs in the presence of the first order terms, wherein Gebhart includes viscous dissipation effects and in the present work it refers to chemical kinetics. Therefore, the following Table 9 has been drawn up to show the significant difference in the final numerical results obtained for $Pr = Sc = 0.01$ and 100 in the first order approximation terms.

$Sc = Pr$	Gebhart's (1962) $\phi_1'(0)$	Author's Results $-c_1'(0)$
0.01	0.003497	$n = 1$: 0.0477435 $n = 2$: 0.0325043
100	0.4877	$n = 1$ 15.72654 $n = 2$ 11.2733

Table 9: Numerical results for the 1st order approximation.

Initial Concentration Distributed along the Plate

The following discussions, for the distributed concentration along the plate, are based on the calculations using the theory of Chapter III.

The results of the numerical solutions for concentration and velocity distributions at Sc from 0.01, to 10^3, $n = 0$ and $p = 1$ are given in Fig. 25 and Fig. 26 respectively. The concentration and velocity profiles are drawn against the dimensionless similarity variable η. The boundary layer region decreases in thickness as the Schmidt number increases; thus for high Schmidt number fluids, mass diffusion takes place within a thin layer. This agrees with the results discussed by many authors including Morgan and Warner (1956), Ostrach (1953), Sparrow and Gregg (1956) and Schlichting (1955).

Fig. 27 shows the effect of chemical reaction upon mass transfer at the surface of the plate. From these results it appears that the amount of mass flowing with reaction is considerably greater than that without reaction and the transfer coefficient is a rapidly increasing monotonic function of Schmidt number, up to Sc = 10^3 at $n = 0$.

The choice of distributed as against uniform initial concentrations at the plate, to be used for the purpose of determining the effect of distribution (discussed previously in the preliminary remarks), is shown in Fig. 28.

By averaging the initial distribution concentration at the plate and choosing this average value to be equal to the uniform concentration value, a comparison between the concentration profiles in these two cases is possible. Fig. 29 shows the comparison between the concentrations at $y' = 0.1$ (near the plate), whereas Fig. 30 shows the comparison of the concentrations at $y' = .8$ (far from the plate), for Sc = 0.01 and n = 0. The figures 28, 29 and 30 reveal that for the uniform case, the concentration profile decreases in magnitude from the maximum constant value along the plate to a much lower range far from the plate. Near the plate and over most of the domain of x', the concentration profile is close to the uniform value, while indicating irregularity and a steep gradient in a neighbourhood of the leading edge at $x' = 0$. Sufficiently far from the plate, the irregularity apparently disappears and the profile reduces to a more smoothly increasing function of x'. For the distributed case, the same figures show that the profile decreases uniformly from its initial distribution at the plate to the minimum curve far from the plate, with little apparent change in shape characteristics.

A striking feature of these results is that, although the distributed curve at the plate varies widely above and below the

uniform case (Fig. 28), a concentration profile is produced away from the plate (Fig.30) which is uniformly above that of the uniform case and not essentially different in shape. This suggests that, if an initial concentration is maintained in a functional variation along the plate, then the results produced in the ambient fluid after some distance from the plate may not differ greatly in character from that produced if the initial concentration had been distributed uniformly.

Fig. 31 and Fig. 32 give the results of the series solutions of concentration and velocity distributions obtained for the distributed problem. Numerical results of concentration profiles are shown in Fig. 33 for this problem. These results for various values of reaction orders cannot be compared due to the fact that the plate surface concentration distribution depends upon the order of reaction, thus comprising independent problems for each order of reaction, so these results show only independent behaviour for each n.

Finally, the following table shows a comparison of our results for the cases of negligible (p = 0.01) and zero (p = 0) reaction-rate with those of Sparrow and Gregg (1958), which illustrates the expected similarity in the magnitude of the surface gradient terms.

Sc = Pr	Sparrow and Gregg	Author's Results	
	$-\phi'(0)$	$-c'(0)$	
	Power law n = 1	First order reaction	
		p = 0.01	p = 0
1.0 0.7	0.9898 0.8806	0.8469 0.7546	0.8632 0.7876
	Exponential case	3/2 order reaction	
		p = 0.01	p = 0
1.0 0.7	0.832 0.735	0.8203476 0.7330996	0.823695 0.735827

Table 10: Comparison of Results of Sparrow and Gregg (1958) with author's results.

This table shows the excellent agreement between the Sparrow et.al's results and the author's results for negligible reaction rate.

6.2   Concluding Remarks:

Steady-state natural convection flow over a semi-
infinite vertical plate has been studied for the specific
case in which the plate is of   given concentration in a
chemical species and convection arises as a result of
chemical reaction and diffusion within an ambient fluid
surrounding the plate. The formulation of the problem
has been based on the classical assumptions of the boundary-
layer theory, using the Navier-Stokes equations with
typical laws of chemical diffusion and reaction rate
kinetics applied to a two-dimensional field. The objective
in this study has been to determine solutions of the basic
equations which will yield the two-dimensional concentration
and flow fields away from the plate, when a given con-
centration distribution is maintained along the plate
surface.

In the case of uniform concentration along the plate,
the problem has been reduced to finding similarity-type
solutions for various order terms in perturbation expansions
about an effective reaction number. Application of the
results is therefore restricted to low reaction numbers,
or as is further shown, for a given reaction-rate, the

domain of validity must consequently be restricted to a small region down-stream from the leading edge. Solutions have been prepared using both analytical and numerical techniques. In the analytical case, truncated Taylor series have been constructed for the concentration distributions and stream functions, but these are found to be valid for small Schmidt numbers, of order 0.01 or less. From non-dimensionalisation of the basic equations, it has been found that the problem is essentially two-parameter, comprising the reaction-rate order (n) and Schmidt number (Sc). A numerical technique based on the Nacht-Sheim method has been developed and applied to this problem. Solutions have been calculated and presented for $Sc = 10^{-2}$, 10^2 and 10^4 at $n = 2$. It is generally found that normal concentration gradients are large and non-uniform near the leading edge, rapidly decreasing and becoming more uniform for points downstream. Also the boundary-layer thickness appears to increase with decreasing orders of Sc. The chemical reaction-rate (k) is not an explicit parameter and therefore contributes as a dimensional scaling factor only. It has been found that increasing the value of k, while keeping other parameters fixed, has

the effect of scaling curves of constant concentration outward from the plate. This means that an increase in reaction-rate may be expected to considerably increase the spatial penetration of the diffusing chemical species.

It has also been found that increasing the magnitude of the reaction order n for fixed Schmidt number Sc has the effect of expanding the effective diffusion and convection layers, while there is some indication that initial mass transfer at the plate decreases slightly. It therefore seems that the presence of chemical reaction in general will result in an apparent increase in diffusion-convection effects, with larger, but less distinct (as indicated by lower normal gradients) boundary layers.

In the case where the initial concentration at the plate is nonuniform, a study has been made which applies only to distributions whose mathematical form is dependent on the reaction order n. When this is assumed, it has been found that complete similarity solutions are available. That is, the partial differential equations which govern the problem may be reduced to a system of ordinary differential equations. Solutions for negligible reaction-rate are compared to those of Sparrow et al (1958) for two

Schmidt number values 0.7 and 1.0. The comparison shows good agreement with our results. From these results, for fixed n = 0, it has been found that the depth of diffusion and extent of the velocity field both increase with decreasing Sc; this conforms to what might be expected physically, namely, that the diffusion and convective effects would be expanded with an increase in diffusivity.

The features of this study which are essentially new derive from including reaction-rate kinetics in natural convection flow. When the initial concentration at the plate surface is uniform, quantitative application of results will be necessarily restricted to cases where either the reaction rate or the domain of definition downstream of the leading edge is small. However, similarity solutions for the distributed concentration along the plate permit calculation even in those cases where the reaction-rate is dominant, but where the flow remains laminar; but we must accept a plate surface concentration distribution whose mathematical form is itself prescribed by the order of the reaction. Although stability and transition are defined in terms of Grashof number limits, and the reaction-rate parameter is independent of Grashof number, still, for appreciable effects of reaction-rate, the flow may not remain laminar.
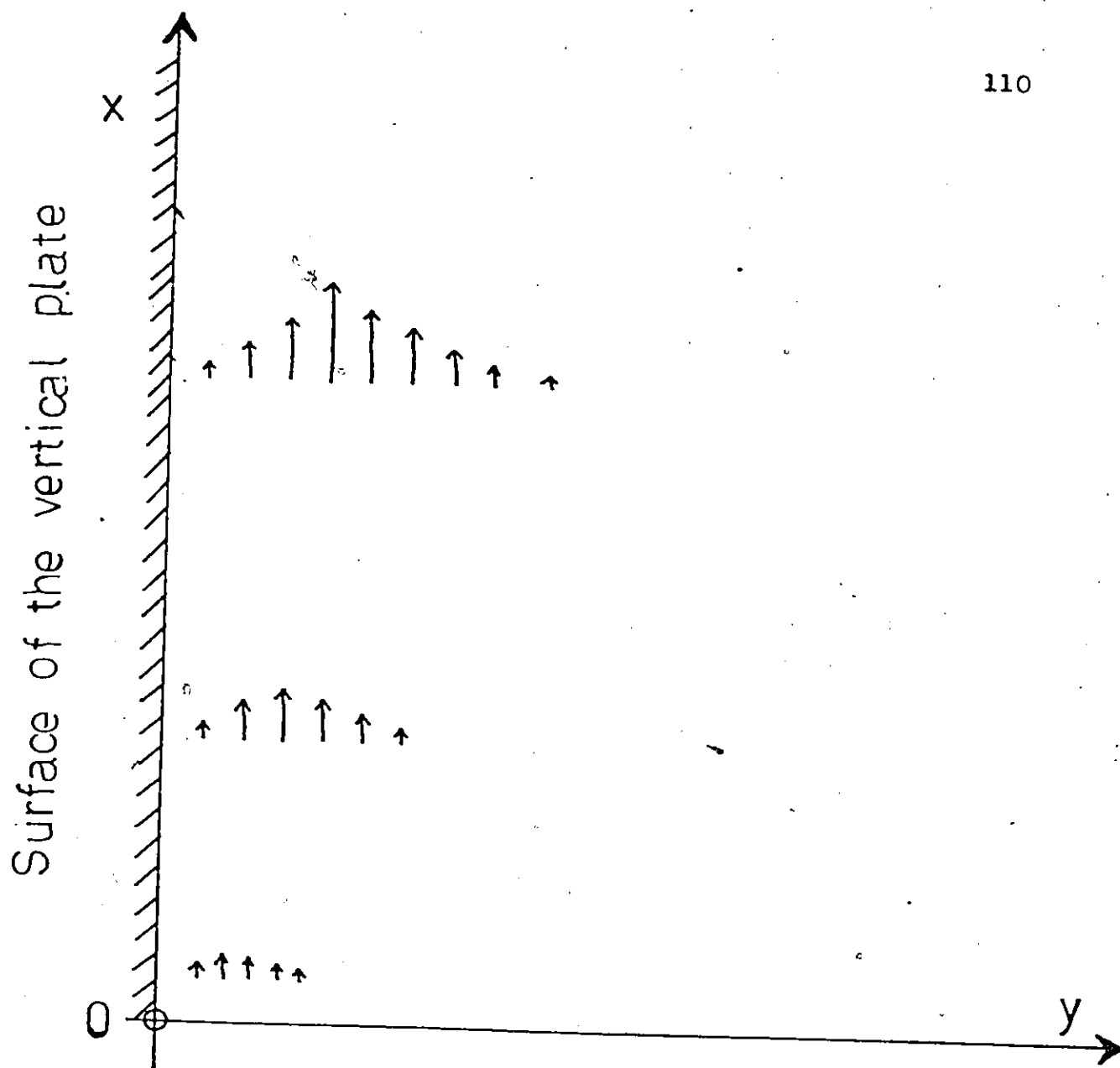
Fig.1 :   Physical plane of velocity
field in natural convection.
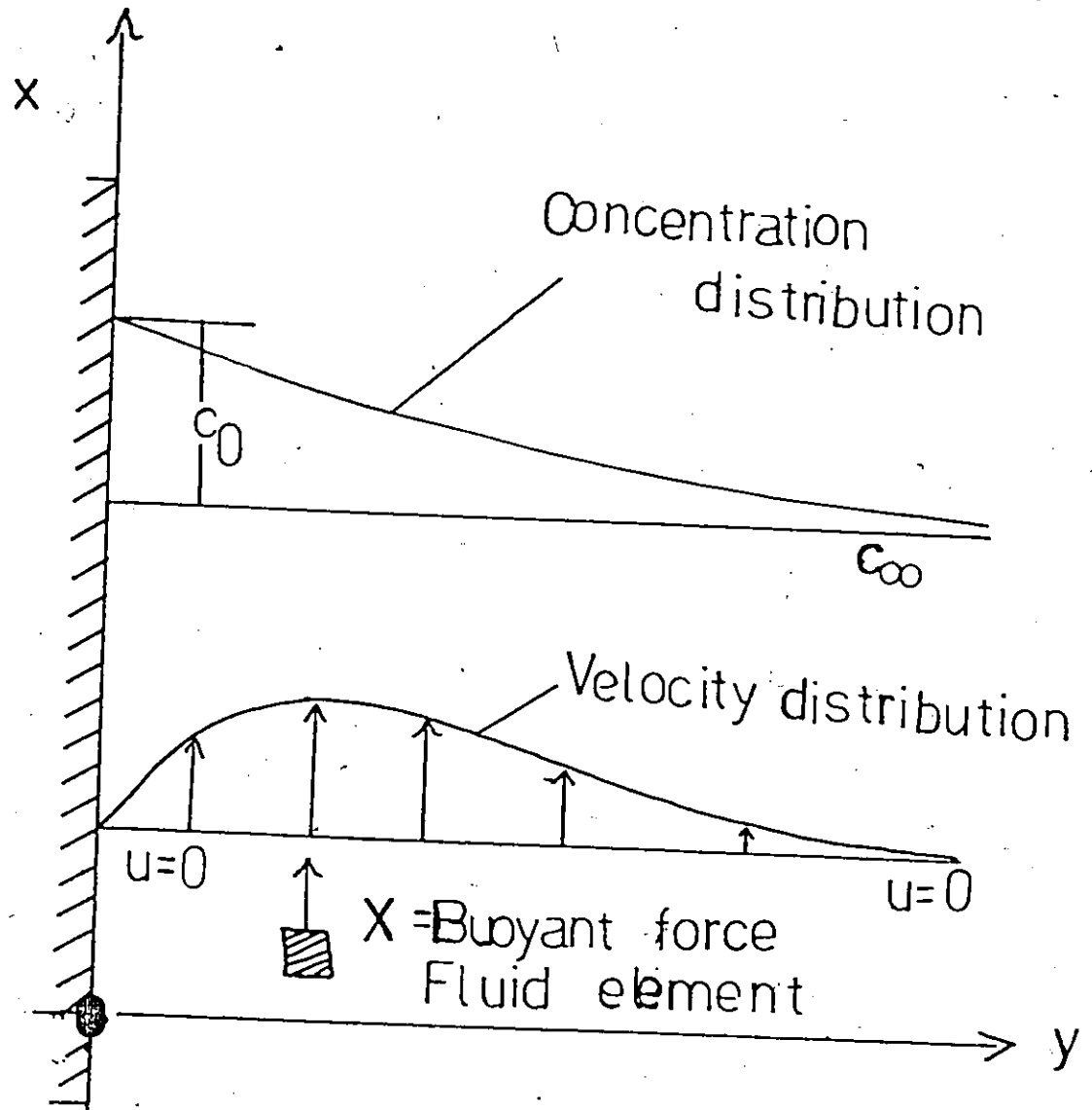
Fig 2: Velocity and Concentration distributions in the physical plane
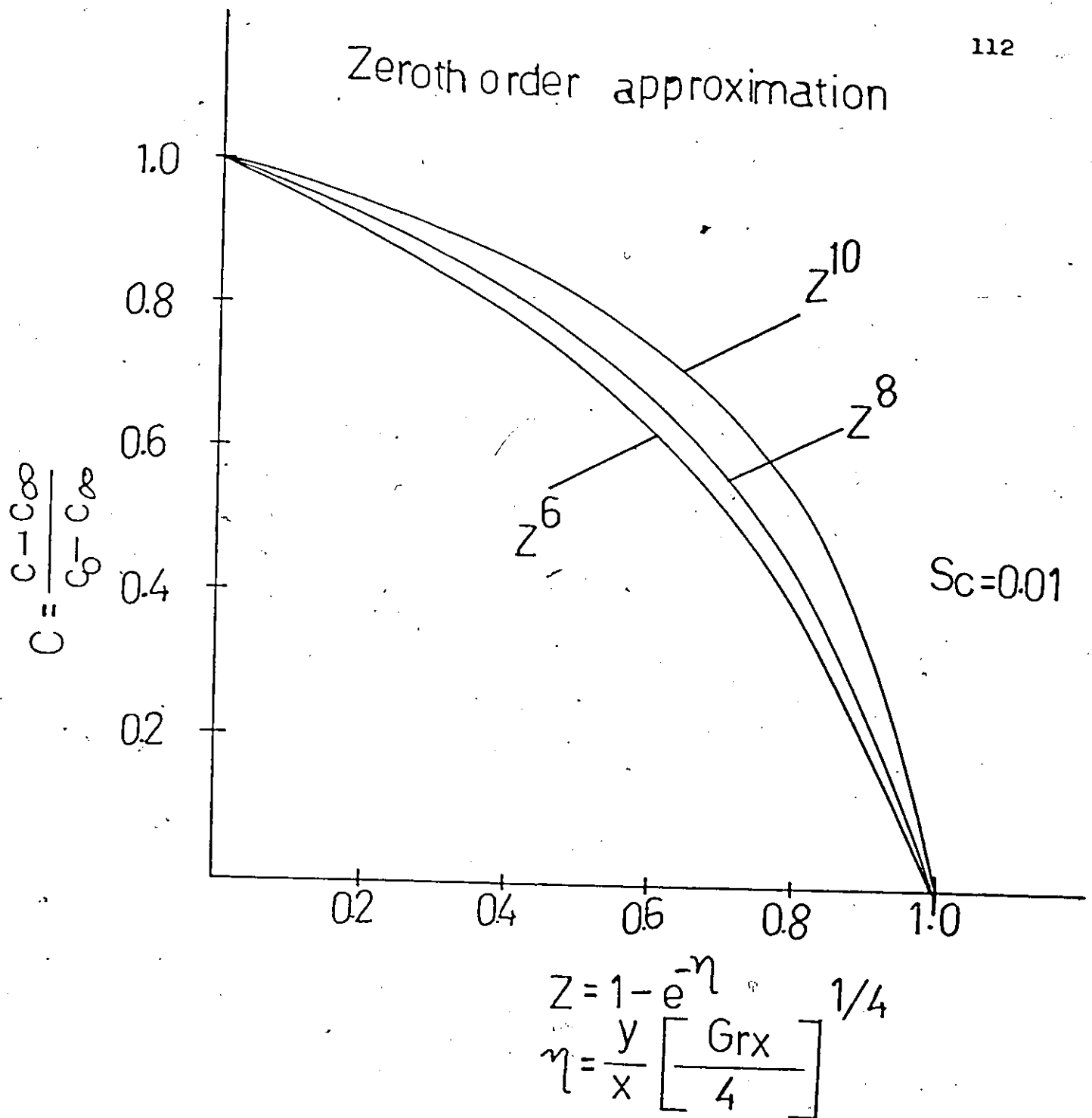
Fig. 3 : Comparison of series solutions upto Z^6, Z^8 and Z^{10} of the Concentration profiles without reaction for uniform Concentration at the plate

Z^8

$S_c = 0.01$
$n = 1$

Z
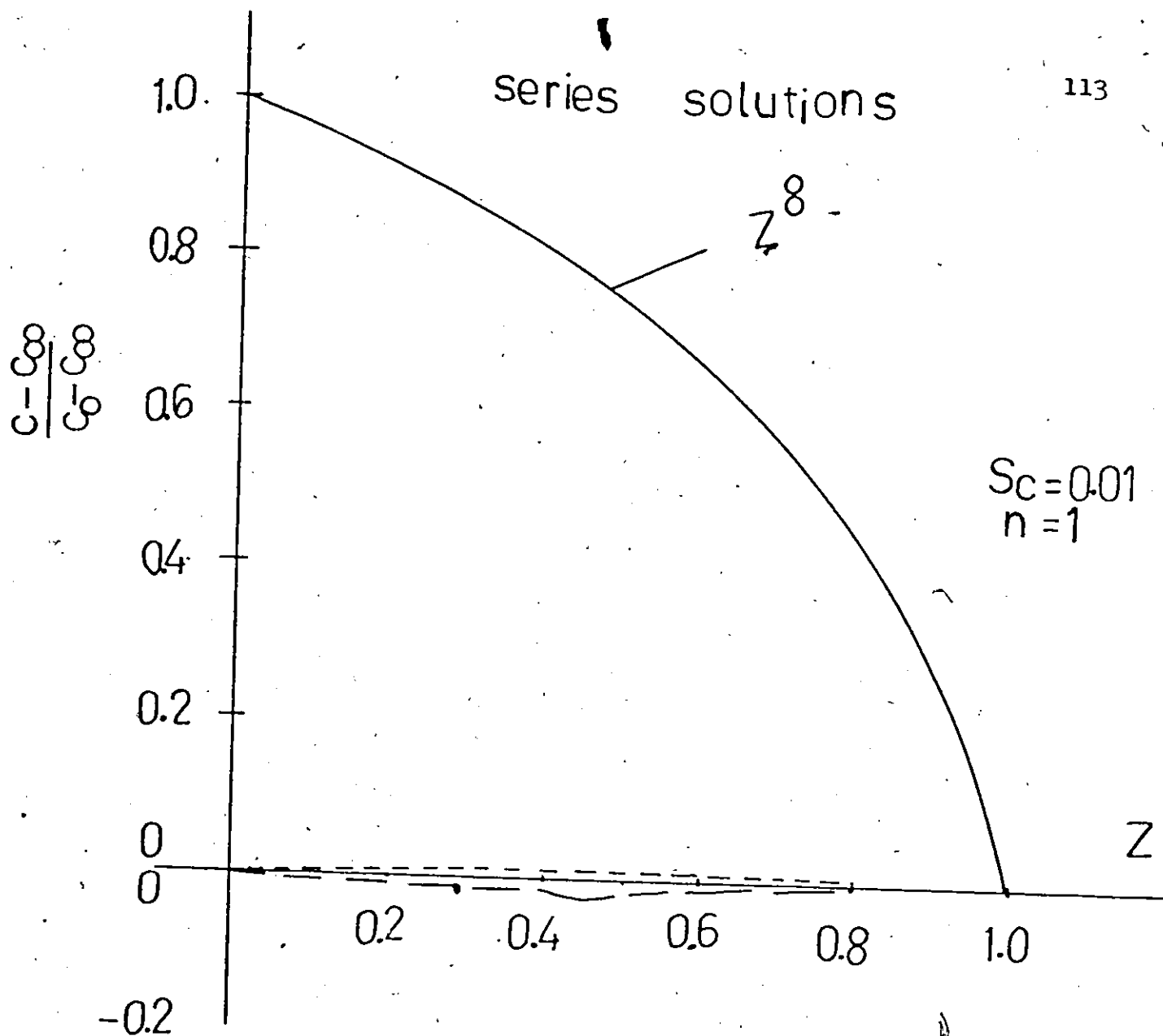
Fig. 4: Comparison of zeroth, first
and second order approximations

zeroth —————————
first — — — — —
second -----------
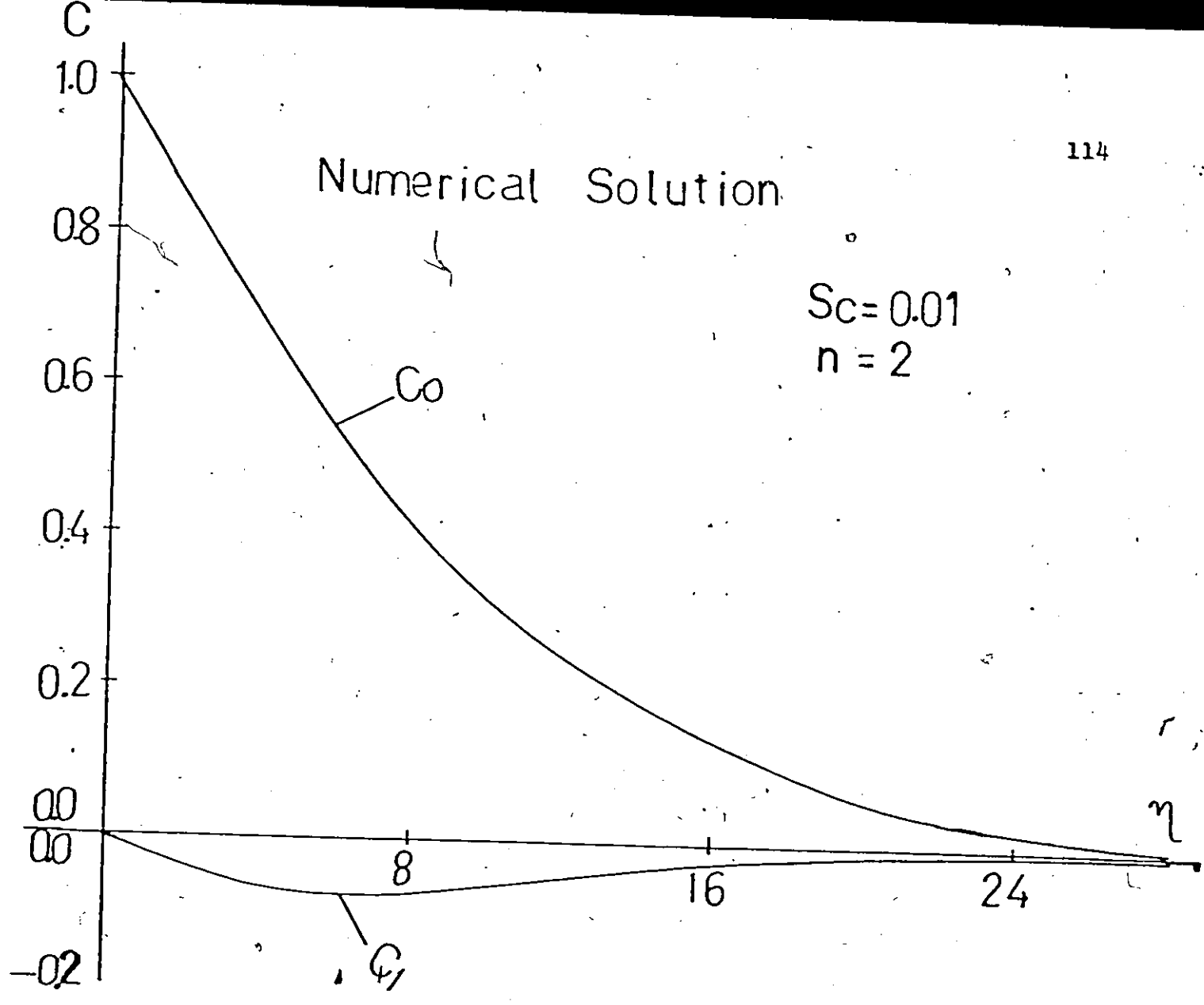
Fig. 5 : Concentration distributions in the boundary layer for uniform concentration along the plate

Fig. 6 : Concentration distributions in the boundary layer for uniform concentration along the plate
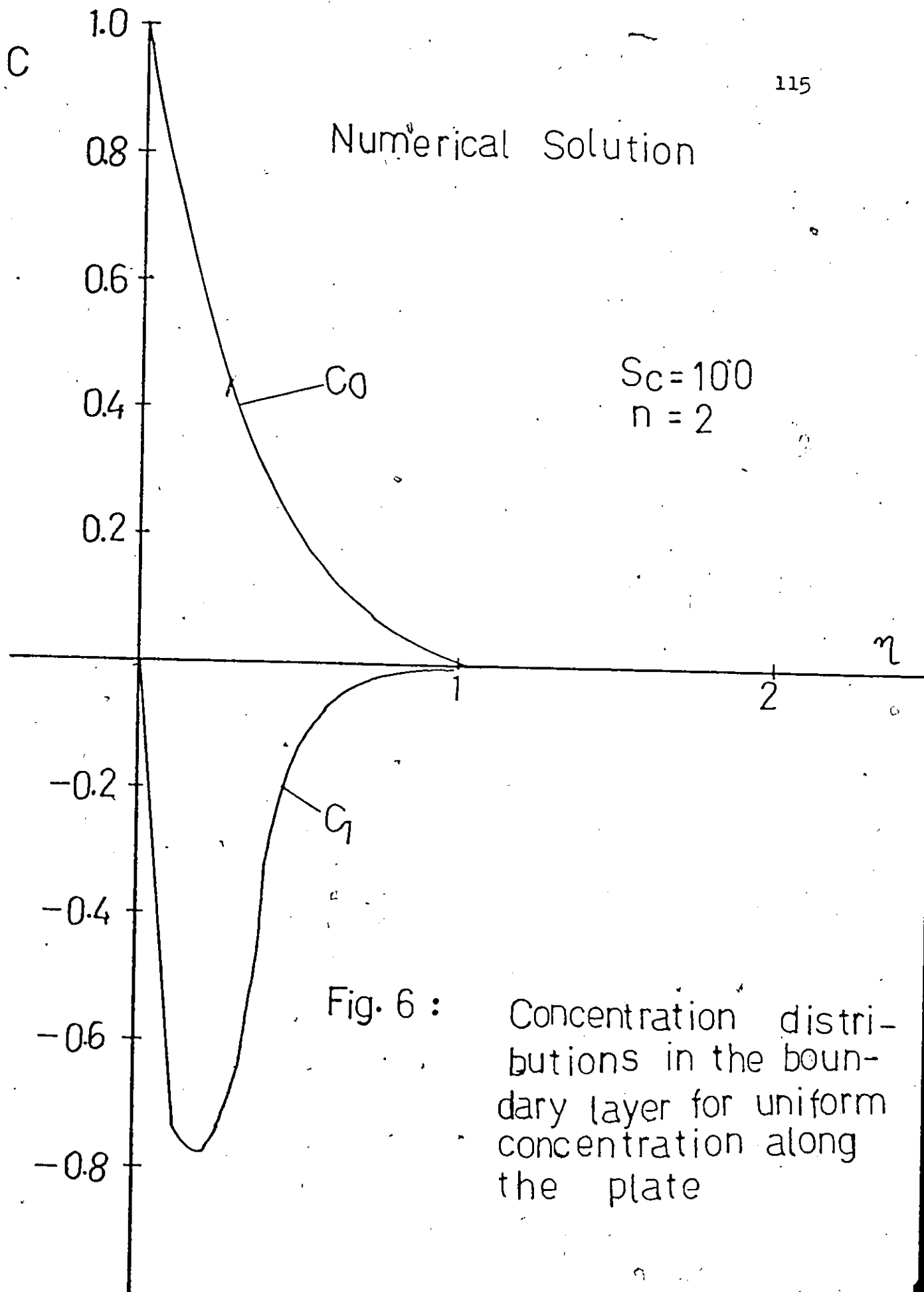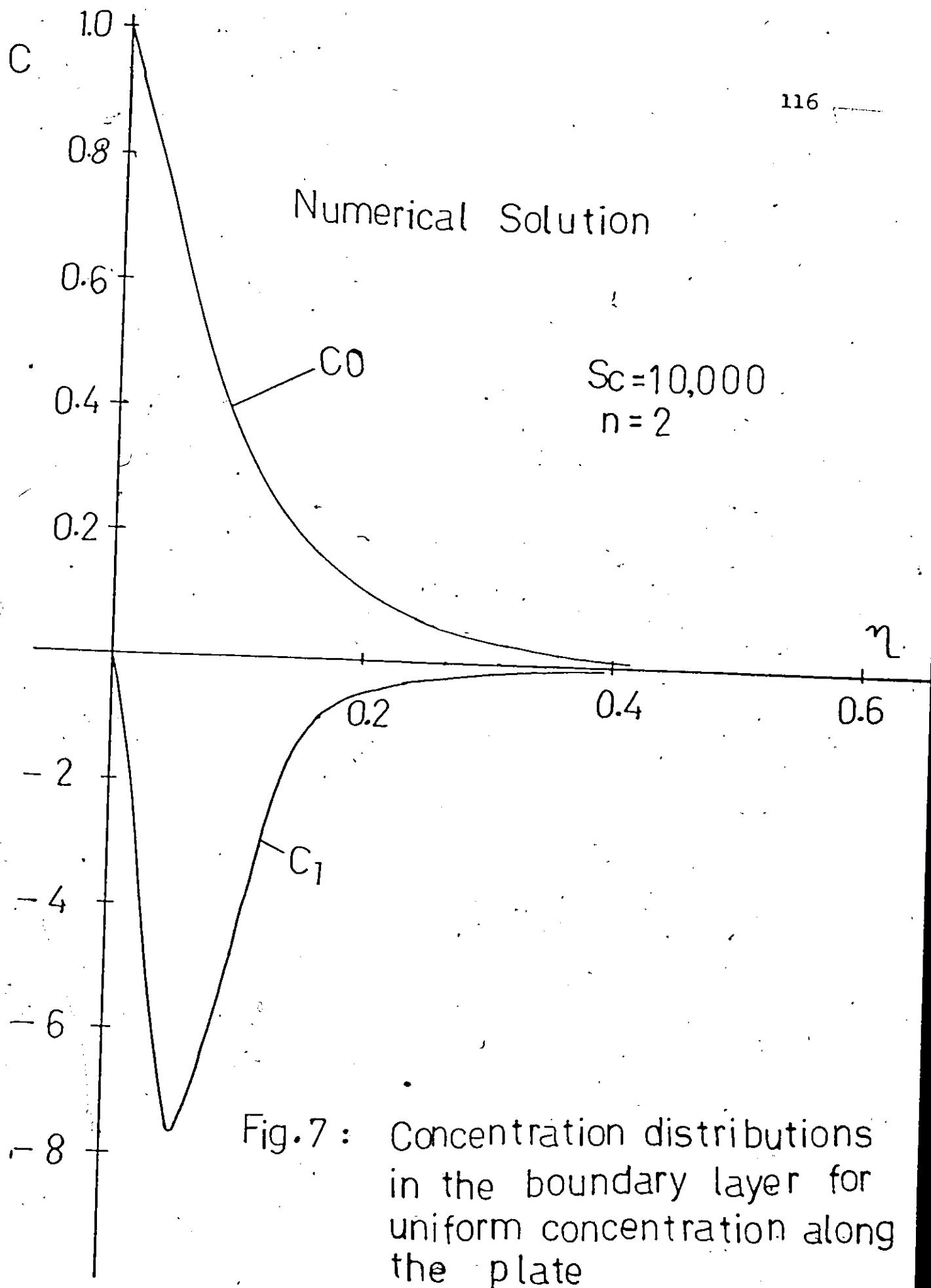
Fig.7 : Concentration distributions in the boundary layer for uniform concentration along the plate
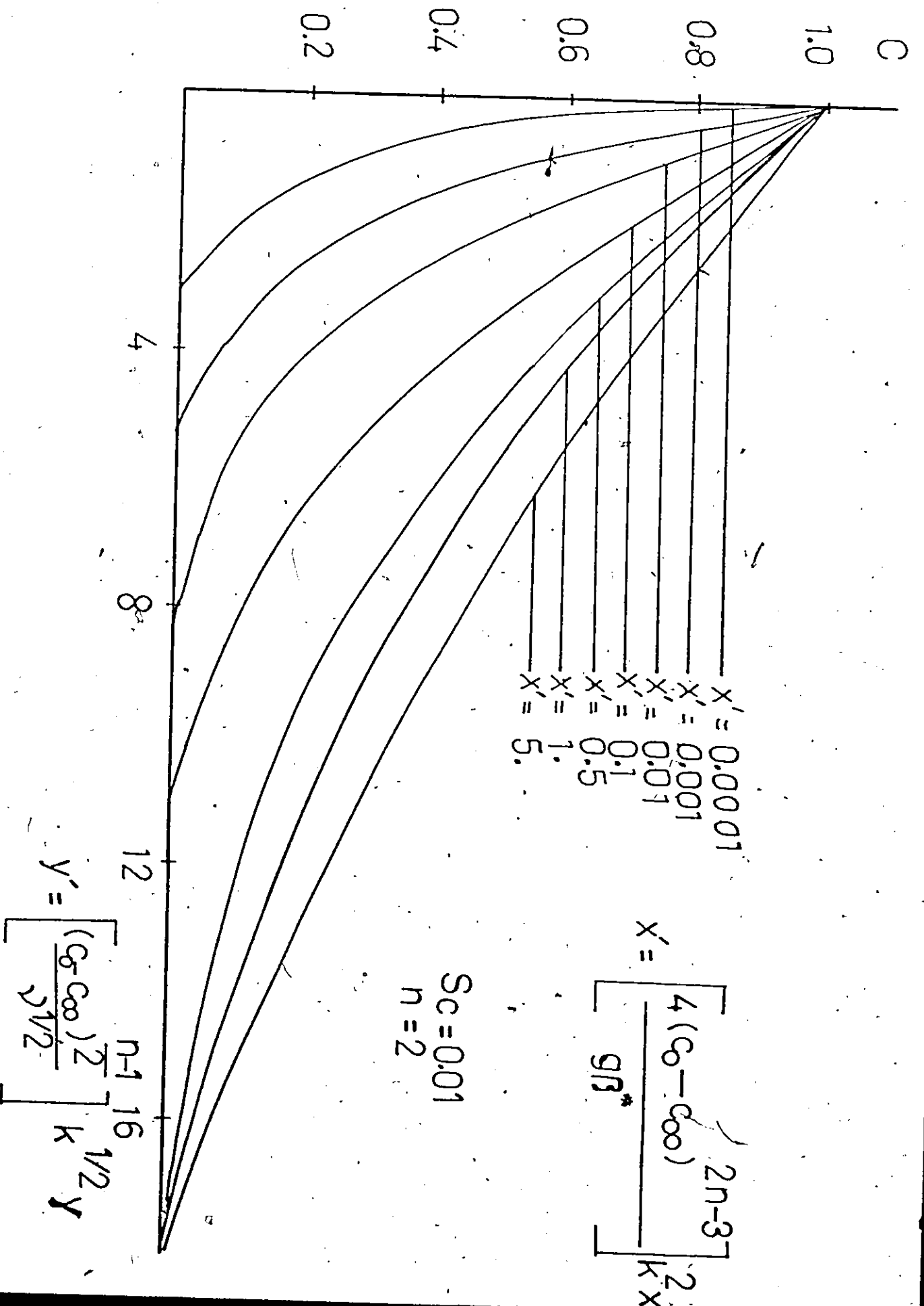
Fig.8 : Concentration distributions from first order perturbation solution

$$C$$

1.0
0.8
0.6
0.4
0.2

4

8

12

16

$$y' = \left[\frac{(C_0 - C_\infty)^{\frac{n-1}{2}}}{\nu^{1/2}} \right] k^{1/2} y$$

$$x' = \left[\frac{4(C_0 - C_\infty)^{2n-3}}{g\beta} \right]^2 k^2 x$$

$$Sc = 0.01$$
$$n = 2$$

$x' = 0.0001$
$x' = 0.001$
$x' = 0.01$
$x' = 0.1$
$x' = 0.5$
$x' = 1.$
$x' = 5.$
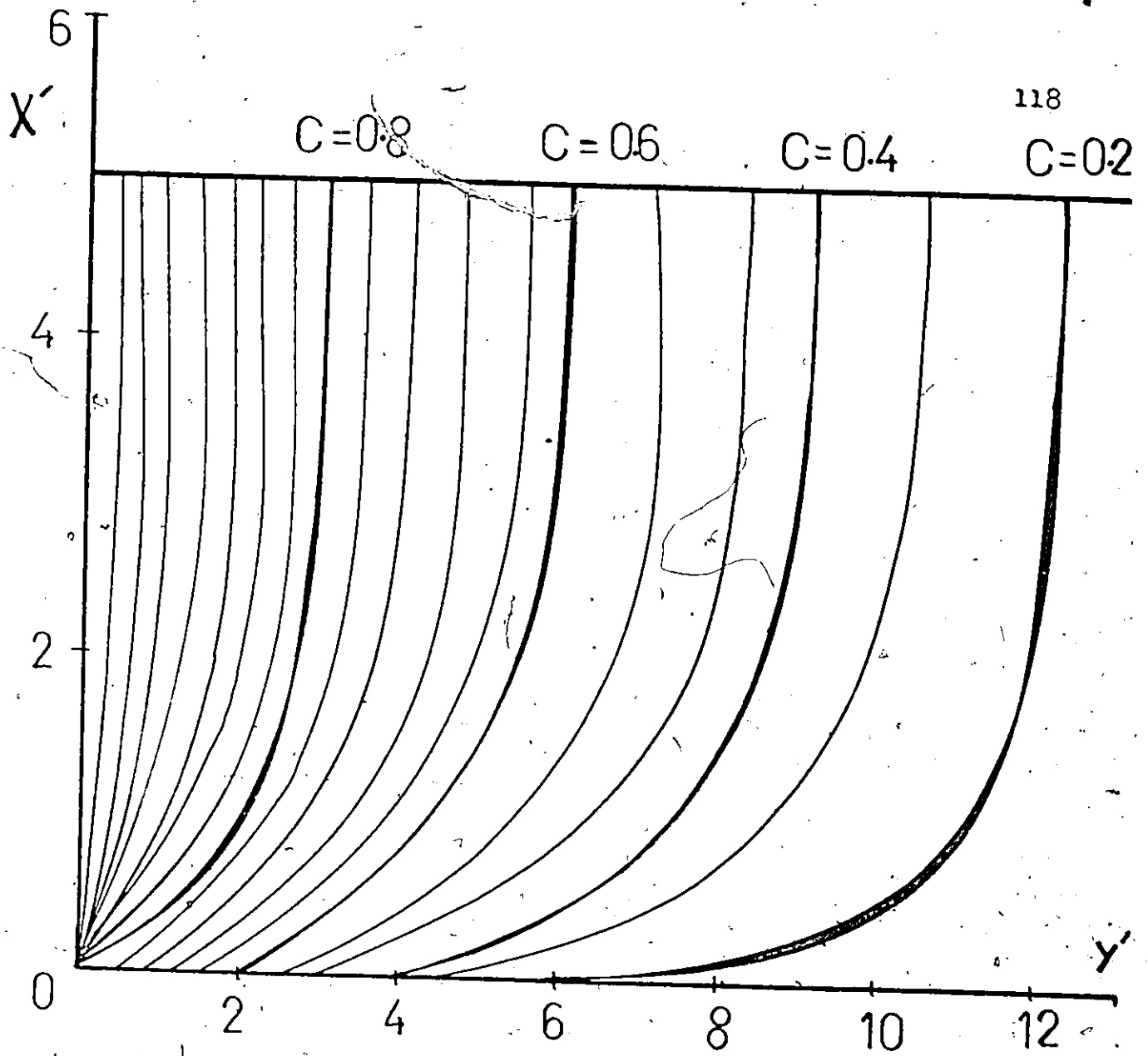
Fig. 9 : Concentration picture in the
x′-y′ plane
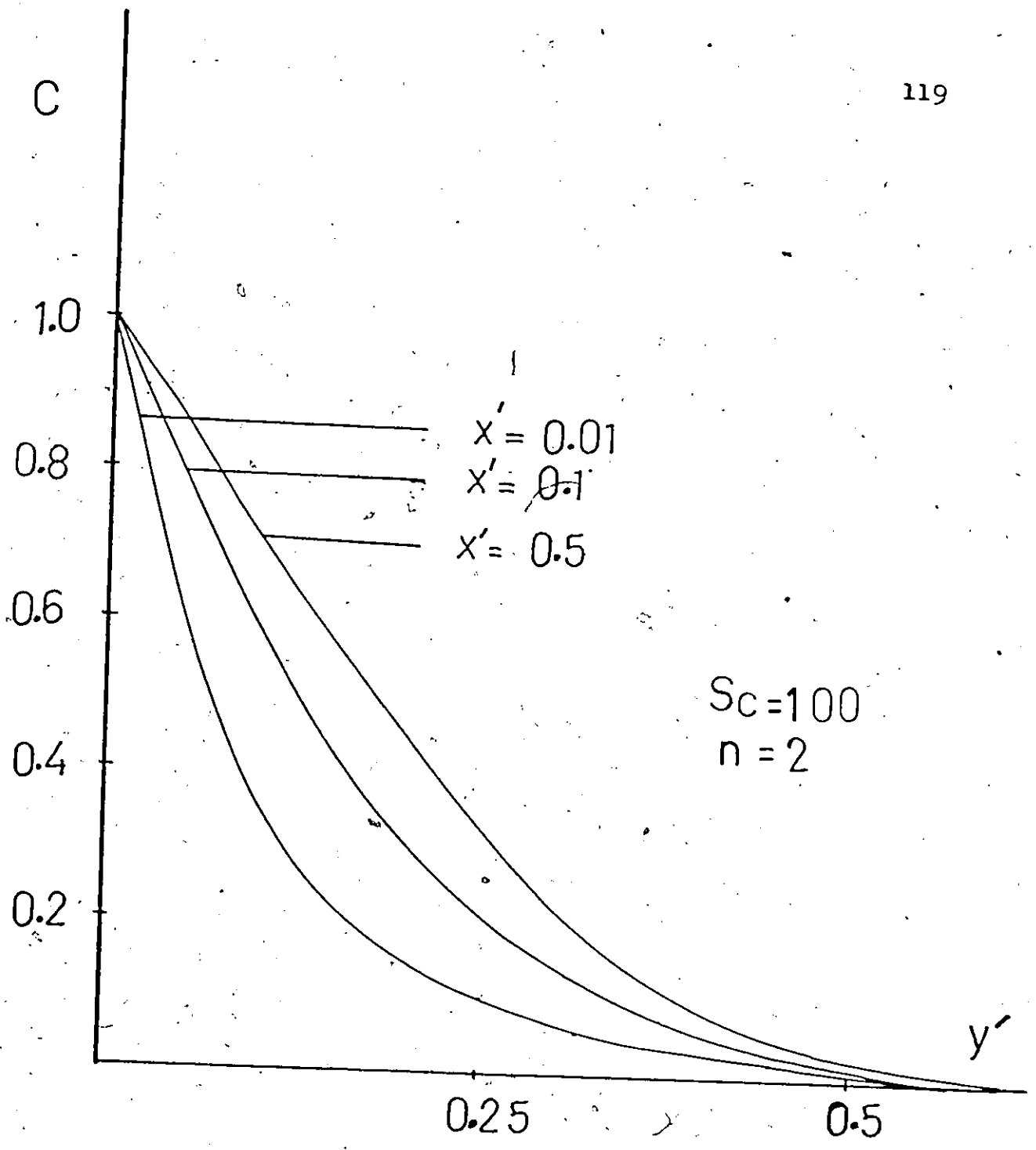
Fig.10: Concentration distributions for various x′
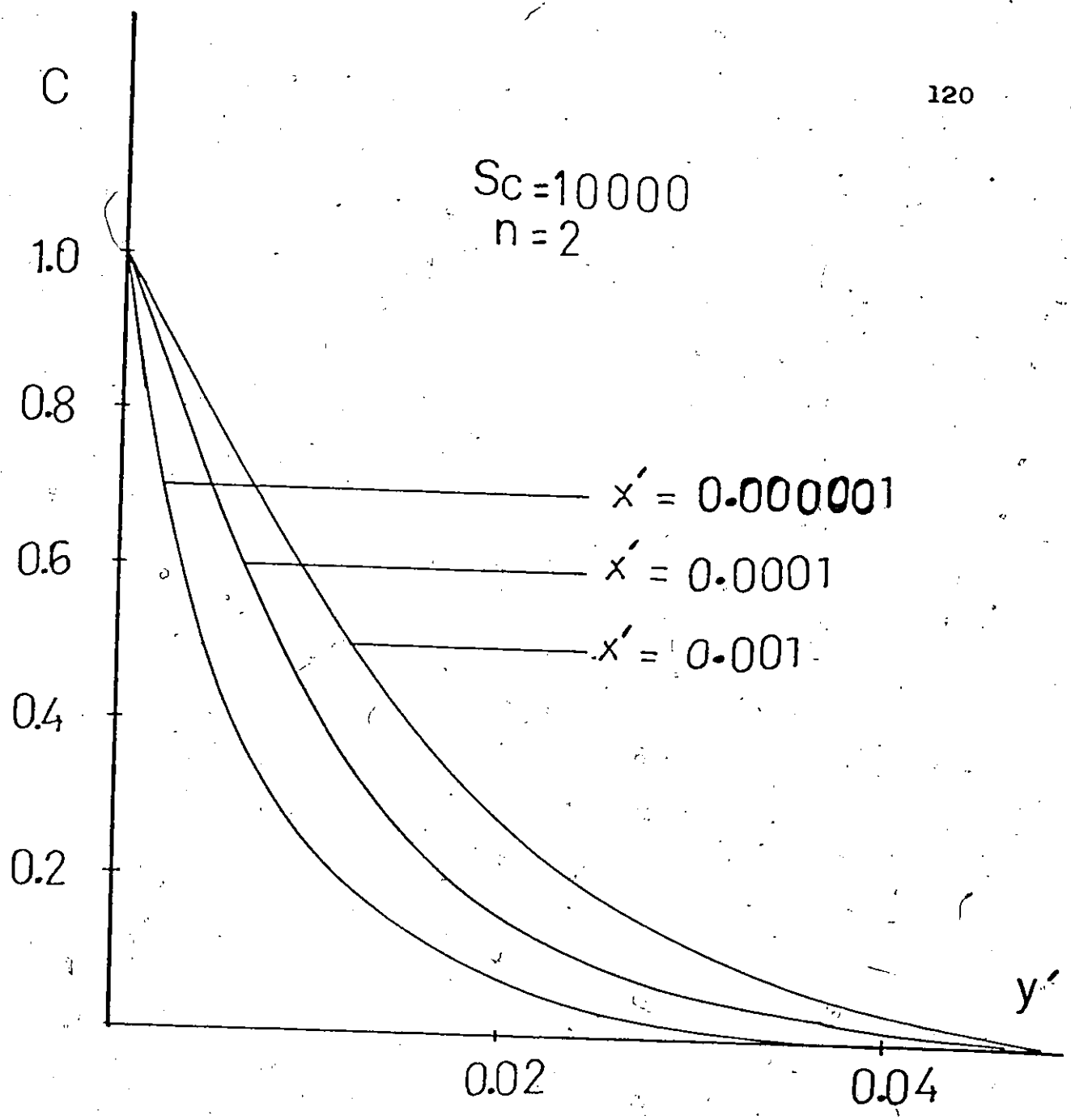
Fig·11: Concentration distributions for various x′
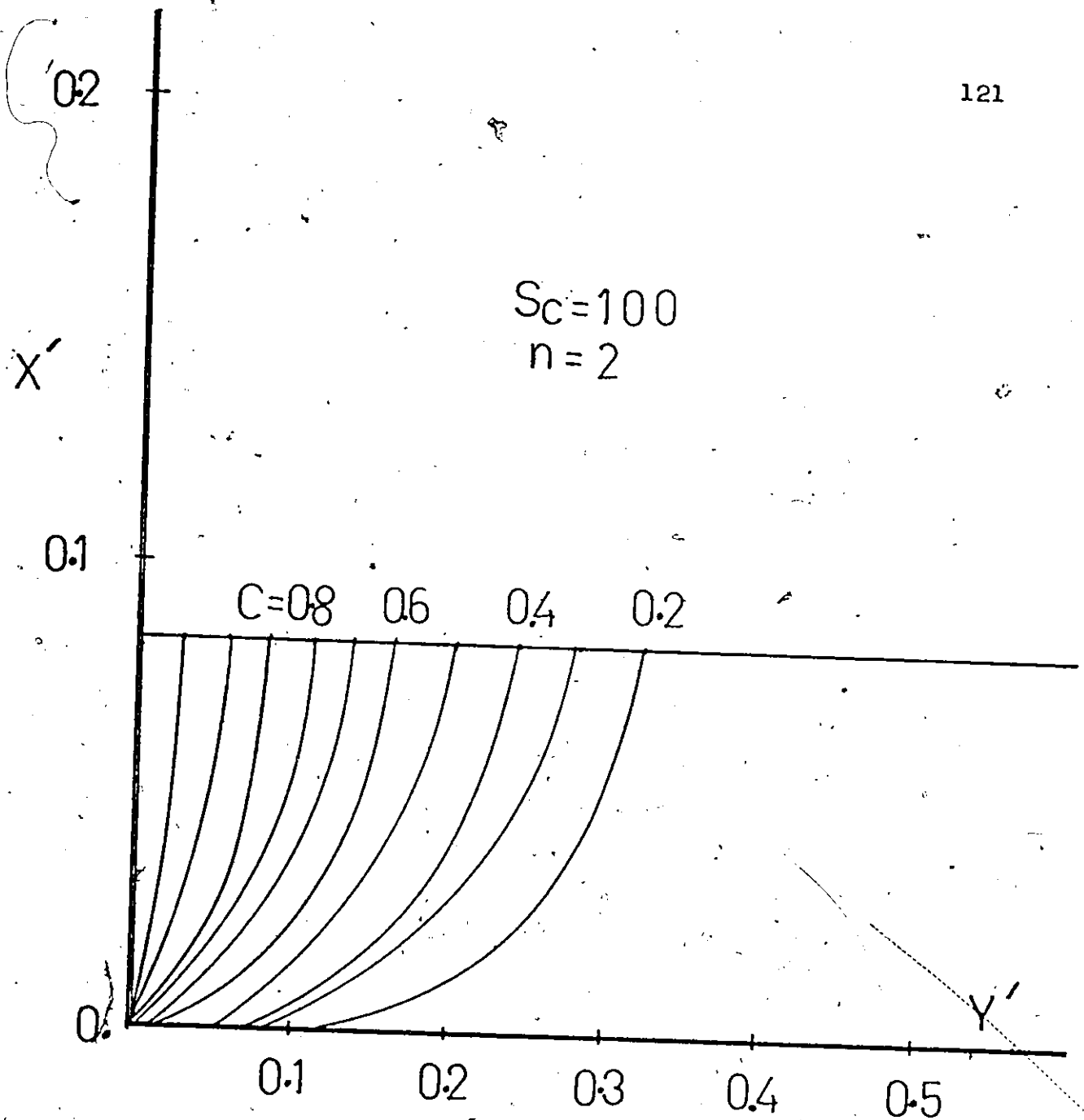
Fig.12: concentration picture in the x́-ý plane
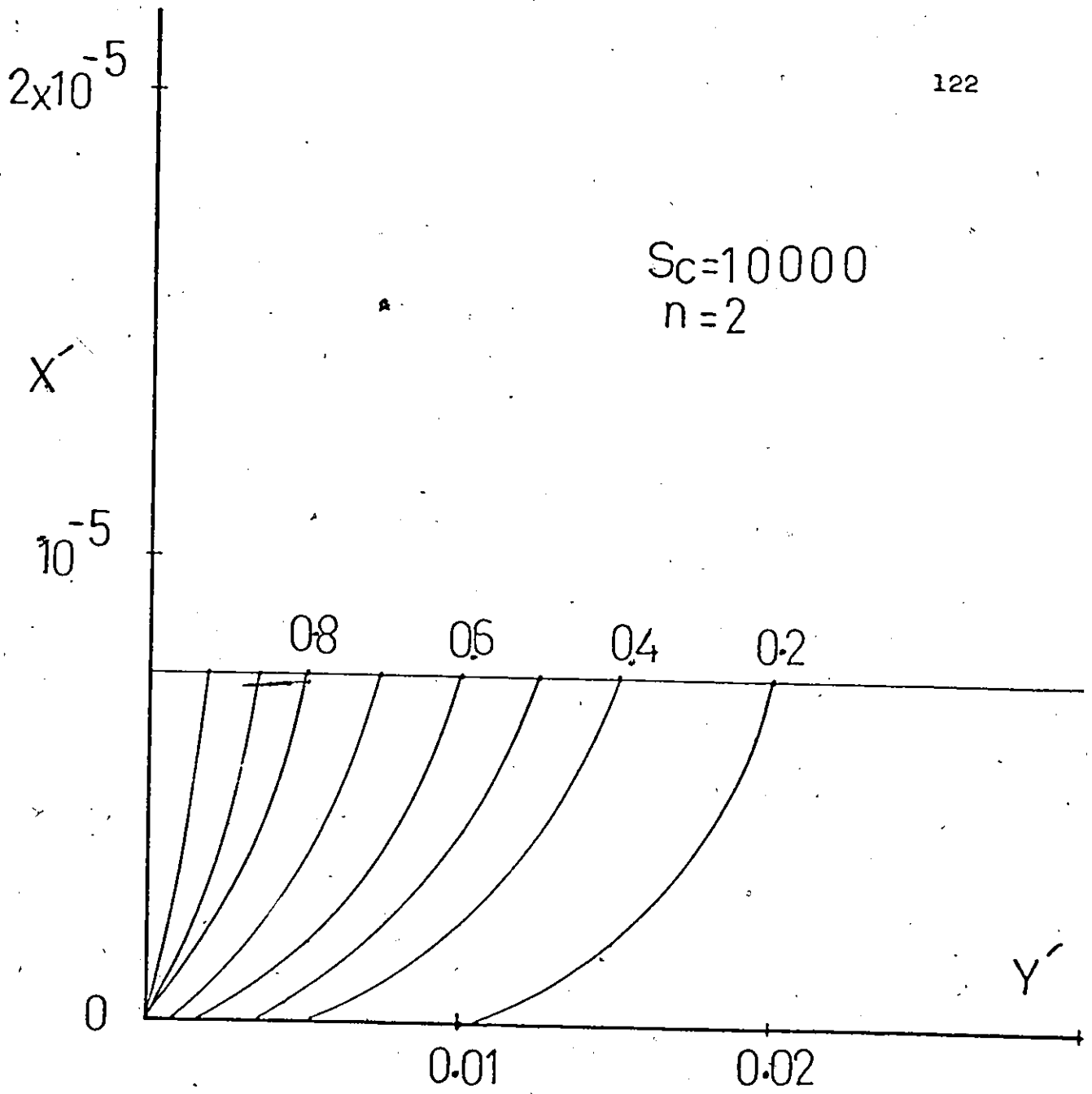
Fig.13 : concentration picture in the x'-y' plane

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$$u' = \frac{u}{(g\beta^*)/k(c_0 - c_\infty)^2}$$
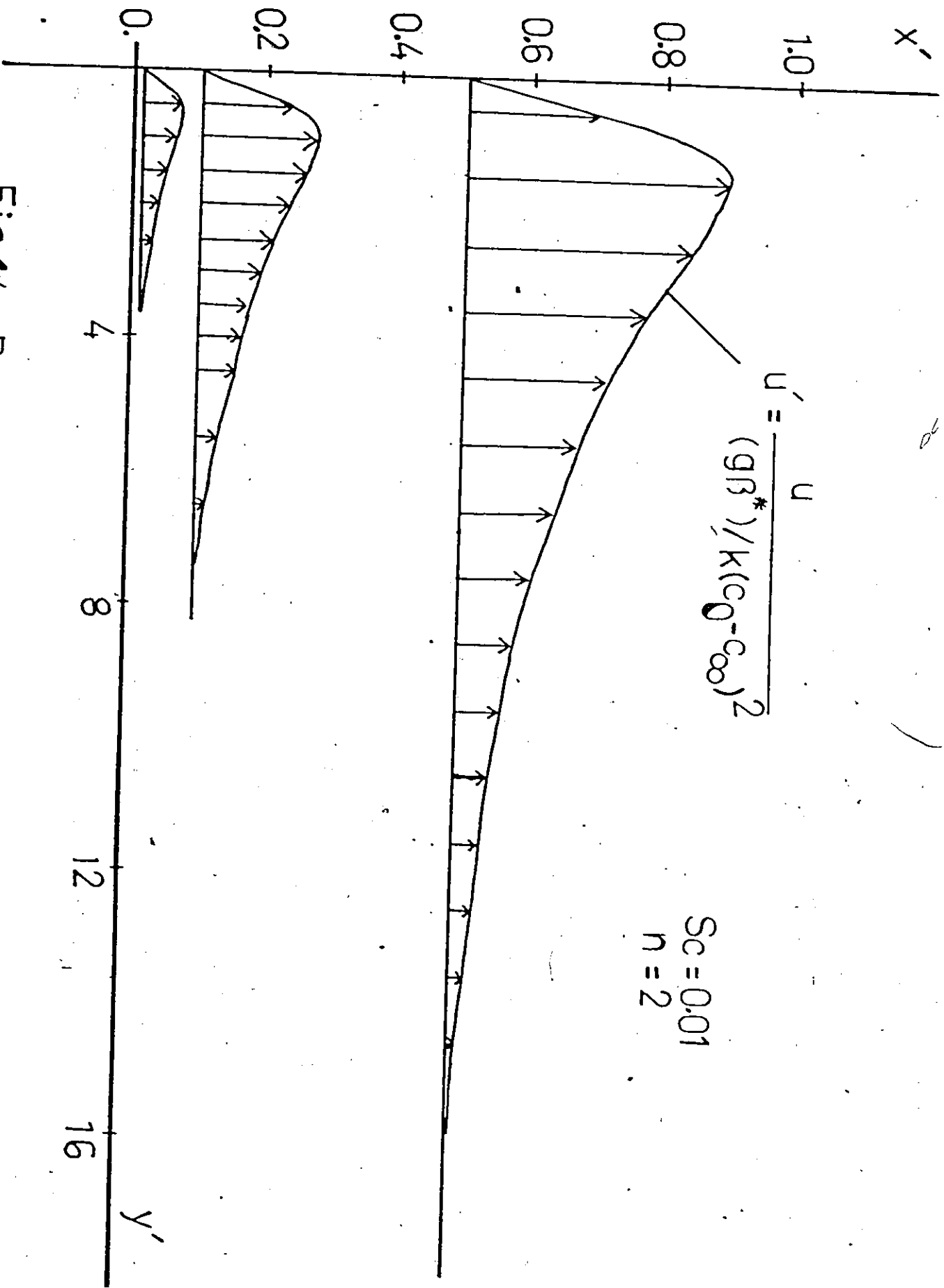
Sc = 0.01
n = 2

Fig.14 : Boundary layer growth
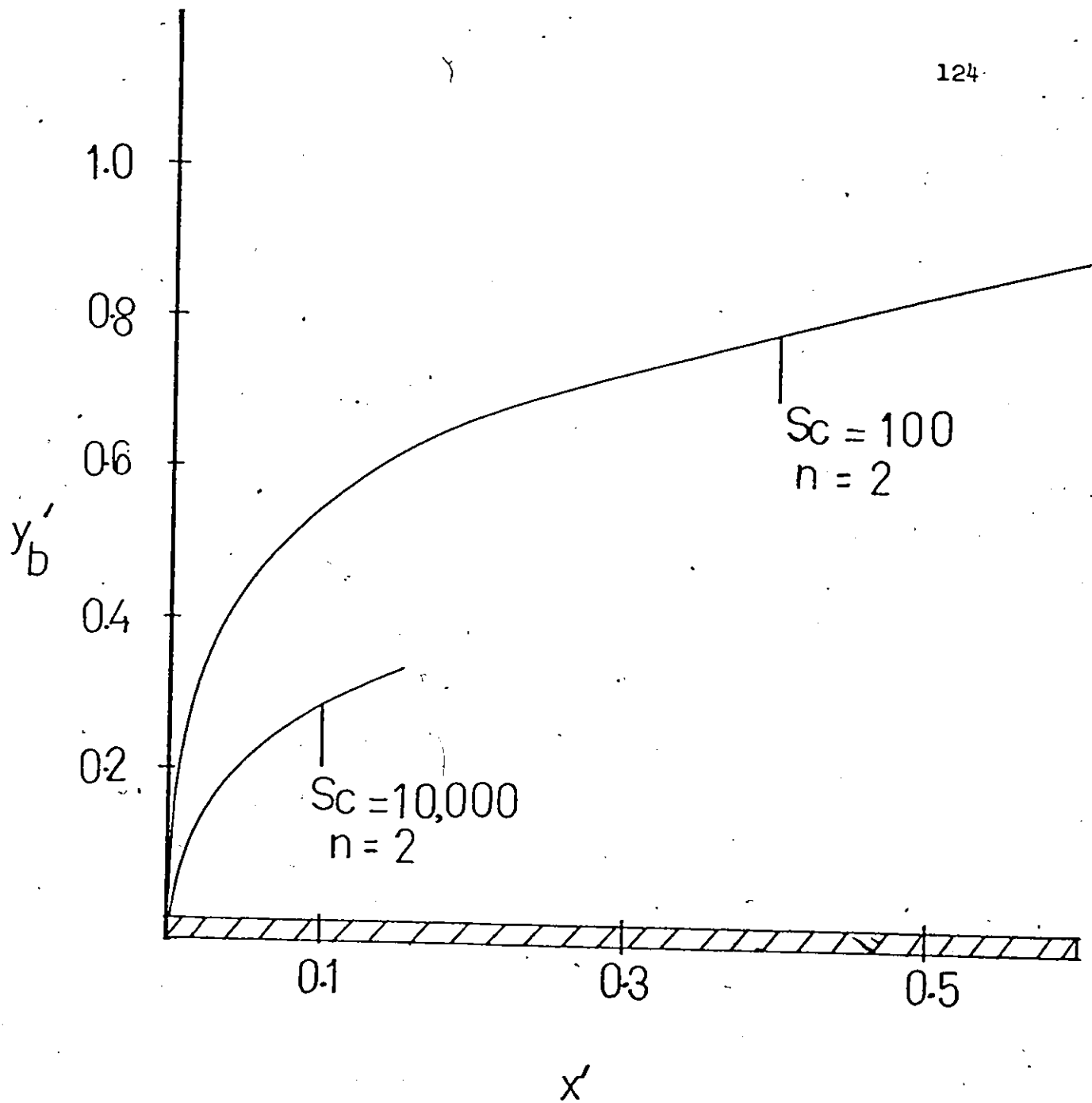
Fig. 15 : Boundary layer thickness in the $x'-y'_b$ plane
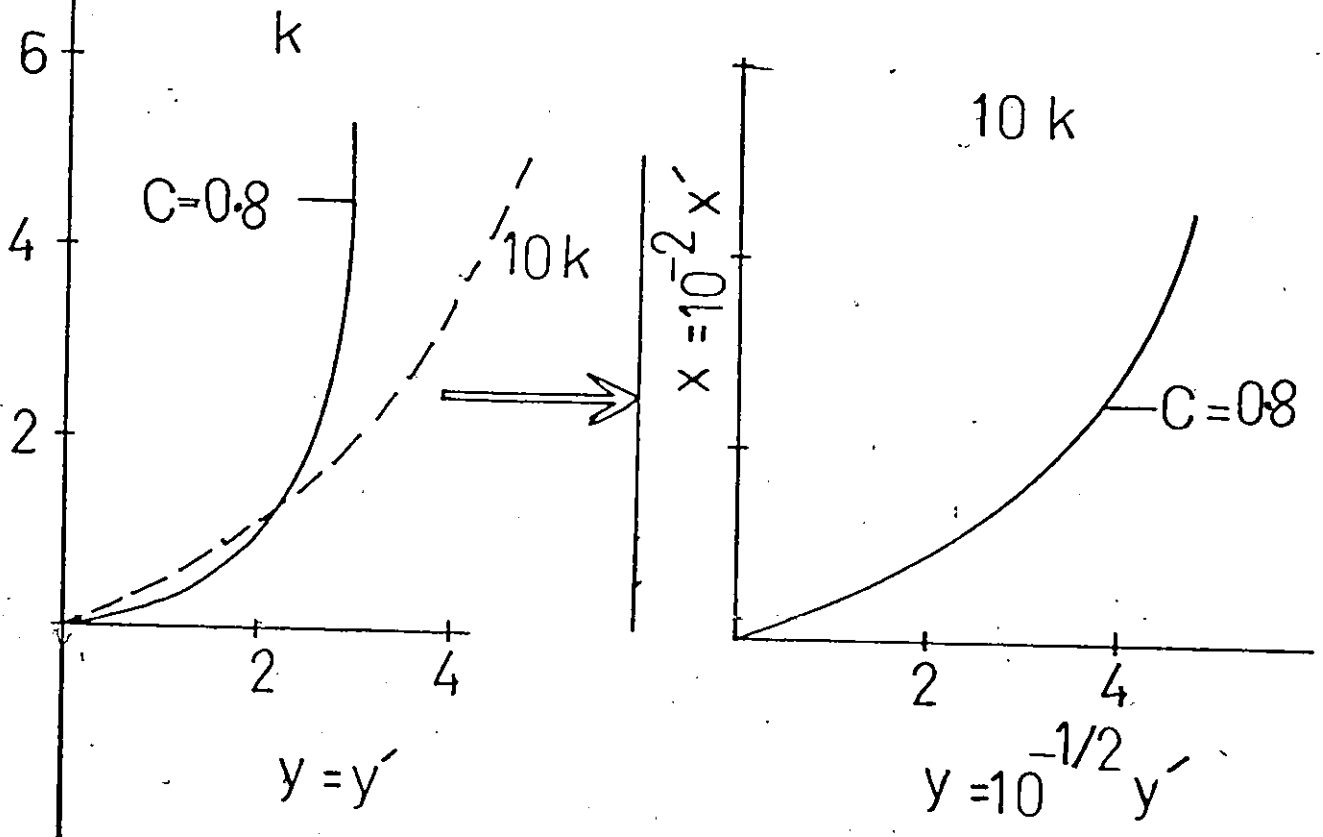
Fig.16: Effect of chemical reaction
rate on concentration
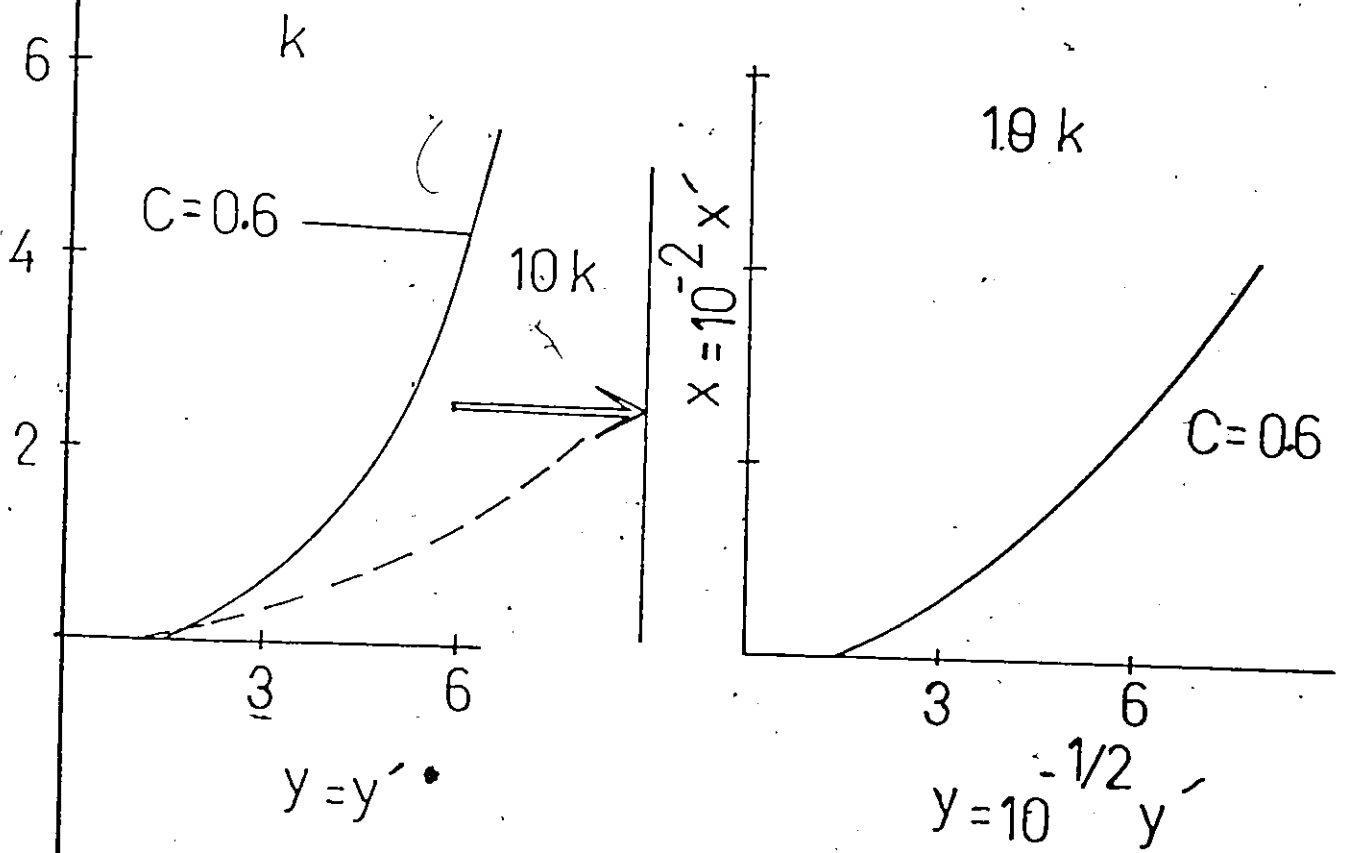
Fig·17: effect of reaction rate on concentration
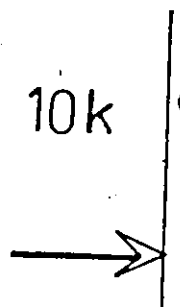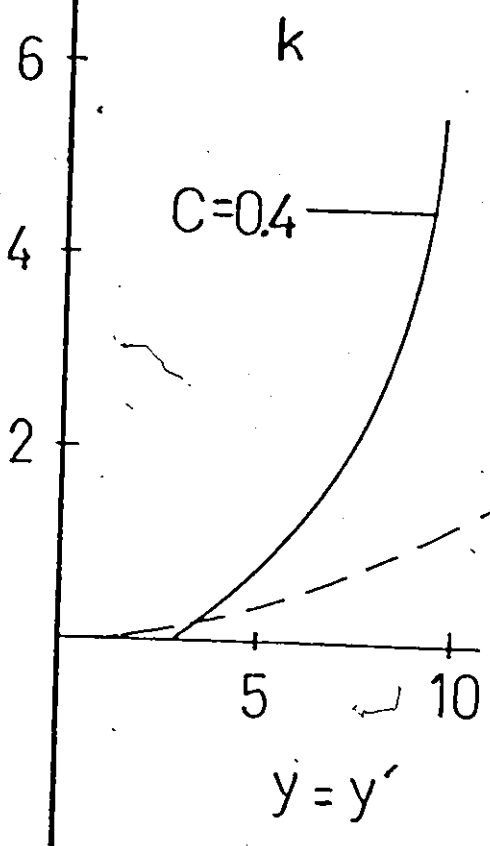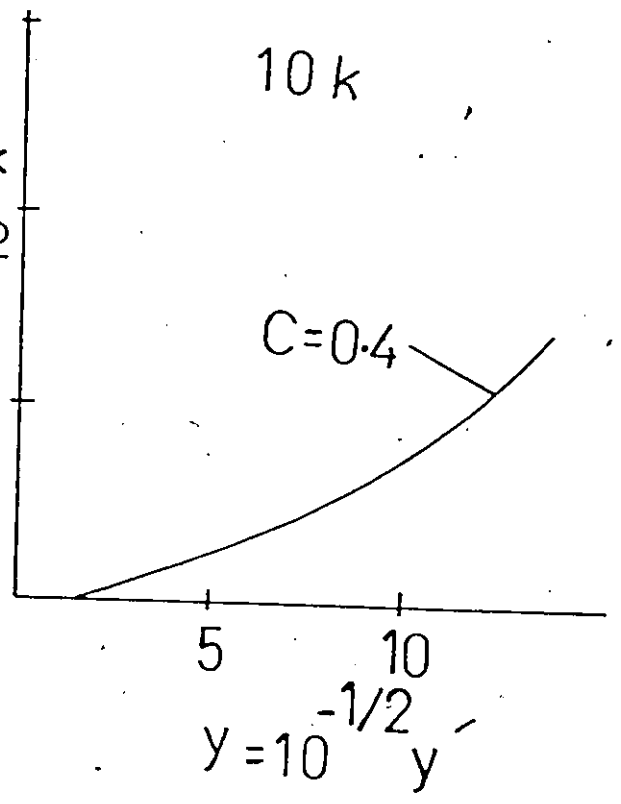
Fig.18: effect of reaction rate on concentration
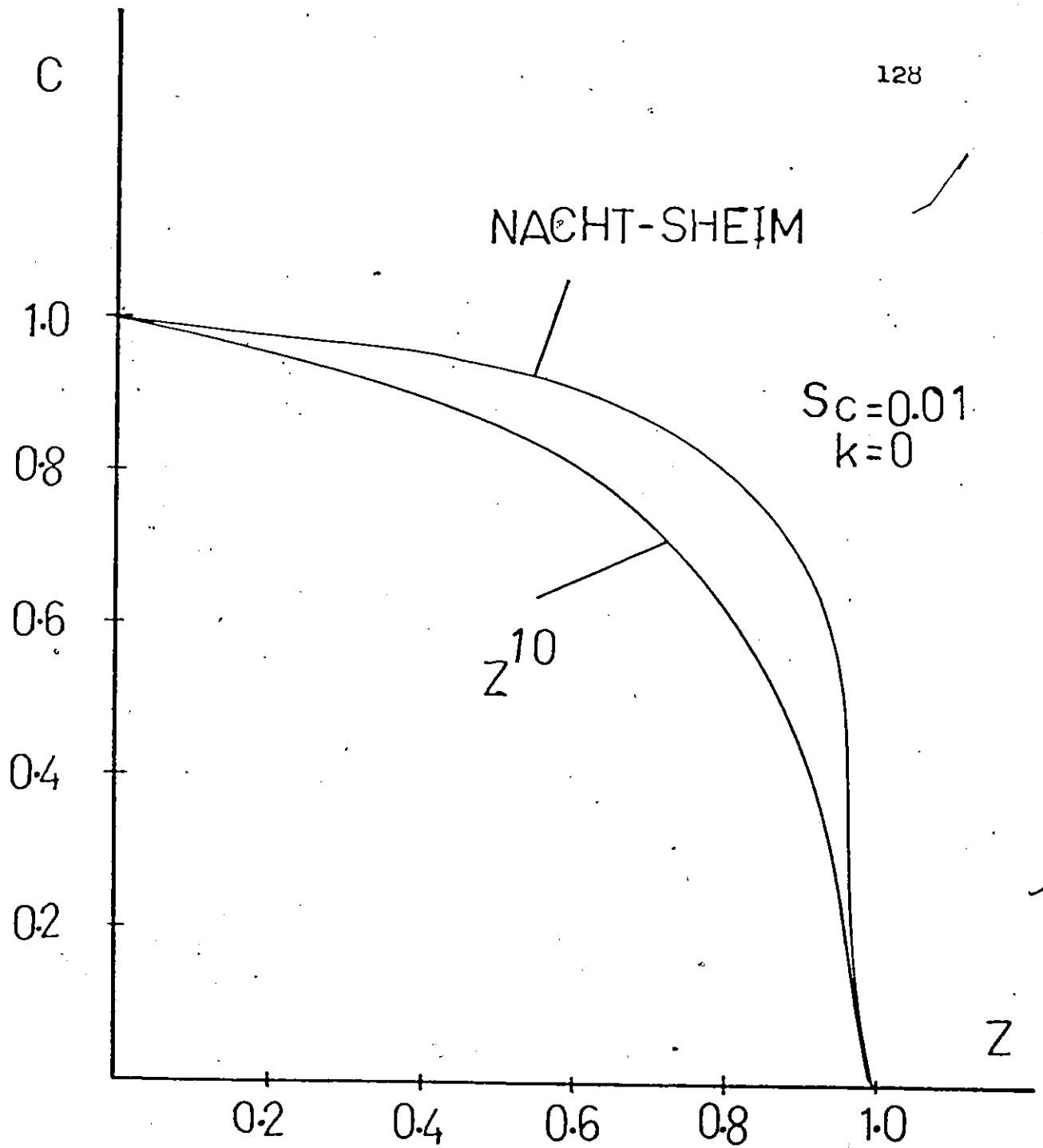
Fig. 19.: Comparison between numerical
and series solutions of
concentration without reaction
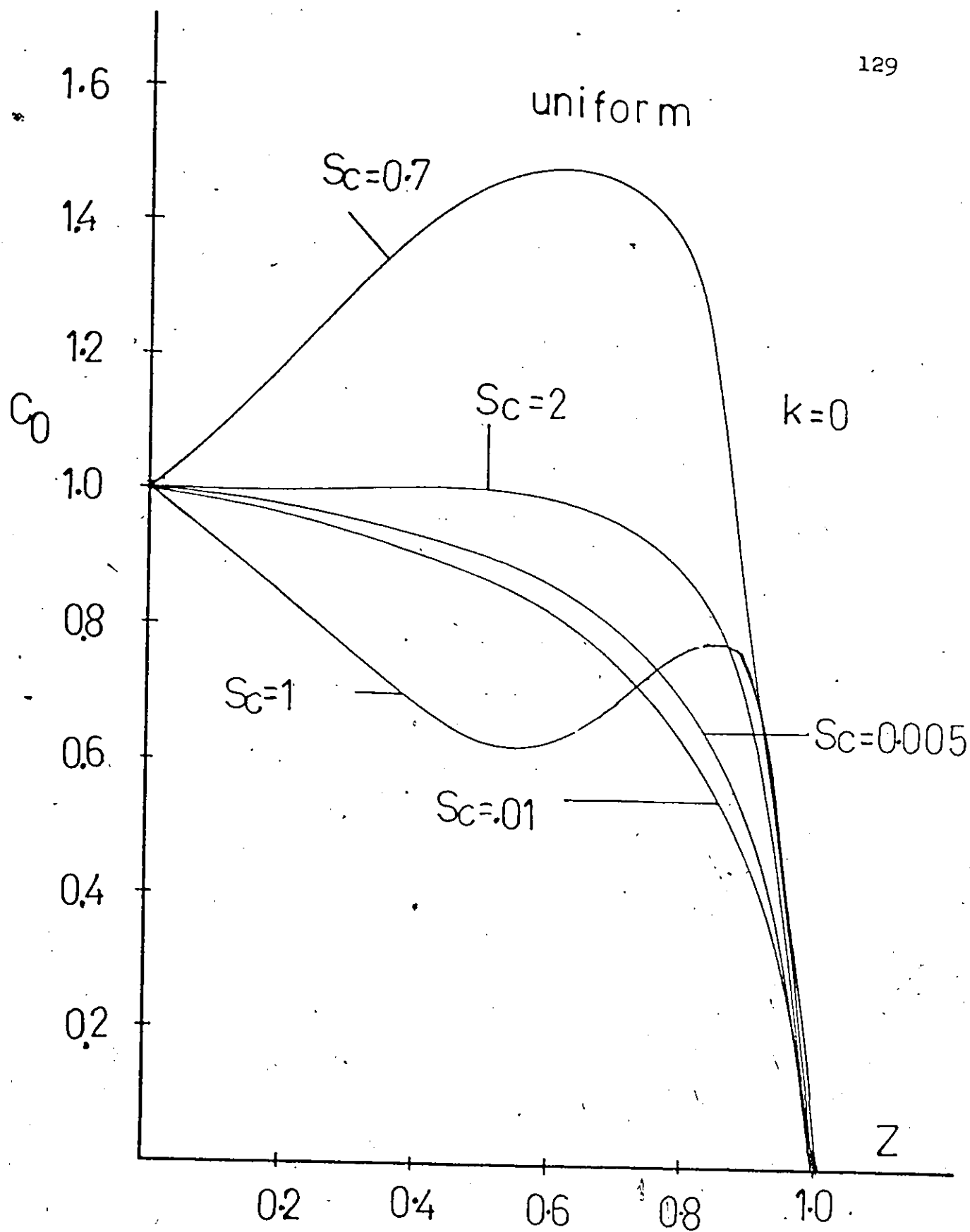
Fig.20: stability of series solution upto Z^{10}

series solution upto Z^8

$$Sc = 0.01$$
$$n = 1$$

$$\left|\frac{C_2}{C_1}\right|$$

.002

.001

2   4   6   8   10   12

η
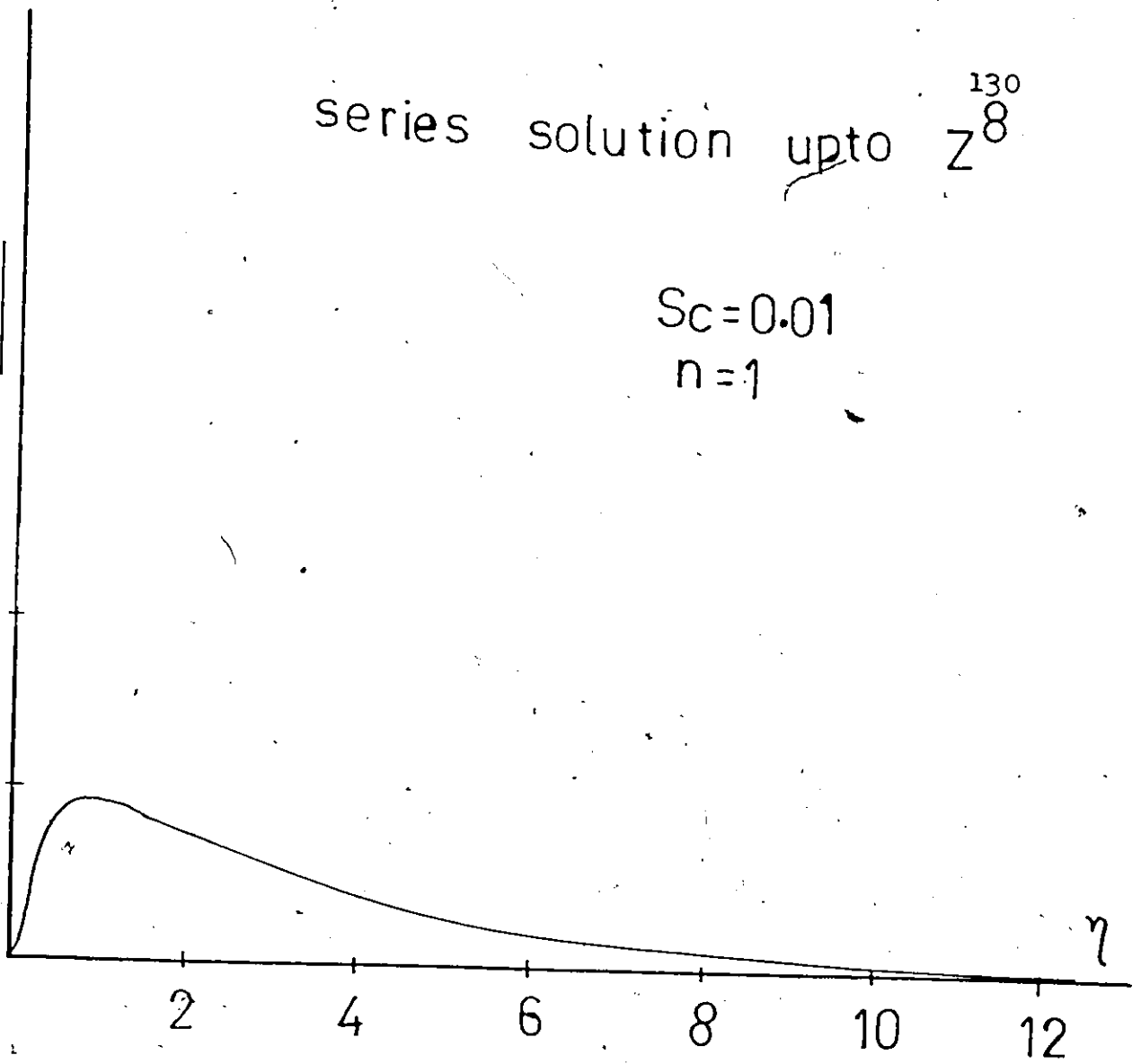
Fig. 21: graph of $\left|\dfrac{C_2}{C_1}\right|$ as a function

of η
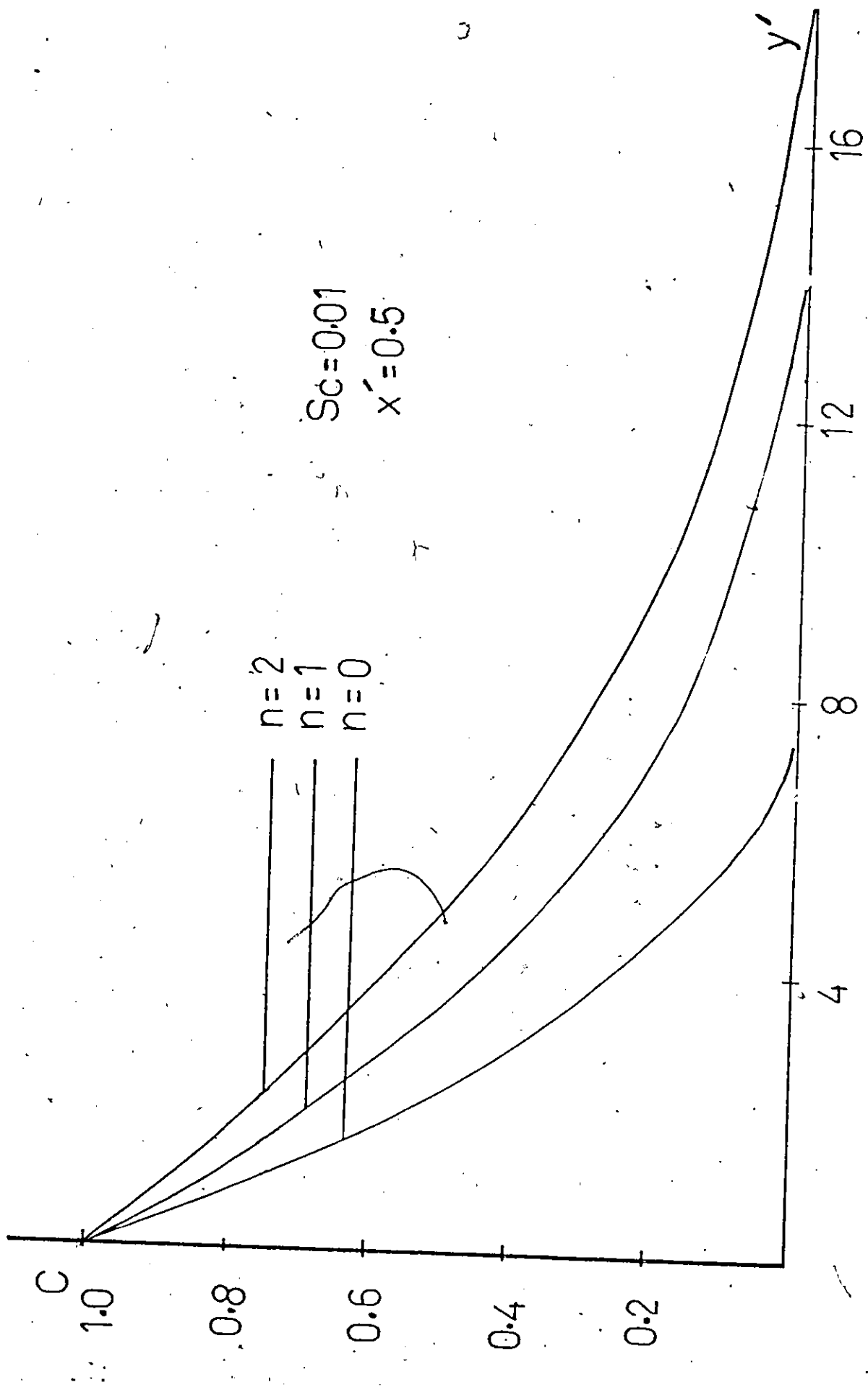
Fig. 22: numerical solutions of concentrations for uniform concentration at the plate

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$$u' = \frac{u}{(g\beta^*)/k(C_0^* - C_\infty)2n-2}$$

$$Sc = 0.01$$
$$x' = 0.5$$

n=2
n=1
n=0
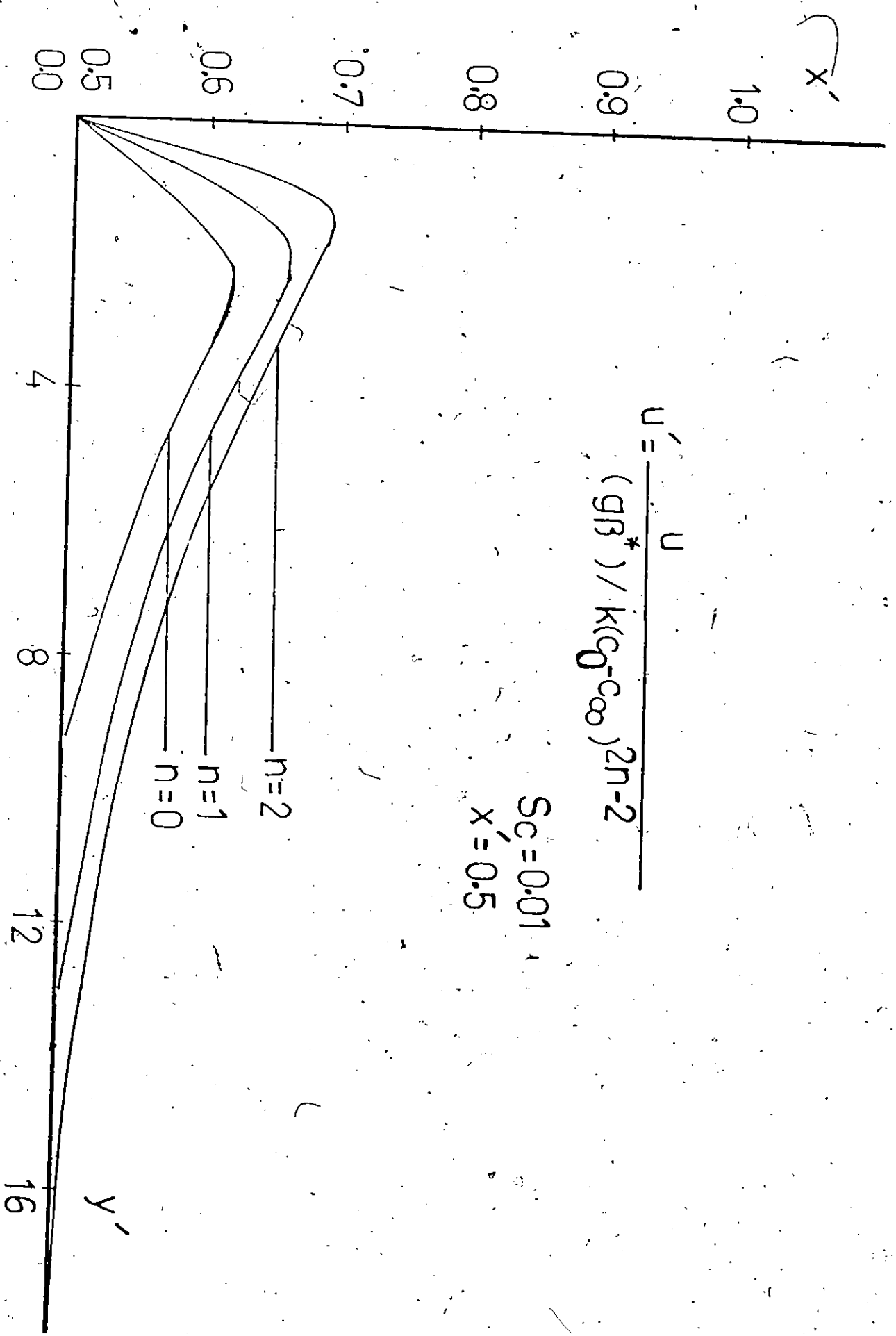
Fig.23: numerical solutions of velocity for uniform concentration at the plate
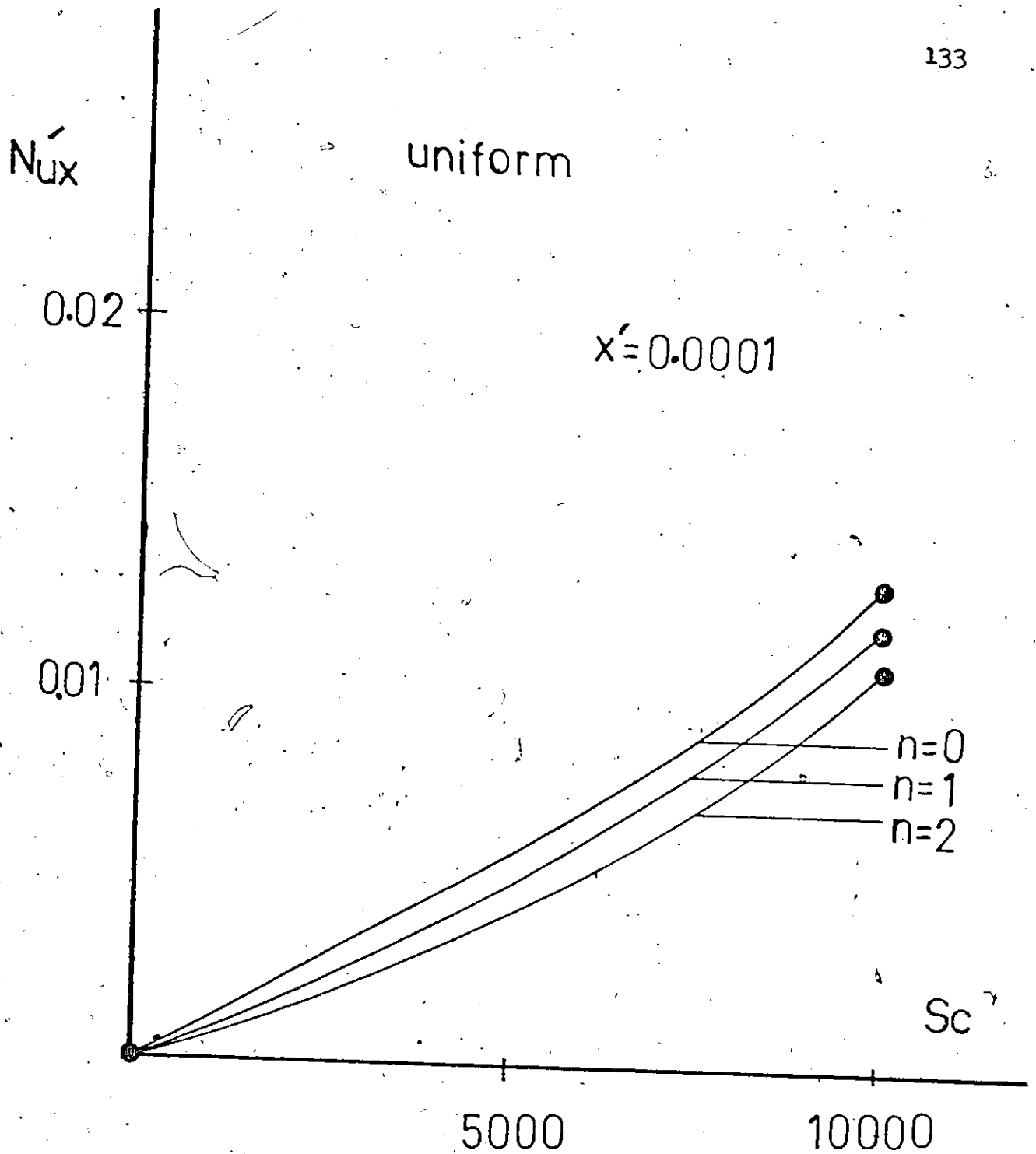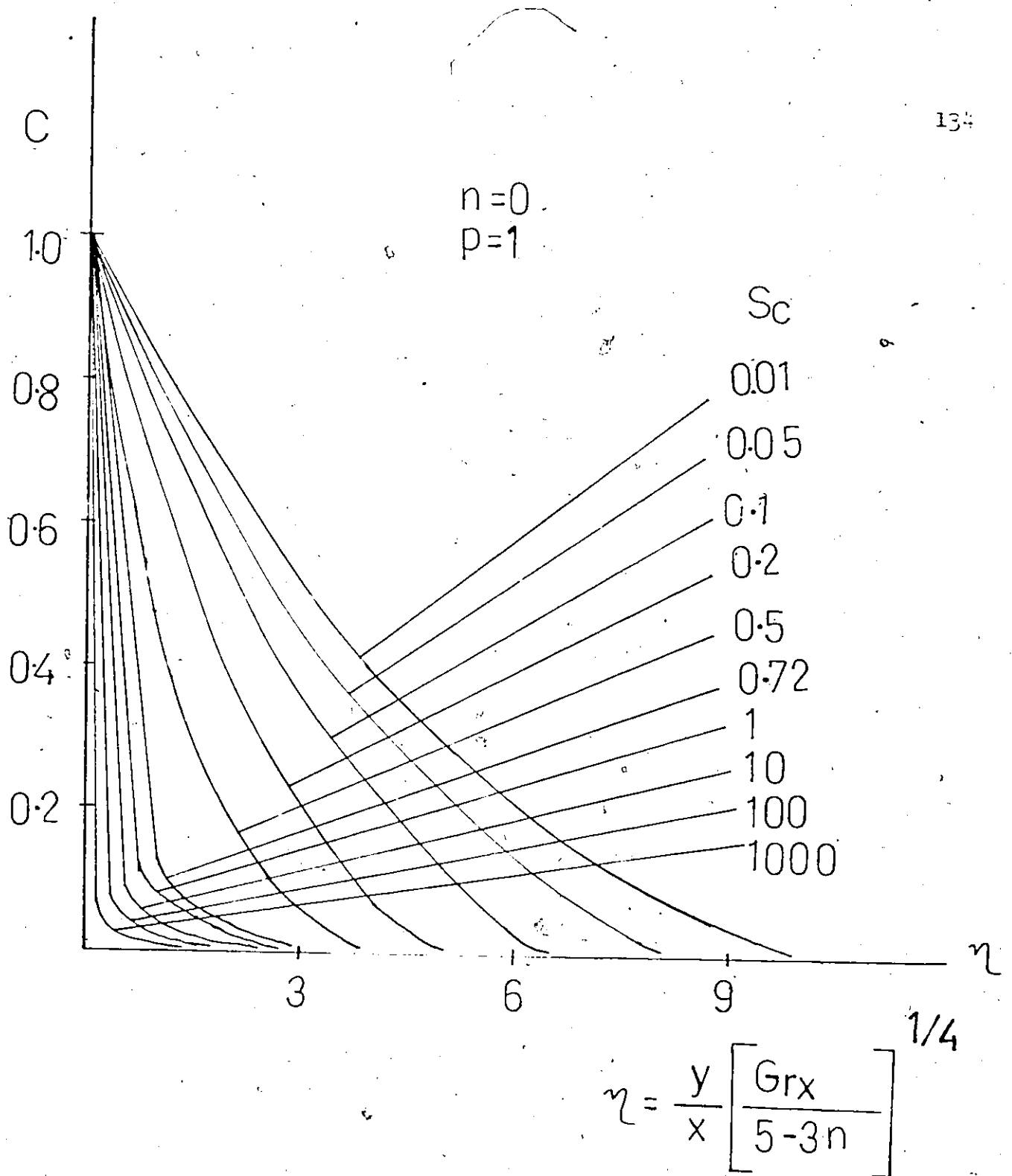
Fig. 24: mass flux as a function of Schmidt number

C

1.0

0.8

0.6

0.4

0.2

n = 0
p = 1

Sc

0.01
0.05
0.1
0.2
0.5
0.72
1
10
100
1000

3   6   9 η

$$\eta = \frac{y}{x}\left[\frac{Gr_x}{5-3n}\right]^{1/4}$$

Fig. 25: results of numerical solutions of concentration distributions for the distributed concentration along the plate
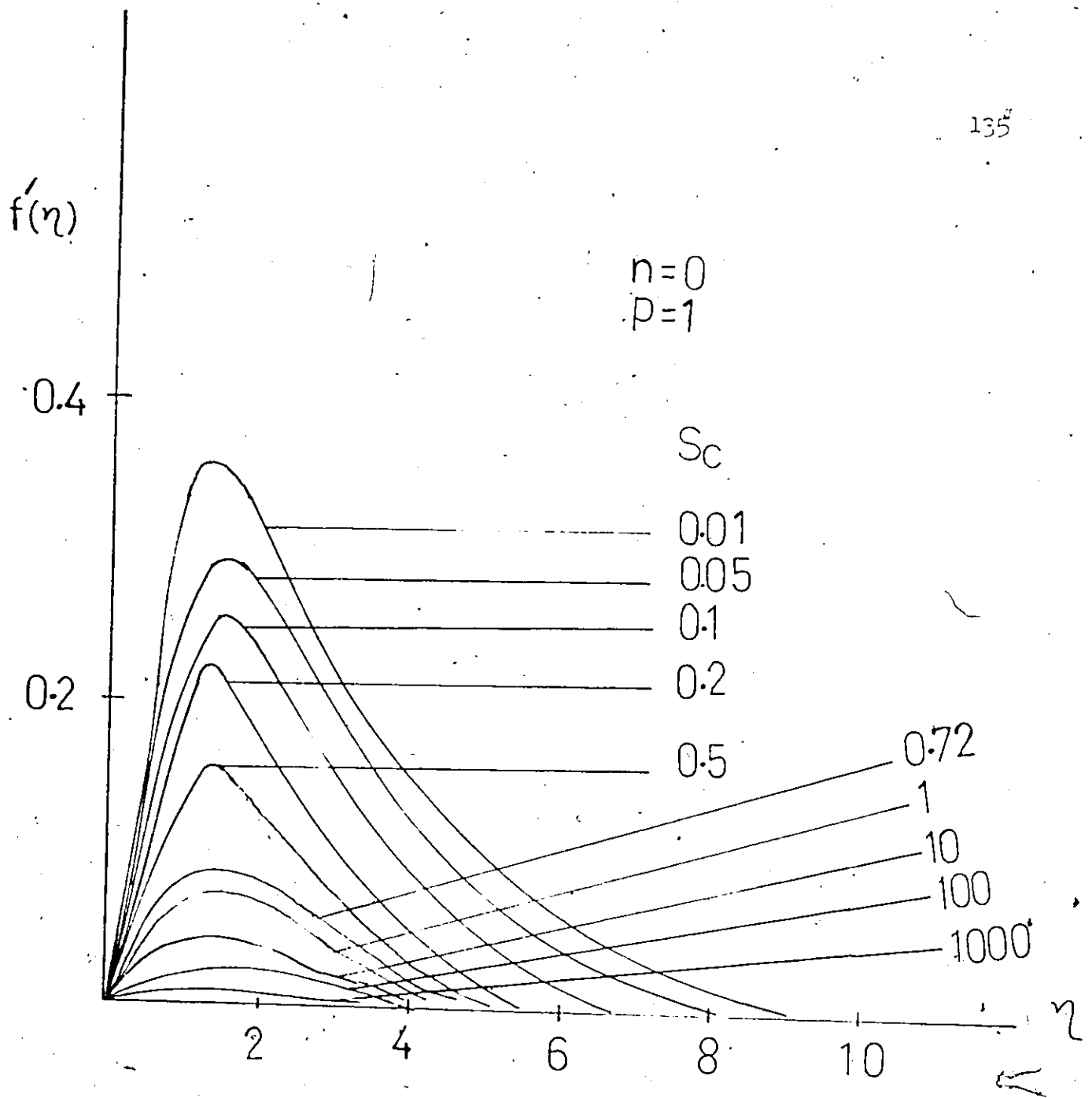
Fig·26: results of numerical solutions of velocity distributions for the distributed concentration along the plate
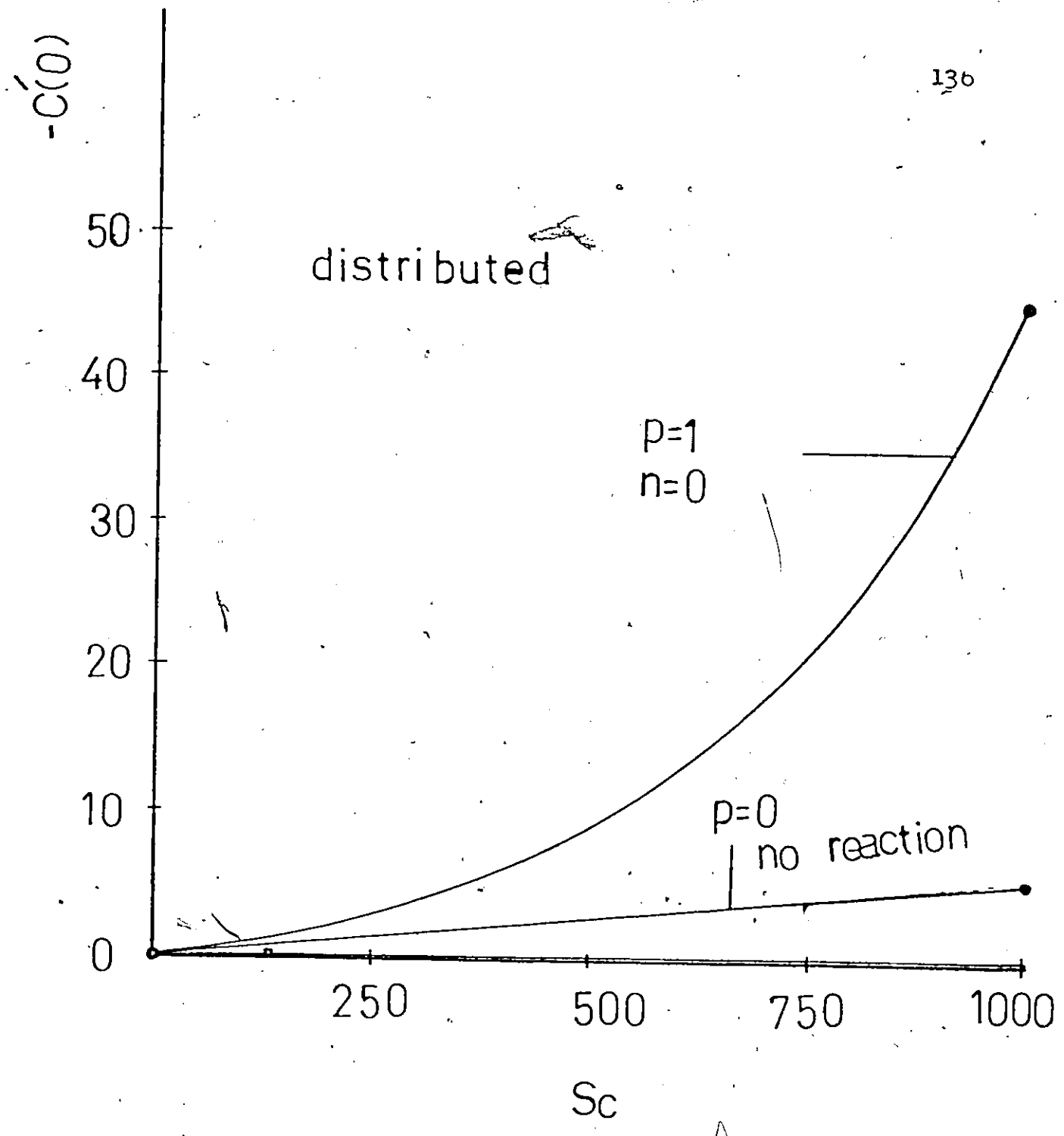
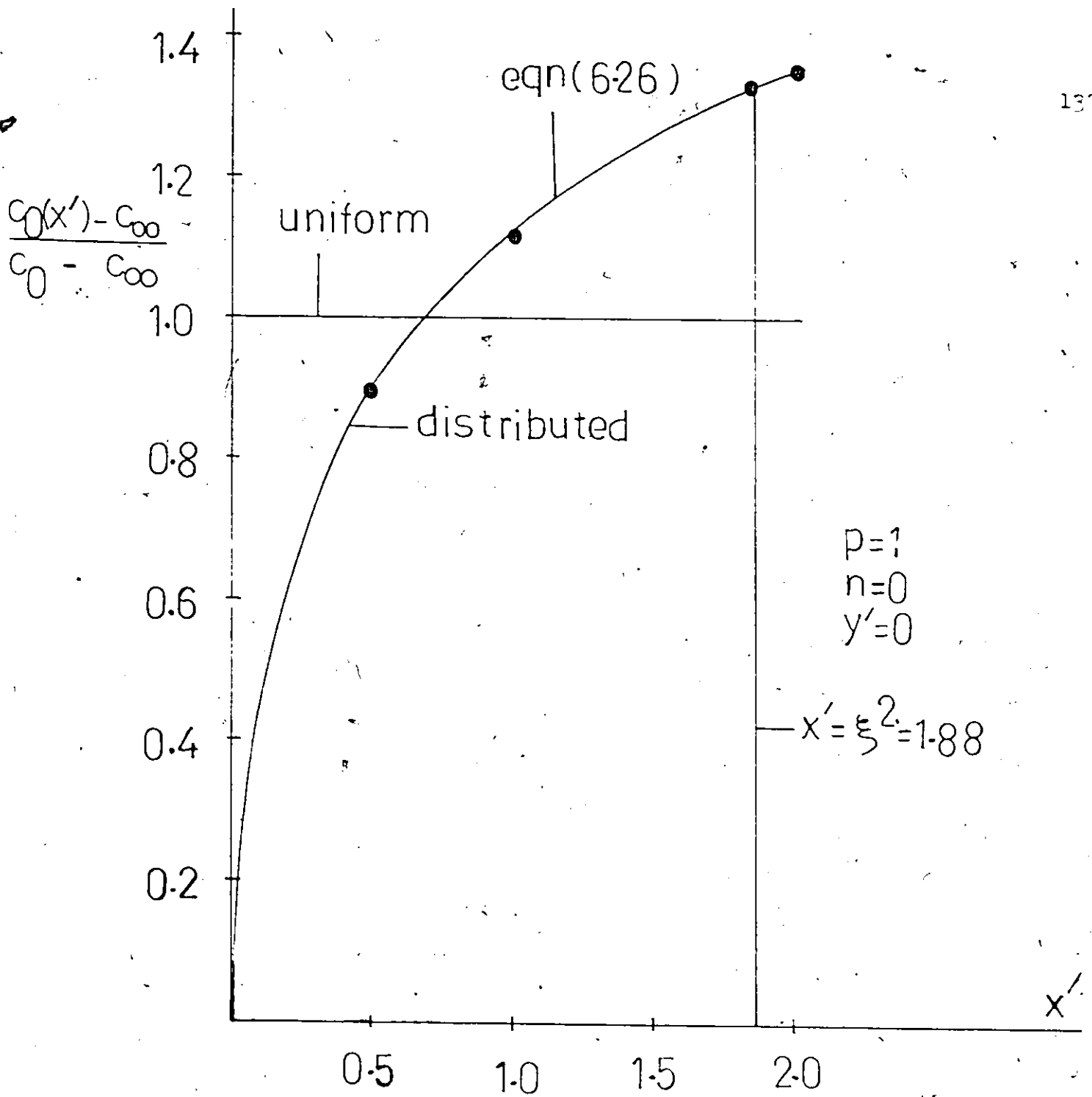Fig.27: effects of reaction upon mass-transfer

Fig·28: initial concentrations at the plate
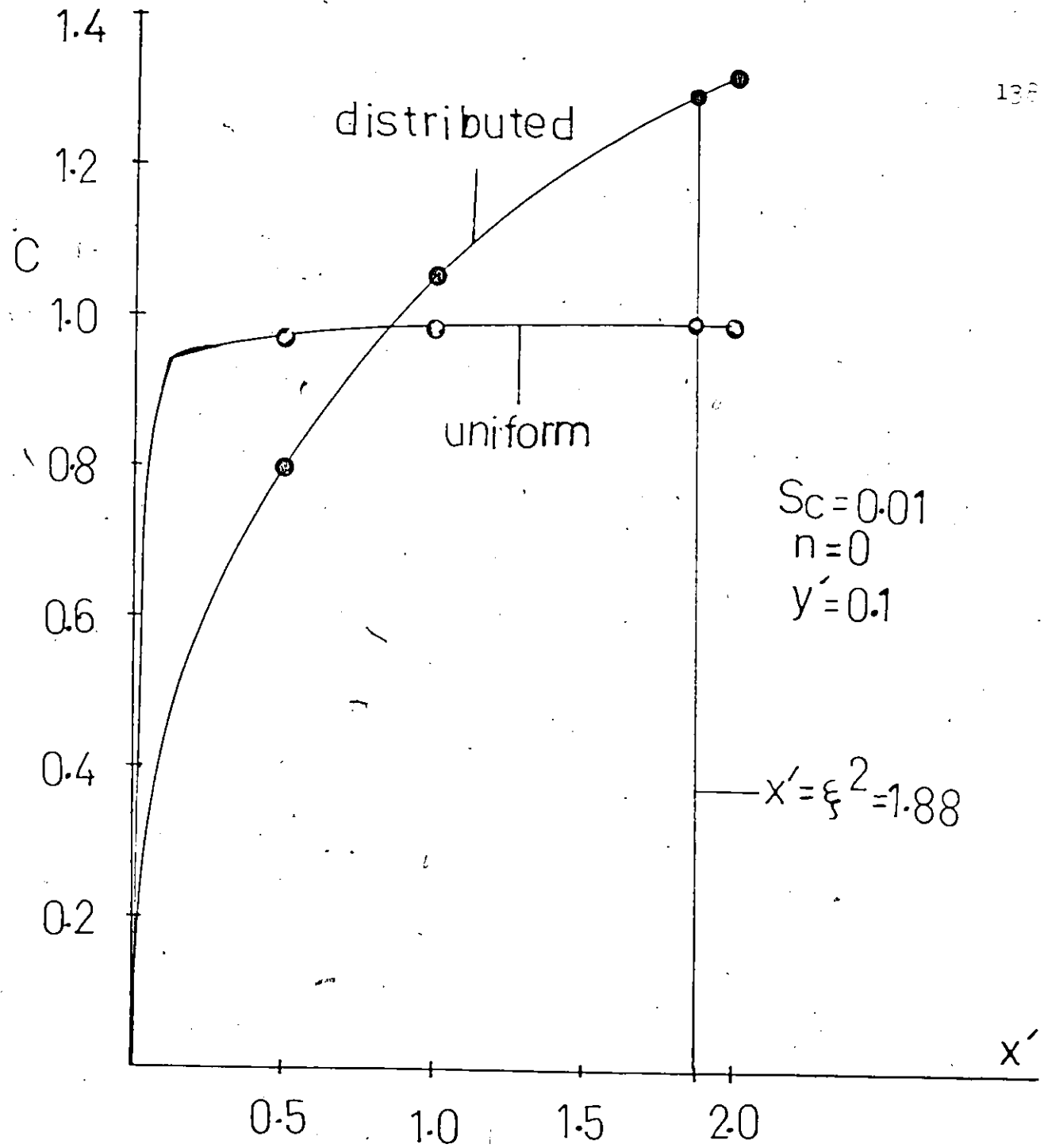for uniform and distributed
problems at $y'=0$

Fig. 29: comparison of concentration profiles
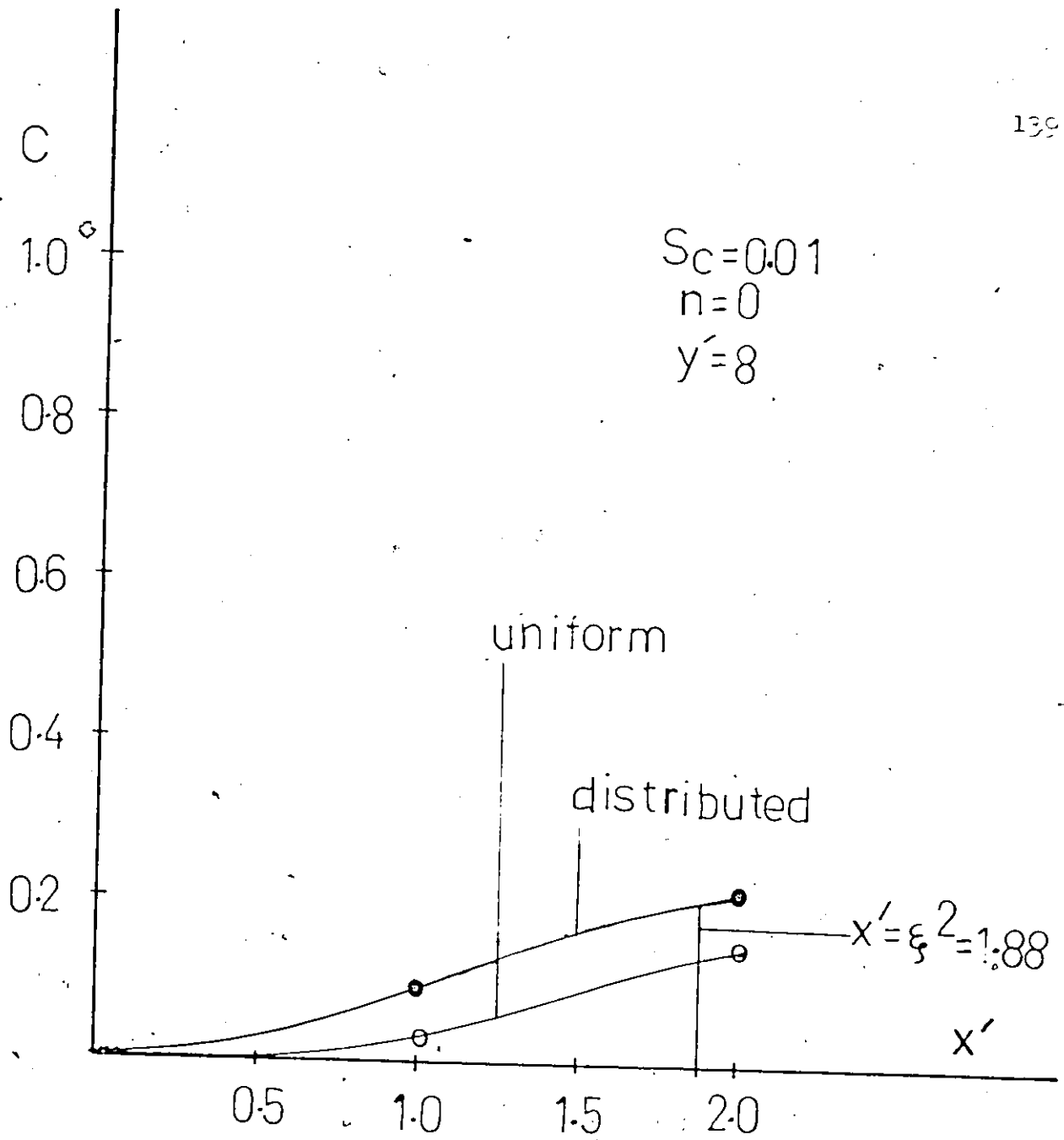between uniform and distributed
problems at y'=0.1

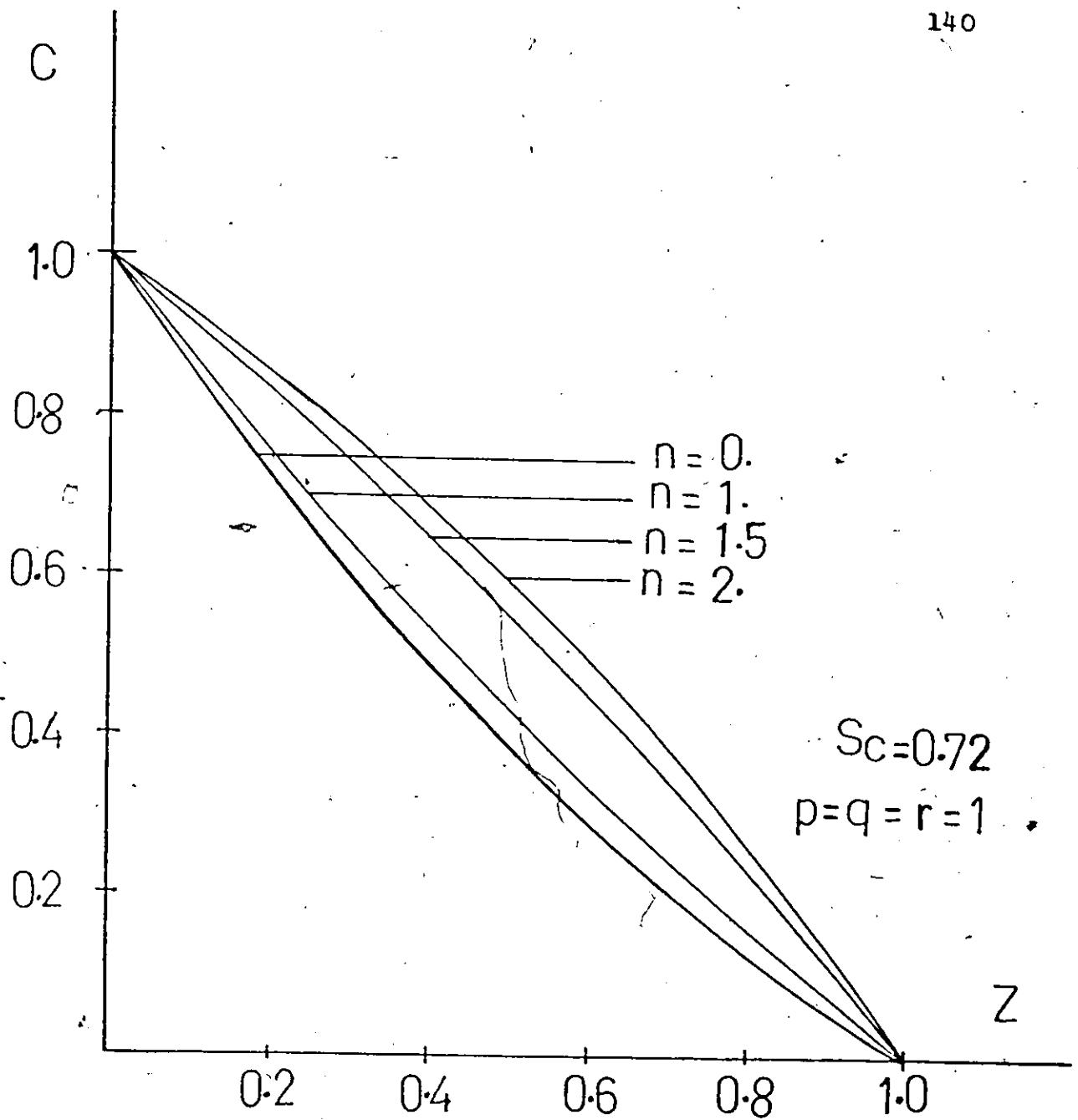Fig. 30: comparison of concentration profiles between uniform and distributed problems at $y'=8$

Fig. 31 : Series solutions of concentra-
tion for the distributed
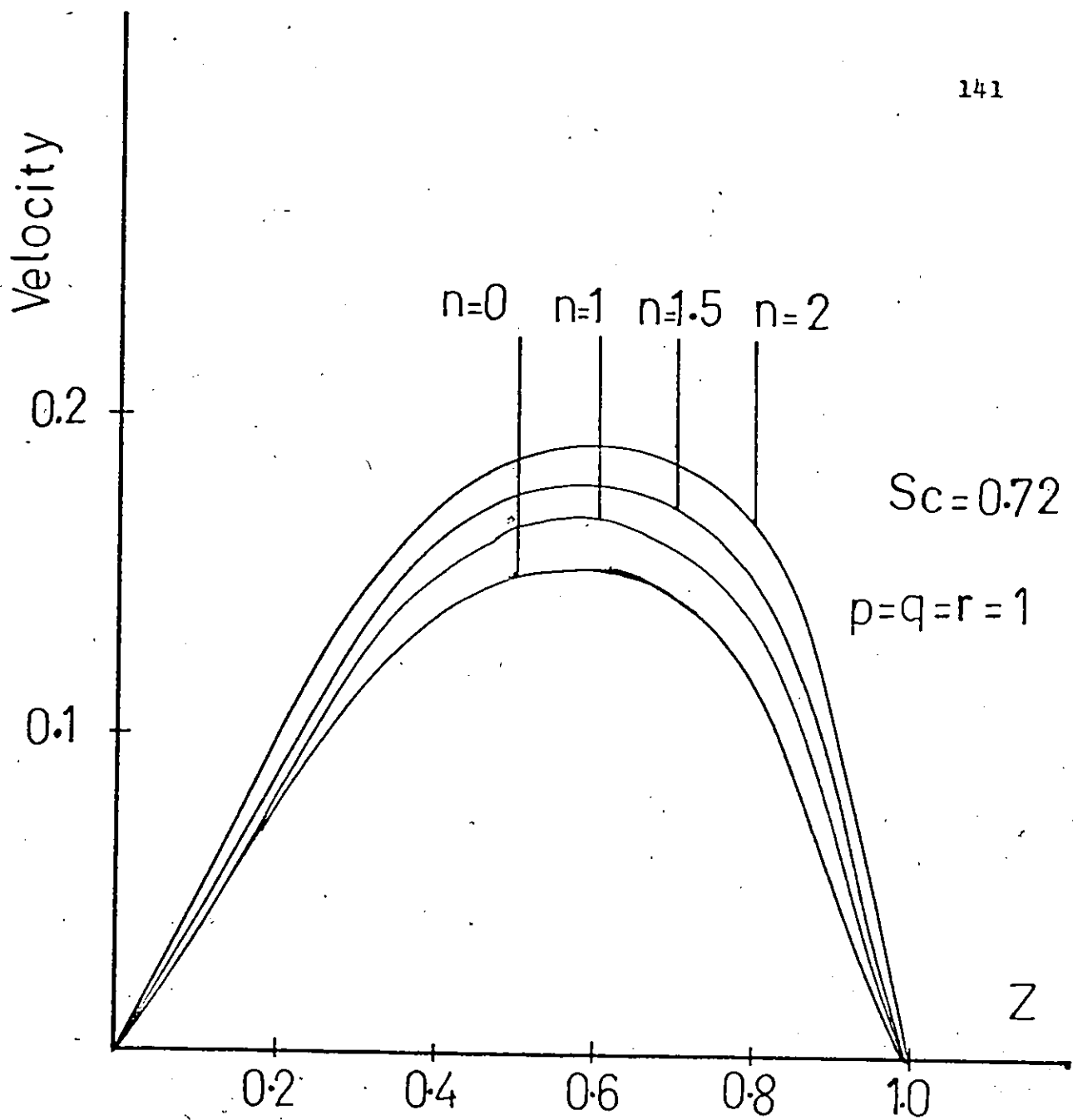concentration along the plate

Fig.32: Series solutions of velocity distributions for the distributed concentration along the plate
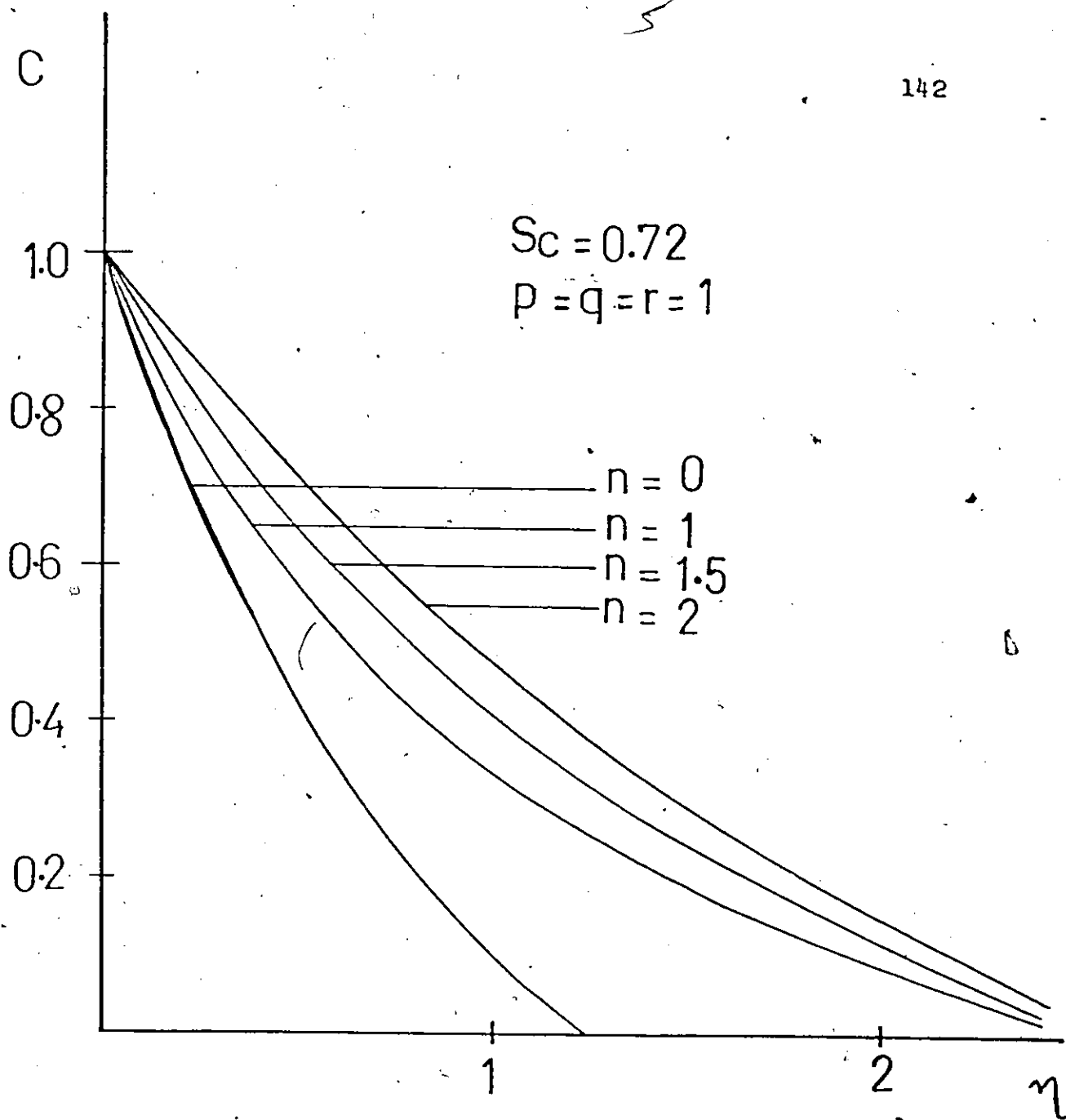
Fig.33 : Results of numerical solutions of concentration distributions for several reaction orders for distributed concentration along the plate

APPENDIX

DESCRIPTION OF THE REACTION KINETIC THEORY.

In this appendix we discuss chemical Kinetics which arise in the problem.

Let us define the rate of reaction: Consider a reaction in which substances A and B react to form the product C.

$$A + B \longrightarrow C$$

Suppose, C_A = concentration of A

C_B = concentration of B

C_C = concentration of C

V = volume of the mixture

N_A = number of moles of A in V

N_B = number of moles of B in V

N_C = number of moles of C in V

then,

$$C_A = \frac{N_A}{V}$$
$$C_B = \frac{N_B}{V}$$
$$C_C = \frac{N_C}{V}$$

The reaction rate r_C with respect to C is defined as the rate per unit volume of C reacting fluid at which the substance C is being produced or lost by reaction.

Symbolically,

$$r_C = \frac{1}{V}\frac{d(N_C)}{dt}$$

$$= \frac{1}{V}\frac{d(VC_C)}{dt}$$

and in our notation,

$$\dot{c}_C''' = r_C = \frac{1}{V} \frac{d(Vc_C)}{dt} \tag{A-1}$$

If the volume V of the system is constant then (A-1) can be written as,

$$\dot{c}_C''' = r_C = \frac{dc_C}{dt} \tag{A-2}$$

Again from experiment and from theory, it is known that for simple gas reactions, the reaction rate is proportional to the product of small integral powers α and β of the concentration of the reagents,

thus if the order of a reaction is α w.r.t. substance A,

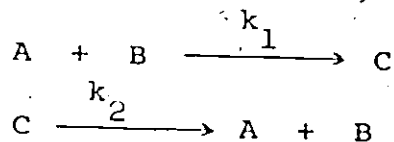β w.r.t. substance B,

the rate equation may be written as

$$r = k\, c_A^\alpha\, c_B^\beta \tag{A-3}$$

where k = rate constant.

In general, these powers α and β may be fractional or integral including zero. This order of reaction is determined by an experimental procedure. In general case, the units of k in the metric-system, would be:

$$(g\ moles)^{1-\alpha-\beta} \qquad (litres)^{\alpha+\beta-1} \qquad (sec)^{-1}$$

For reversible reaction, say

$$A + B \xrightarrow{\ k_1\ } C$$

$$C \xrightarrow{\ k_2\ } A + B$$

the rate of reaction of the substance C can be written as,

$$r_C = k_1\, c_A^\alpha c_B^\beta - k_2 c_C^\gamma$$

The rate constant k generally obeys the following relation,

$$k = k_0 e^{-E/RT}$$

This equation known as the Arrhenius equation has k_0=constant

E = activation energy, commonly in the range 10,000 to 50,000 cal/(gm. moles)
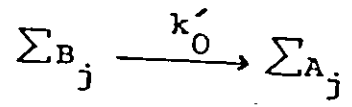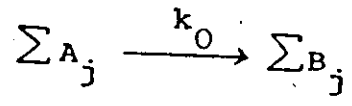
R = universal gas constant,

and, T = absolute temperature.

In general, for homogeneous reversible reaction, we can write the rate as follows:

$$r = k_0 e^{-E/RT} \prod c_j^{\alpha j} - k_0' e^{-E'/RT'} \prod c_j'^{\beta j}$$

where the reaction is:

$$\sum A_j \xrightarrow{k_0} \sum B_j$$

$$\sum B_j \xrightarrow{k_0'} \sum A_j$$

c_j - concentration of A_j

c_j' - concentration of B_j

where r is the rate of production of B_j.

Consider the following reaction:

$$2NaCl + H_2SO_4 = Na_2SO_4 + 2HCl$$

2NaCl	H₂SO₄	Na₂SO₄	2HCl
Sodium Chloride	Sulphuric Acid	Sodium Sulphate	Hydrochloric Acid
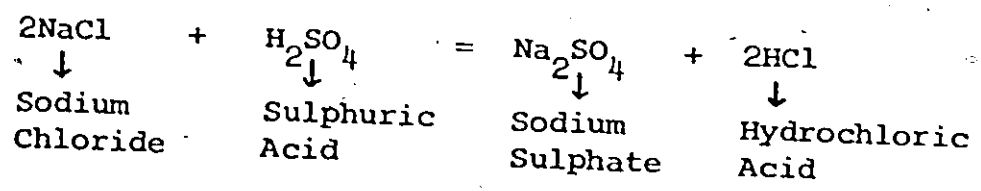
If the dissociation of NaCl in the presence of an aqueous dilute solution of Sulphuric Acid is of the nth order, then the concentration C of NaCl satisfies

$$\frac{dc}{dt} = -kc^n \qquad \text{(A-4)}$$

Similarly, we can define zeroth, first or fractional orders.

The equation (A-4) states that the rate of decrease of concentration C is proportional to C^n, where n is the order of reaction. If the reaction rate is fast, then k is large, if it is slow, then k is small and if there is no reaction then k = 0.

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