NUMERICAL SOLUTION OF A DIFFUSION-REACTION EQUATION

by

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Abstract

This thesis is concerned with the numerical solution of the reaction-diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 (u^m)}{\partial x^2} - cu^p, \qquad c \geq 0,\ p>1,\ m>1. \tag{1}$$

Modified versions of the algorithms of Graveleau & Jamet and Tomoeda are first tested on the simpler porous medium equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 (u^m)}{\partial x^2}$$

and then applied to the initial value problem for (1) and initial data with finite support. The results are compared with the analytic large time solution for various regimes in p-m parameter space.

ACKNOWLEDGMENT

I wish to express my sincere thanks to my supervisor, Dr R E Grundy, who has always encouraged my interest and advised me on numerous problems I have met throughout. Indeed, I found his helpfulness and patience has always been inexhaustible.

Last but not least I would like to thank all my friends, colleagues and members of staff of the Department of Mathematics, University of St.Andrews.

Finally I wish to dedicate this work to my mother and my late father, Amine Koutbeiy.

DECLARATION

I Majdi Amine Koutbeiy hereby certify that this thesis has been composed by myself, that it is a record of my own work, and that it has not been accepted in partial or complete fulfilment of any other degree or professional qualification.

Signed

Date 18th. June. 1986

CONTENTS

1. INTRODUCTION

In this thesis we study the initial and initial-boundary value problems associated with the nonlinear diffusion-reaction equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2(u^m)}{\partial x^2} - c u^p \qquad ; x \in \mathbb{R}^1 , t \geqslant 0 \qquad (1.1)$$

where m>1; c⩾0 and p>0. This equation serves as a model in many fields of applied mathematics such as population dynamics (Okubo((1980)), flow of chemically reacting fluids (Aris (1975)) and in plasma physics where (1.1) describes the evolution of a temperature jump in a plasma with a power law conductivity and nonlinear absorption.

In each of these areas of activity two problems associated with (1.1) are important. The first is of initial value type where (1.1) is solved subject to

$$u(x,0) = u_0(x) \qquad (1.2)$$

where $u_0(x) \geqslant 0$ has finite support. We call this problem I. The second is the initial-boundary value problem where we are required to solve (1.1) together with (1.2) for x⩾0, and the boundary condition

$$u(0,t) = U(t) \qquad ; t \geqslant 0 \qquad (1.3)$$

This is called problem II.

As a preliminary to studying these problems for (1.1) we first consider the simplified equation with the reaction term absent

$$\frac{\partial u}{\partial t} = \frac{\partial^2(u^m)}{\partial x^2} \qquad (1.4)$$

which, because of its utility as a model for flow in a porous medium; is often referred to as the porous medium equation. Our motivation in studying (1.4) is twofold. In the first place the solution of (1.4) has many features in common with that of (1.1) and since it has a more complete general theory, it is useful and instructive to deal with this first. Furthermore as (1.4) is a simpler equation the numerical schemes

2. THE POROUS MEDIUM EQUATION

One of the earliest analytic solution to the porous medium equation was due independently to Barenblatt (1952) and Pattle (1959). This has the form of a similarity solution and can be written as

$$u(x,t) = \begin{cases} \frac{1}{\lambda(t)} \left\{ 1 - \left[\frac{x}{\lambda(t)}\right]^2 \right\}^{1/(m-1)} & ; |x| \leq \lambda(t) \\ 0 & ; |x| \geq \lambda(t) \end{cases} \tag{2.1}$$

$$\text{where} \quad \lambda(t) = \left\{ \frac{2m(m+1)}{(m-1)} \; t \right\}^{1/(m+1)} \quad ; t \geq 0 \tag{2.2}$$

and the origin of t is arbitrary so can be replaced by $t+t_0$. This so-called Barenblatt-Pattle solution reveals an important general property of solutions to the porous medium equation namely if the support is finite at some time $t=T_1$ then it remains so for $t>T_1$. The paths in the (x,t) plane separating regions where $u>0$ from those where $u=0$ are called interfaces or fronts. In the case of the Barenblatt-Pattle solution these are given by

$$x = \pm \lambda(t) \tag{2.3}$$

with δ-function initial data. In general, any positive initial data with finite support will generate two interfaces $S_i(t)$, $i=1,2$ with $S_1(0)<S_2(0)$, which must be determined as part of the solution. It was shown by Kalashnikov (1967) that for $t>T$, $T\varepsilon[0,\infty)$ then

$$(-1)^i S_i(t) \quad ; i=1,2 \tag{2.4}$$

is a non-decreasing function of t. Knerr (1977) went a little further and proved that there exists a $T_i \geq 0$ such that $(-1)^i S_i(t)$ is strictly increasing and $S_i(t) = S_i(0)$ if $0 \leq t \leq T_i$. Furthermore Knerr gave an important result concerning the velocity of the interfaces; viz.,

$$\frac{dS_i}{dt} = -\frac{m}{(m-1)} \left\{ \frac{\partial(u^{m-1})}{\partial x} \right\}_{x=S_i(t)} \equiv \frac{-m}{(m-1)} \left(\frac{\partial v}{\partial x} \right)_{x=S_i(t)} \tag{2.5}$$

As we shall see later (2.5) forms the basis of schemes for the numerical tracking of interfaces. The existence of interfaces prompts several questions, the most important being that of what boundary conditions hold there. Clearly u=0 on $S=S_i(t)$ (2.6) and, as far as most applications go, the other is concerned with the flux

$$\frac{\partial(u^m)}{\partial x}$$

which can either be negative or zero. So we have the conditions, additional to (2.6),

$$\frac{\partial(u^m)}{\partial x} = -L \quad , L > 0 \qquad (2.7)$$

or

$$\frac{\partial(u^m)}{\partial x} = 0 \qquad (2.8)$$

on $S=S_i(t)$.

By for the most relevant is (2.8) which is sometimes called the zero-flux boundary condition. Although the condition (2.7) has physical relevance, particularly in heat conduction problems, it has been rarely used in mathematical analyses of the porous medium equation. So for the purposes of this thesis we require (2.6) and (2.8) to hold on any interface.

The results of Knerr leads one to the question of the waiting time. This is the time lag, from the applications of the initial data, during which an interface is stationary. In the above notation this is denoted by T_i. It has been known for some time that an interface where u=0 can either move immediately or remain stationary for a finite time and then move off. In this connection there are two distinct situations to consider, distinguished by the mechanism by which the interface beings to move. The first is where the initial motion is governed purely by the initial data at the interface and the second by conditions within the support of $u_0(x)$. The former has come to be called the local case and the latter global.

At this stage it is convenient to make the change of variable $v=u^{m-1}$ and consider the equation

$$\frac{\partial v}{\partial t} = \frac{m}{(m-1)}\left(\frac{\partial v}{\partial x}\right)^2 + mv\,\frac{\partial^2 v}{\partial x^2} \qquad (2.9)$$

In the analysis that follows we may treat each interface separately and for convenience we take this to be initially at x=0. In order that the solution for v(x,t) is unique (2.9) has to be supplemented by two boundary conditions (2.6) and (2.8) on the interface x=S(t),

$$v(S(t),t) = 0 \qquad (2.10)$$

and

$$\left\{v^{\frac{1}{(m-1)}}\,\frac{\partial v}{\partial x}\right\}_{x=S(t)} = 0 \qquad (2.11)$$

Considerable insight into the nature of the waiting time problem was gained by Kath & Cohen (1982) who took the limit $m\to 1$. This led Grundy (1983) and Lacey (1983), to formulate the following results. With initial data

$$v_0 = \left\{u_0(x)\right\}^{m-1} = f(x) \qquad (2.12)$$

where $f(x) \sim Ax^{\alpha}$, $x\to 0$.

Three cases can be distinguished

(1) $\alpha<2$. Here the left-hand interface moves immediately and the waiting-time is zero. The initial motion of this unknown boundary is governed purely by the local behaviour of f(x) as $x\to 0$. This is termed a local case.

(2) $\alpha>2$. Here the interface begins to move when a singularity, characterized by a discontinuity in $(\partial v/\partial x)$ which develops within the support of f(x), reaches x=0. The waiting-time t^* is positive and, since the initial motion of the boundary is governed by the nature of f(x) away from x=0, we call this a global case.

(3) $\alpha=2$. Here two possibilities may occur.

(a) If $f''(x)$ is a maximum at $x=0$ then the singularity will form at $x=0$ and the interface begins to move when $t=t^*=\{2f''(0)\}^{-1}$. This is considered a local case.

(b) If $f''(x)$ has a maximum at some point in the interior of the support of $f(x)$ then the singularity develops at this point and the interface begins to move when this reaches $x=0$. This is a global case.

The local structures of the solution as $x\to0$ and $t\to t^*$ in the global case when $t\to0$ in the local cases can be found by the similarity solution of Lacey, Ockendon and Taylor (1982). Estimates of waiting times have recently been given by Aronson, Caffarelli and Kamin (1983).

By for the most important role played by the Barenblatt-Pattle solution in particular and similarity solutions in general is in the large time limit of the solutions to problem I and II for the porous medium equation. It was shown by Kamin (1973) that for problem I with $u=0$ and $\frac{\partial(u^m)}{\partial x} = 0$ on the interface then $u(x,t)$ as $t\to\infty$ approached the Barenblatt-Pattle similarity solution. The eigenvalues of this solution were obtained by Grundy & McLaughlin (1982a) thus determining in principal the asymptotic expansion of $u(x,t)$ as $t\to\infty$. For problem II with $u=0$ and $\frac{\partial(u^m)}{\partial x} = 0$ on the interface a similar exercise can be undertaken, and Peletier (1971) showed that as $t\to\infty$ the solution converged to the similarity solution

$$u(x,t) = \eta_0^2 \, h^{1/(m-1)}(\xi) \tag{2.13}$$

$$\xi = x/\eta_0 t^{1/2} \tag{2.14}$$

where $h(\xi)$ satisfies the boundary value problem

$$mhh'' + \frac{m}{(m-1)}(h')^2 + \frac{\xi}{2}h' = 0 \tag{2.15}$$

$$h(1) = 0 \quad , \; h'(1) = -(m-1)/2m \qquad \text{and} \tag{2.16}$$

$$h(0) = U_0^{(m-1)}/\eta_0^2 \tag{2.17}$$

Here η_0 is determined numerically by integrating (2.15) from $\xi=1$ to $\xi=0$ to obtain h(0).

Whence

$$\eta_0 = \left\{ U_0^{(m-1)} / h(0) \right\}^{1/2} \tag{2.18}$$

and so the interface is given by

$$S(t) = \eta_0 \, t^{1/2} \tag{2.19}$$

To complete the picture Grundy & McLaughlin (1982 b) constructed a rational asymptotic expansion of u(x,t) as $t \to \infty$ with the above similarity solution as the leading term.

The analytic properties of the porous medium equation which we have outlined above will be used in section 4 to provide a quantitative test of the numerical procedures. Of particular importance in this respect is the waiting time analysis and the large time comparison.

We now go on to give a similar, but necessarily less complete review of the reaction diffusion equation. Questions regarding waiting times for these equations are still open as is a large portion of the theory for the initial-boundary value problem, problem II.
The only aspect of the theory which we can deal with with any certainty is the pure initial value problem which, for initial data with finite support, has an almost complete description. This we deal with in the next section.

3. THE INITIAL VALUE PROBLEM FOR THE DIFFUSION-REACTION EQUATION

Here we consider the large time solution for the inital value problem for (1.1) with (1.2). (Problem I). In general it is known that for m>1 and initial data with finite support there exist two interfaces along which u=0. In many model situations involving (1.1) the addition boundary condition,

$$\frac{\partial(u^m)}{\partial x} = 0$$

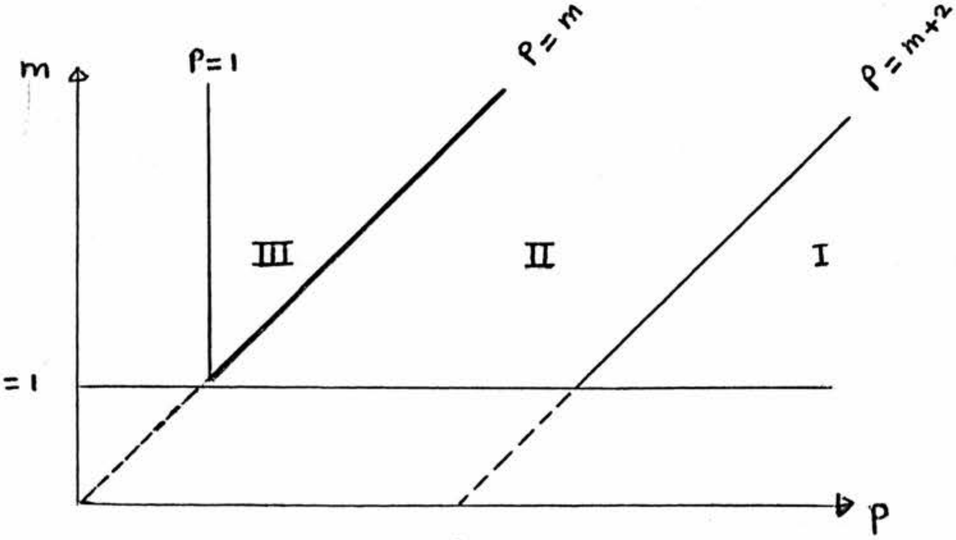
usually holds at the interface. So we solve (1.1) and (1.2) with

$$\left.\begin{array}{l} u = 0 \\ \text{and} \quad \dfrac{\partial(u^m)}{\partial x} = 0 \end{array}\right\} \qquad (3.1)$$

along left and right interfaces

$$x = S_i(t) \qquad , \quad i = 1, 2 . \qquad (3.2)$$

The results we describe below are due to Grundy (1986) and are, by necessity, somewhat more involved than that for the porous medium equation, in that the nature of the asymptotic solution depends on the location in (p-m) parameter space. The situation is shown schematically below.



3.1 p>m+2

In this regime of parameter space the result we base our analysis on is due independently to Kersner (1979) and Knerr (1979). This states that if $S(t) = |S_i(t)|$, i=1,2, then as $t \to \infty$

$$A t^{1/(m+1)} \leqslant S(t) \leqslant B t^{1/(m+1)} \quad ; \; t \geqslant 1 \qquad (3.1.1)$$

where A and B are positive constants. This result suggests we consider the similarity variable

$$\eta = x \, t^{-1/(m+1)} \qquad (3.1.2)$$

and put

$$u(x,t) = t^{\alpha} \, v(\eta, t) \qquad (3.1.3)$$

where $v(\eta,t)$ is bounded as $t \to \infty$, $\eta = O(1)$. Thus the exponent α gives the temporal decay of $u(x,t)$ as $t \to \infty$.

In terms of η and v (1.1) becomes

$$(m+1) t \frac{\partial v}{\partial t} + \alpha (m+1) v - \eta \frac{\partial v}{\partial \eta} = (m+1) \, t^{\alpha(m-1) + \frac{m-1}{m+1}} \, \frac{\partial^2 (v^m)}{\partial \eta^2} - (m+1) \, t^{\alpha(p-1)+1} \, v^p \qquad (3.1.4)$$

A non trivial second order equation for v emerges if the first term on the right hand side of (3.1.4) dominates the second term as $t\to\infty$, and at the same time balancing the order unity terms. This happens if

$$\alpha = -1/(m+1) \tag{3.1.5}$$

and

$$p > m+2 \tag{3.1.6}$$

Proceeding further we formally expand

$$v(\eta,t) = v_0(\eta) + t^{\gamma_1} v_1(\eta) + \cdots \tag{3.1.7}$$

in the limit $t\to\infty$, $\eta=0(1)$ with $\mathrm{Re}\,\gamma_1<0$.

This gives

$$v_0 + \eta v_0' + (m+1)(v_0^m)'' - (m+1)\, t^{(2+m-p)/(m+1)}\, v_0^p +$$

$$\left\{v_1 + \eta v_1' - \gamma_1(m+1)v_1 + m(m+1)(v_1 v_0^{m-1})''\right\} t^{\gamma_1} + \cdots = 0 \tag{3.1.8}$$

Thus equating terms of 0(1) gives

$$v_0 + \eta v_0' + (m+1)(v_0^m)'' = 0 \tag{3.1.9}$$

For the next order we have two possibilities.

First

$$\gamma_1 = (2+m-p)/(m+1) \tag{3.1.10}$$

and

$$m(m+1)(v_1 v_0^{m-1})'' + \eta v_1' + (p-m-1)v_1 - (m+1)v_0^p = 0 \tag{3.1.11}$$

or

$$\mathrm{Re}(\gamma_1) < (2+m-p)/(m+1)$$

and

$$m(m+1)(v_1 v_0^{m-1})'' + \eta v_1' + v_1\left\{1-\gamma_1(m+1)\right\} = 0 \tag{3.1.12}$$

The equations (3.1.9), (3.1.11), (3.1.12) have to be solved subject to the appropriate boundary conditions at the interface. For (3.1.9) this means

$$v_0 = (v_0^m)' = 0 \qquad \text{at} \quad \eta = \eta_i \quad , \; i=1,2 \tag{3.1.13}$$

where the interfaces have the expansions

$$S_1(t) = \eta_1 t^{1/(m+1)} \{1 + o(1)\}$$

$$S_2(t) = \eta_2 t^{1/(m+1)} \{1 + o(1)\}$$

as $t\to\infty$. A straightforward integration of (3.1.9) subject to (3.1.13) yields the Barenblatt-Pattle similarity solution

$$v_0 = \left\{\frac{(m-1)}{2m(m+1)}\right\}^{1/(m-1)} (\eta_0^2 - \eta^2)^{1/(m-1)} \tag{3.1.14}$$

and so $\eta_1=-\eta_2=\eta_0$. Since (1.1) does not have a mass invariance property, η_0 cannot be determined by such considerations. It will, one suspects, depend in some way on the initial conditions.

As far as the error term goes γ_1 is either given by (3.1.10) or the solution of the eigenvalue problem (3.1.12) with the appropriate boundary conditions. For a discussion of this problem see Barenblatt (1952) or Grundy & McLaughlin (1982a).

3.2 $m<p\leq m+2$

The analysis of the previous section depended on the reaction term in (3.1.4) being negligible as $t\to\infty$. This is no longer true when $p=m+2$. In fact as we shall see, throughout the regime $m<p\leq m+2$ we need to seek an alternative expansion for u as $t\to\infty$. The starting point is a result due to Bertsch, Kersner and Peletier (1982) which states that

$$At^{\beta} \leq S(t) \leq Bt^{\beta} \quad , \quad t \geq 1 \tag{3.2.1}$$

where

$$\beta = (p-m)/2(p-1)$$

and A and B are positive constants. So with (3.2.1) in mind we introduce the similarity variable

$$\eta = x t^{-\beta} \tag{3.2.2}$$

and put

$$u(x,t) = t^{-1/(p-1)} v(\eta, t) \tag{3.2.3}$$

It was noted in the above paper that this substitution makes the reaction and diffusion term of the same order as $t \to \infty$. If we now formally expand

$$v(\eta, t) = v_0(\eta) + O(1) \qquad (3.2.4)$$

then v_0 satisfies

$$v_0 + \frac{(p-m)}{2} \eta v_0' + (p-1)(v_0^m)'' - (p-1) v_0^p = 0 \qquad (3.2.5)$$

The boundary conditions on v_0 are

$$v_0 = (v_0^m)' = 0 \qquad \text{on} \quad \eta = \eta_i \quad ; \; i = 1,2 \qquad (3.2.6)$$

Since the support is increasing for all time we look for solutions of (3.2.5) and (3.2.6) which are even about $\eta=0$. So putting

$$\eta_i = \eta_0 \qquad ; \; i = 1,2$$

and

$$\xi = \eta / \eta_0$$

(3.2.5) and (3.2.6) can be recast as the eigenvalue problem

$$\left.\begin{aligned} &(p-1)(v_0^m)'' + \eta_0^2 \left\{ v_0 + \frac{(p-m)}{2} \xi v_0' - (p-1) v_0^p \right\} = 0 \\ &v_0 = (v_0^m)' = 0 \qquad \text{when} \qquad \xi = -1 \\ &v_0' = 0 \qquad\qquad\qquad\qquad\quad\; \xi = 0 \end{aligned}\right\} \qquad (3.2.7)$$

Numerical experiments with this eigenvalue problem indicate that it has a unique solution. This can be obtained by a shooting method using the series solution to start the integration at $\xi=-1$. For the particular case $p=3$, $m=2$ we have $\eta_0=3.4$ to one decimal place.

3.3 $1<p<m$

We defer for the moment our discussion of the case $p=m$ and consider the form of the solution in the regime $1<p<m$ which turns out to be of a completely different character to that for $p>m$. Here the support remains bounded, a conclusion originally due to Kalashnikov (1974).

Thus we may write

$$S(t) \longrightarrow x_0 \qquad , \quad t \longrightarrow \infty \quad . \tag{3.3.1}$$

The result which forms the basis of our analysis is again due to Bertsch, Kersner and Peletier (1982) and states that for any fixed $x \varepsilon (-x_0, x_0)$ then

$$u(x,t) \longrightarrow (p-1)^{-1/(p-1)} \quad t^{-1/(p-1)} \tag{3.3.2}$$

as $t \to \infty$. We note two aspects of this result, firstly that the end points are excluded and consequently the asymptotic solution does not satisfy the boundary conditions at the interface. In other words (3.3.2) is not a uniformly valid approximation in x to the solution of (1.1). It turns out however that (3.3.2) defines the leading term in an outer expansion when $t \to \infty$, x fixed $\varepsilon (-x_0, x_0)$. So we construct the expansion.

$$u(x,t) = (p-1)^{-1/(p-1)} \quad t^{-1/(p-1)} \quad \{1 + \Delta_1(x,t) + \cdots\} \tag{3.3.3}$$

where $\Delta_1 \to 0$ as $t \to \infty$, x fixed. In order to satisfy the boundary conditions at the interfaces this expansion has to be supplemented by an inner expansion valid where the similarity variable

$$\zeta = (x \pm x_0) \; t^{\delta} = O(1) \tag{3.3.4}$$

We then construct an inner expansion

$$u(x,t) = t^{\alpha} \{ v_0(\zeta) + o(1) \} \tag{3.3.5}$$

valid as $t \to \infty$, ζ fixed and $O(1)$. The indices α and δ are chosen so that (3.3.5) matches with (3.3.3) and secondly so that $v_0(\zeta)$ satisfies a second order equation enabling the boundary conditions at each interface to be satisfied. As we will see below the choice

$$\alpha = -1/(p-1) \qquad , \qquad \delta = (m-p)/2(p-1) > 0 \tag{3.3.6}$$

satisfies these criteria.

The first step is to insert (3.3.5) with (3.3.4) and (3.3.6) into equation (1.1) with boundary conditions (3.1).

We find that $v_0(\zeta)$ satisfies

$$(p-1)(v_0^m)'' - (p-1)v_0^p + v_0 - \frac{(m-p)}{2}\zeta v_0' = 0 \qquad (3.3.7)$$

subject to the boundary condition

$$(v_0^m)' = v_0 = 0 \qquad (3.3.8)$$

at $\zeta=\zeta_0$, where ζ_0 is at the moment unknown. Matching to first order with the outer solution (3.3.3) requires that

$$v_0 \to (p-1)^{-1/(p-1)} \quad ; \quad |\zeta| \to \infty \qquad (3.3.9)$$

where $\zeta>0$ at the left hand interface and $\zeta<0$ at the right hand one. The problem (3.3.7)-(3.3.9) is an eigenvalue problem for ζ_0 and may be conveniently recast by scaling $|\zeta|$ with $|\zeta_0|$. Limits on $|\zeta_0|$ can be obtained for this problem using a shooting method and a series solution about $\xi=0$. As an example we obtained $3.3170 < |\zeta_0| < 3.3172$ for $p=1.5$, $m=2$.

3.4 p=m

We now deal with the borderline case p=m which as we shall see has certain features in common with both the cases considered above.

Bertsch, Kersner and Peletier showed for this case that

$$A \operatorname{Log} t \leqslant S(t) \leqslant B \operatorname{Log} t \qquad (3.4.1)$$

So this suggests the variable

$$\xi = x - \zeta_0 \operatorname{Log} t \qquad (3.4.2)$$

together with the substitution

$$u(x,t) = t^{\alpha} v(\xi, t) \qquad (3.4.3)$$

where ζ_0 is at the moment unknown.

In terms of v and ξ (1.1) becomes

$$t\frac{\partial v}{\partial t} + \alpha v - \zeta_0 \frac{\partial v}{\partial \xi} = t^{\alpha m+1-\alpha}\left\{\frac{\partial^2(v^m)}{\partial \xi^2} - v^m\right\} \qquad (3.4.4)$$

Remembering we require a second order equation so that the boundary conditions are satisfied at the interface, we choose

$$\alpha = -1/(m-1).$$

At the same time we expand

$$v(\xi, t) = v_0(\xi) + o(1) \tag{3.4.5}$$

in the limit $t \to \infty$, $\xi = 0(1)$. The equation satisfied by v_0 is therefore

$$\alpha v_0 - \zeta_0 v_0' = (v_0^m)'' - v_0^m \tag{3.4.6}$$

The boundary conditions at the interface where

$\xi = \xi_0$, say, are

$$v_0 = (v_0^m)' = 0 \tag{3.4.7}$$

The outer expansion in this case valid for $t \to \infty$, $x = 0(1)$ is simply

$$u = \left(\frac{1}{m-1}\right)^{1/(m-1)} t^{-1/(m-1)} \left\{ 1 + o(1) \right\} \tag{3.4.8}$$

and so the matching condition on v_0 is

$$v_0 \longrightarrow \left(\frac{1}{m-1}\right)^{1/(m-1)} , \quad |\xi| \to \infty \tag{3.4.9}$$

Hence $\zeta_0 > 0$ and $\xi \to -\infty$ for matching at right hand interface while $\zeta_0 < 0$, $\xi \to +\infty$ for matching at the left hand one.

We determine ζ_0 as follows. Putting

$$v_0 = W^{1/(m-1)} \quad , \quad W' = -\zeta_0 P \quad , \quad P > 0 \tag{3.4.10}$$

reduces (3.4.6) to

$$\frac{dP}{dW} = \frac{(m-1)^2 \alpha^2 W^2 - m P^2 - (m-1)\alpha^2 W + (m-1) P}{m(m-1) W P} \tag{3.4.11}$$

where $\alpha^2 = 1/\zeta_0^{\,2}$.

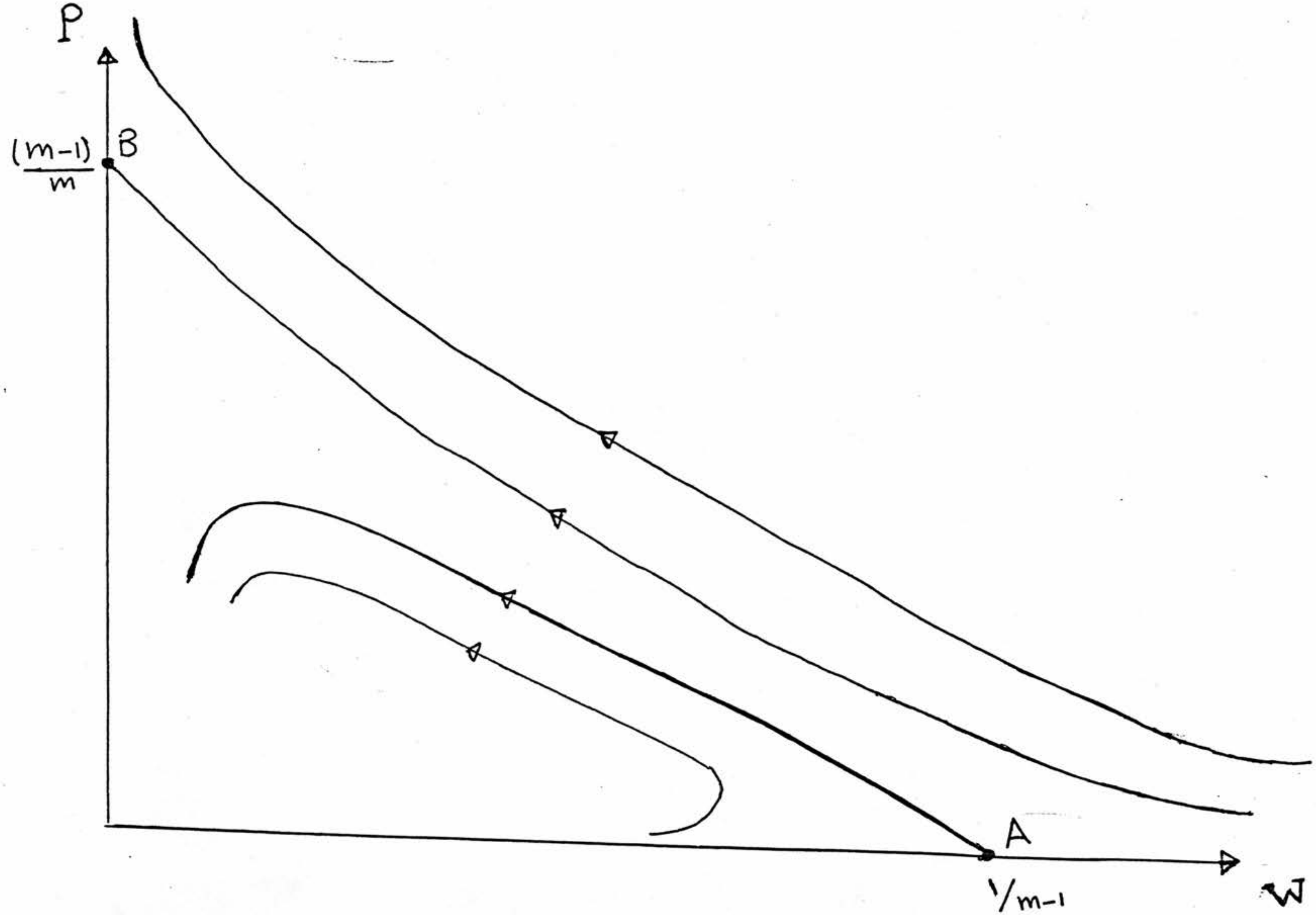
Referring to Fig.(1) there are two singular points of relevance; one is at $P=0$, $W=1/m-1$ (A) and the other is at $P=(m-1)/m$, $W=0$ (B). The first is a saddle point with a left hand separatrix

$$P = \beta (W - 1/(m-1)) \tag{3.4.12}$$

$$\beta = \left\{ +(m-1) - \sqrt{(m-1)^2 + 4\alpha^2 m(m-1)} \right\} / 2m$$

while the other is also a saddle point with a right hand separatrix

$$P = \frac{(m-1)}{m} - \frac{\alpha^2 W}{m} \tag{3.4.13}$$



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Now at the interface we can show that

$$W = -\zeta_0 \frac{(m-1)}{m}(\xi - \xi_0) - \frac{(m-1)(\xi-\xi_0)^2}{2m^2} + \cdots\cdots \tag{3.4.14}$$

and

$$W' = -\zeta_0 \frac{(m-1)}{m} - \frac{(m-1)(\xi-\xi_0)}{m^2} + \cdots\cdot \tag{3.4.15}$$

We can invert (3.4.14) to give

$$(\xi - \xi_0) = \frac{-mW}{\zeta_0(m-1)} - \frac{mW^2}{2\zeta_0^3(m-1)^2}$$

Substituting into (3.4.15) gives

$$P = \frac{(m-1)}{m} - \frac{\alpha^2 W}{m}$$

at the interface, which is precisely the condition along the separatrix at the saddle point (B) in the W-P plane. The matching condition (3.4.9) is equivalent to

$$W = \frac{1}{m-1} \qquad ; \; W' = -\zeta_0 P = 0$$

which can only be approached along the separatrix at the saddle point (A). A study of the phase plane reveals that there is only one value of ζ_0. which allows the separatrix emanating from B to enter A and this can be found numerically. After some numerical experiments it was realised that the exact solution

$$mP = (m-1) - (m-1)^2 W \tag{3.4.16}$$

with

$$\zeta_0 = \pm \frac{1}{(m-1)}$$

satisfied these requirements.

Returning now to the eigenvalue problem associated with (3.4.6) then we can see from (3.4.16) and (3.4.10) that the solution for v_0 is given by

$$v_0 = \left\{\frac{1}{m-1}\right\}^{1/(m-1)} \left\{1 - e^{\pm[(\frac{m-1}{m})(\xi-\xi_0)]}\right\}^{1/(m-1)} \tag{3.4.17}$$

which satisfies the conditions (3.4.7) and (3.4.9). So ξ_0 is not in fact given by the asymptotic analysis and must remain unknown. Thus, returning to (3.4.2) the interface is given by

$$X(t) = \pm \frac{1}{(m-1)} \operatorname{Log} t + \xi_0 + \cdots \qquad (3.4.18)$$

as $t \to \infty$.

4. THE NUMERICAL SCHEMES

4.1 Introduction

In fact there are many different explicit and implicit numerical schemes for solving the initial value problem of the porous medium equation. So we found throughout our numerical experiments that the explicit method which is mentioned by Mitchell & Griffiths (1980) is unstable. However we are interested in two of the implicit finite difference schemes. The first scheme is due to GRAVELEAU-Jamet (1971). This was specifically designed for the porous medium equation but has the reputation of not tracking the interface accurately. To remedy this the boundary condition at the interface, which is implied in Graveleau and Jamet scheme, was specifically included in the formulation and gave extremely accurate results for the motion of the interface. This amendment to their scheme is described later. The other scheme is due to Tomoeda (preprint). This appears to be the only one for the diffusion-reaction equation which tracks the interface. However it has features which demand rather cumbersome programing and it was decided to modify the scheme particularly in the way the variable time step is chosen. The details of these modifications will be described in 4.4.

4.2 The GRAVELEAU and Jamet algorithm

To describe the scheme, Graveleau and Jamet transformed (1.4), (1.2) by setting $v=u^{m-1}$ to

$$\frac{\partial v}{\partial t} = m v \frac{\partial^2 v}{\partial x^2} + \frac{m}{m-1}\left(\frac{\partial v}{\partial x}\right)^2 \qquad (4.2.1)$$

$$v(x,0) = v^0(x) = (u_0(x))^{m-1} \qquad (4.2.2)$$

Equation (4.2.1) is split into two parts, via,

$$\frac{\partial v}{\partial t} = m v \frac{\partial^2 v}{\partial x^2} \qquad (4.2.3)$$

$$\frac{\partial v}{\partial t} = a\left(\frac{\partial v}{\partial x}\right)^2 \quad ; \quad \left(a = \frac{m}{m-1}\right) \qquad (4.2.4)$$

The difference scheme is based on dividing the operator

$$Av = mv\,\frac{\partial^2 v}{\partial x^2} + a\left(\frac{\partial v}{\partial x}\right)^2 \tag{4.2.5}$$

into two components

$$A_1 v = mv\,\frac{\partial^2 v}{\partial x^2} \tag{4.2.6}$$

$$A_2 v = a\left(\frac{\partial v}{\partial x}\right)^2 \tag{4.2.7}$$

with $a = m/(m-1)$

So we define the difference operators

$$A_{1,h}\, v_i^n = m\, v_i^n\, \frac{v_{i+1}^n - 2v_i^n + v_{i-1}^n}{h^2} \tag{4.2.8}$$

and

$$A_{2,h}\, v_i^n = a[\delta v_i^n(|\delta v_i^n| + \delta v_i^n) - \delta v_{i-1}^n(|\delta v_{i-1}^n| - \delta v_{i-1}^n)]/2 \tag{4.2.9}$$

where $v_i^n = v(ih,nk)$; $ih=x$; $nk=t$; $(i,n)\geq 0$ Integers; h,k are positive numbers and $\delta v_i^n = (v_{i+1}^n - v_i^n)/h$.

Note that $A_{1,h}$ and $A_{2,h}$ are the finite difference analogues of the operator $A_1 v$ defined by (4.2.6) and $A_2 v$ defined by (4.2.7). Then the difference schemes for (4.2.3) with (4.2.2) become

$$(v_i^{n+1} - v_i^n)/K = A_{1,h}\, v_i^n \qquad , \; v_i^0 = v^0(ih)$$

and for (4.2.4) with (4.2.2) we have

$$(v_i^{n+1} - v_i^n)/K = A_{2,h}\, v_i^n \qquad , \; v_i^0 = v^0(ih)$$

Assuming that v_i^n is given for all i then the v_i^{n+1} were computed by means of μ intermediate functions $v_i^{n,r}$, $1 \leq r \leq \mu$:

$$v_i^{n,0} \equiv v_i^n \quad ,$$

$$(v_i^{n,r+1} - v_i^{n,r})/K_1 - A_{1,h}\, v_i^{n,r} = 0 \qquad 0 \leq r \leq \mu - 1 \, ,$$

$$(v_i^{n+1} - v_i^{n,\mu})/K - A_{2,h}\, v_i^{n,\mu} = 0 \, .$$

where μ is a positive integer and $K_1 = K/\mu$. The scheme was started by taking $v^0 = v^0(ih)$ and the stability conditions are:

$$4(K_1/h^2) \leq 1$$

$$2a\,c_1(K/h) \leq 1$$

where $c_1 = \sup_x |d\, v^0(x)/dx|$.

4.3 Tomoeda algorithm

This algorithm deals with (1.1). To describe the algorithm Tomoeda put $v=u^{m-1}$ and recast (1.1), (1.2) as

$$\frac{\partial v}{\partial t} = m v \frac{\partial^2 v}{\partial x^2} + a\left(\frac{\partial v}{\partial x}\right)^2 - (m-1) c v^q \quad , \tag{4.3.1}$$

$$(a = m/(m-1) \quad , \quad q = (m-2+p)/(m-1)) \quad ,$$

$$v(0,x) = v^0(x) = (u^0(x))^{m-1} . \tag{4.3.2}$$

Eq.(4.3.1) is then split into three parts

$$\frac{\partial v}{\partial t} = m v \frac{\partial^2 v}{\partial x^2} = P v \quad , \tag{4.3.3}$$

$$\frac{\partial v}{\partial t} = a\left(\frac{\partial v}{\partial x}\right)^2 = H v \quad , \tag{4.3.4}$$

$$\frac{\partial v}{\partial t} = -(m-1) c v^q = D v . \tag{4.3.5}$$

and so the equation can be rewritten as

$$\frac{\partial v}{\partial t} = (H + P + D) v \tag{4.3.6}$$

This algorithm aimed to construct difference schemes P_h, H_h and D_h for P, H and D respectively and then unify suitably these schemes so as to approximate (4.3.1), (4.3.2) (see (4.3.7)).

I The Difference Scheme

To see how this is done we let h be a positive number and $\{t_n\}$ be an increasing sequence. We denote by $v_h^n(x)$ the difference approximation for the solution of (4.3.1), (4.3.2) at $t=t_n$ and consider the sequence $\{v_h^n\}_{n=0,1,2,\dots} \subset U_h$ such that

$$v_h^{n+1} = (I_h + (K/\nu) D_h)^{\nu} (I_h + (K/\mu) P_h)^{\mu} (I_h + K H_h) v_h^n \tag{4.3.7}$$

where I_h is the identity operator, $K=K_{n+1}=t_{n+1}-t_n$ is a variable time step, $\nu=\nu(n+1)$ and $\mu=\mu(n+1)$ are integers depending on K_{n+1}. U_h is the set of non-negative continuous functions $v_h (\neq 0)$ satisfying the following properties

(i) v_h has compact support,

(ii) v_h is linear on each interval $[x_i, x_{i+1}]$ $(i\varepsilon Z)$.

Here Z is the set of integers and $\{x_i\}_{i\varepsilon Z} \equiv X(\ell, r)$ is the set of nodal points defined by

$$x_i = x_i(\ell, r) = \begin{cases} ih & i \in Z \setminus \{L(\ell)-1, R(r)+1\}, \\ \ell & i = L(\ell)-1, \\ r & i = R(r)+1, \end{cases} \tag{4.3.8}$$

where

$$\ell = \ell(v_h) = \sup\{\xi \in \mathbb{R}^1 ; \quad v(x) = 0 \quad \text{on } (-\infty, \xi)\},$$

$$r = r(v_h) = \inf\{\xi \in \mathbb{R}^1 ; \quad v(x) = 0 \quad \text{on } (\xi, \infty)\},$$

$$L(\ell) = \min\{i \in Z ; \ ih > \ell\},$$

$$R(r) = \max\{i \in Z ; \ ih < r\}.$$

$\ell(v_h)$ and $r(v_h)$ denote the left and right interface of v_h respectively.

II The Difference Operator $H_{h,K} = I_h + KH_h$

For simplicity an operator $H_{h,K}$ mapping from U_h to U_h is introduced instead of H_h. For $v_h \varepsilon U_h$ the numbers ℓ' and r' were defined (which become the interfaces of $H_{h,K}v_h$) by

$$\ell' = \ell - a\,\delta v_{L-1} K \quad , \quad r' = r - a\,\delta v_R K \tag{4.3.9}$$

where $\ell = \ell(v_h)$, $r = r(v_h)$, $L = L(\ell)$, $R = R(r)$ and

$$\delta v_i = \delta v_h(x_i) = \left(v_h(x_{i+1}) - v_h(x_i)\right)/h_i \quad , h_i = x_{i+1} - x_i ,$$

$$(x_i \in X(\ell, r) \quad , \ i \in Z).$$

From the conditions on K (see (4.3.12), (4.3.13)) it follows that

$$L' = L - 1 \quad \text{or} \quad L' = L \ ; \ R' = R+1 \quad \text{or} \quad R' = R \tag{4.3.10}$$

where $L' = L(\ell')$ and $R' = R(r')$. Therefore $(H_{h,K}v_h)(x_i')$ are defined for all $x_i' \varepsilon X(\ell', r')$ by

$$(H_{h,K} v_h')(x_i) = \begin{cases} v_i + a(\delta v_i)^2 K & \text{if} \quad i \in S^+ = S_S^+ \cup S_R^+ , \\ v_i & \text{if} \quad i \in S^0 , \\ v_i + a(\delta v_{i-1})^2 K & \text{if} \quad i \in S^- = S_S^- \cup S_R^- , \\ (L'h - \ell')\,\delta v_{L-1} & \text{if} \quad i = L' = L-1 , \\ (R'h - r')\,\delta v_R & \text{if} \quad i = R' = R+1 , \\ 0 & \text{if} \quad i \in Z \setminus \{L', \dots R'\}. \end{cases} \tag{4.3.11}$$

where

$$S_S^+ = \{ i \in \{L, \ldots, R\} : \delta v_{i-1} < \delta v_i \text{ and } \delta v_{i-1} > \delta v_i \},$$

$$S_S^- = \{ i \in \{L, \ldots, R\} : \delta v_{i-1} < \delta v_i \text{ and } \delta v_{i-1} < -\delta v_i \},$$

$$S_R^+ = \{ i \in \{L, \ldots, R\} : \delta v_{i-1} \geqslant \delta v_i > 0 \},$$

$$S_R^- = \{ i \in \{L, \ldots, R\} : 0 \geqslant \delta v_{i-1} \geqslant \delta v_i \},$$

$$S^0 = \{ i \in \{L, \ldots, R\} : \delta v_{i-1} \geqslant 0 \geqslant \delta v_i \}.$$

Note that the above definition is derived from construction of the solution $v(t,x)$ of (4.3.4) with an initial value

$$v(0,x) = v_h(x) \in U_h \quad \text{so that} \quad v(K, x_i') = H_{h,K} v_h(x_i')$$

holds for all $x_i' \in X(\ell', r')$. Before imposing the condition on K the following lines were defined.

$$y_\ell(t) = \ell - a\,\delta v_{L-1}\, t \quad , \quad y_r(t) = r - a\,\delta v_R\, t \quad ,$$

$$y_i(t) = x_i - a(\delta v_{i-1} + \delta v_i)\, t \quad \text{for } i \in S_S^+ \cup S_S^- \quad ,$$

$$Z_{j1}(t) = x_j - 2a\,\delta v_{j-1}\, t \quad \text{and} \quad Z_{j2}(t) = x_j - 2a\,\delta v_j\, t$$

$$\text{for } j \in S_R^+ \cup S_R^- \cup S^0.$$

Lines y_ℓ, y_r and y_i are called shock lines of the solution of Burgers equation $\frac{\partial w}{\partial t} = a(\frac{\partial w^2}{\partial x})$ obtained by setting $w = \frac{\partial v}{\partial x}$ in (4.3.4). These relations are derived from the Rankine-Hugoniot jump condition. On the wedge determined by two characteristics Z_{j1} and Z_{j2}, the solution w has a rare faction wave which connects the two states δv_{i-1} and δv_i. The following condition on K was imposed:

$$\left\{ \begin{array}{l} \text{The lines } y_i(t),\ Z_{j1}(t),\ Z_{j2}(t),\ y_\ell(t) \text{ and} \\ y_r(t) \text{ do not intersect each other on } (0,K) \quad (4.3.12) \\ \text{and } |y_i(K) - x_i| \leqslant h \ ;\ |Z_{js}(K) - x_j| \leqslant h \quad (s=1,2;\ L \leqslant i,j \leqslant R) \end{array} \right.$$

$$\begin{cases} a\,\delta v_{L-1}\,K \leqslant \frac{h}{4} & \text{if } \delta v_{L-1} > \delta v_L > 0; \\ -a\,\delta v_R\,K \leqslant \frac{h}{4} & \text{if } \delta v_R < \delta v_{R-1} < 0; \\ a\,\delta v_L\,K \leqslant \frac{h}{4} & \text{if } \delta v_L > \delta v_{L+1} > \delta v_{L-1}; \\ -a\,\delta v_{R-1}\,K \leqslant \frac{h}{4} & \text{if } \delta v_{R-1} < \delta v_{R-2} < \delta v_R; \\ K \leqslant c^* h^s & (\text{For simplicity we put } c^*=1 \text{ and } s=\frac{1}{2}) \end{cases} \quad (4.3.13)$$

Under the condition (4.3.12) $H_{h,K}v_h \varepsilon U_h$.

Difference Operator P_h

For $v_h \varepsilon U_h$ let

$$(P_h v_h)(x_i) = m\, v_i\, \delta^2 v_i \qquad \text{for all } x_i \in X(\ell, r) \quad (4.3.14)$$

where $v_i = v_h(x_i)$, $\ell = \ell(v_h)$, $r = r(v_h)$ and

$$\delta^2 v_i = 2\,(\delta v_i - \delta v_{i-1})/(h_i + h_{i-1}) \qquad (h_i = x_{i+1} - x_i).$$

The interfaces of $(I_h + (K/\mu)P_h)v_h$ are the same ones of v_h, and $(I_h + (K/\mu)P_h)v_h \varepsilon U_h$ holds from the following condition:

$$\left.\begin{aligned} & m\,\|v_h\|_\infty\, K'\left[1/h^2 + 2/\{h(h+h_i)\}\right] \leqslant 1 && \text{for } i = L-1, R \\ & 4m\,\|v_{hx}\|_\infty\, K'/(h+h_i) \leqslant 1 && \text{for } i = L-1, R \end{aligned}\right\} \quad (4.3.15)$$

where $K' = K/\mu$, $L = L(\ell)$ and $R = R(r)$.

III The Difference Operator D_h

When $q \geqslant 1$. For $v_h \varepsilon U_h$ let

$$D_h v_h(x_i) = -(m-1)\, c\, (v_i)^q \qquad \text{for all } x_i \in X(\ell, r) \quad (4.3.16)$$

and let the interfaces of $(I_h + (K/\nu)D_h)v_h$ be the same ones of v_h. $(I_h + (K/\nu)D_h)v_h \varepsilon U_h$ holds from the following condition:

$$K'(m-1)\, c\, q\, \|v_h\|_\infty^{q-1} < 1 \qquad (K' = K/\nu). \quad (4.3.17)$$

To start the scheme (4.3.7) we take

$$t_0 = 0, \quad \ell_0 = \ell(v_h^0) \equiv a_1, \quad r_0 = r(v_h^0) \equiv a_2,$$
$$v_h^0(x_i) = v^0(x_i) \quad \text{for all } x_i \in X(\ell_0, r_0).$$

When c=0, equation (1.1) reduced to the porous medium equation and of course the Tomoeda algorithm can be used for that equation. The results are included in section 5.

4.4 The amended algorithms

4.4.1 The GRAVELEAU and Jamet algorithm

We mentioned earlier in this section that this algorithm has the reputation of not tracking the interface accurately. To remedy this we have taken the variable time steps $K^{(n)}$:

$$a \max_i \{|\delta v_i^n|\} K^{(n)}/h = 1$$

where $a = \frac{m}{m-1}$, $\delta v_i^n = (v_{i+1}^n - v_i^n)/h$, $i, n \in \mathbb{Z}$

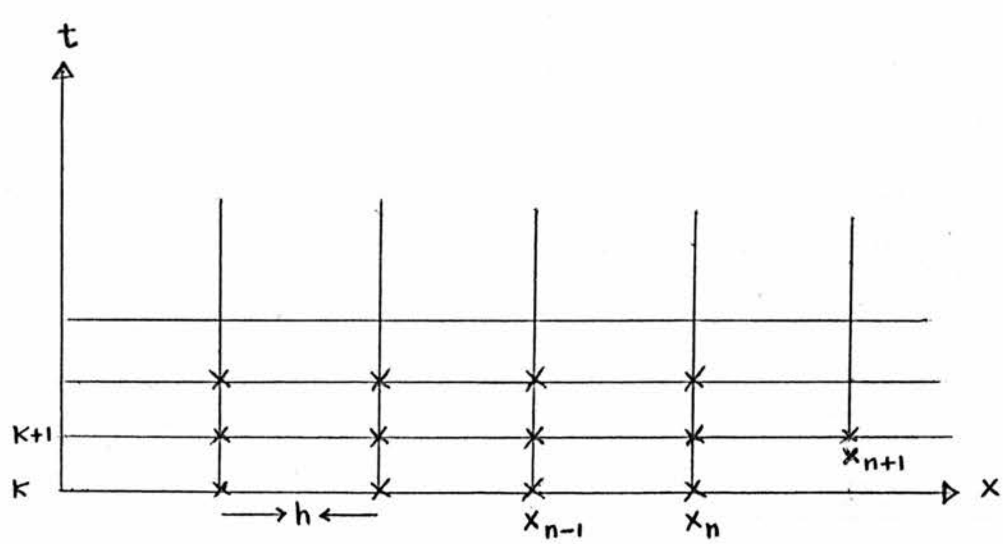
such that the stability condition

$$a\, c_1\, (K/h) \leqslant 1 \qquad (c_1 = \sup_x |dv^0(x)/dx|)$$

and the boundary condition at the interfaces

$$\frac{dS}{dt} = -a\, \frac{\partial(u^{m-1})}{\partial x} \qquad (S = S(t))$$

is satisfied at each step. The interface will therefore move a distance h during the time step K and can be accurately tracked.



At the step K+1 we used linear interpolation to calculate the value of the function at the mesh point x_n using two mesh points: x_{n-1} and x_{n+1}.

To solve problem II for the porous medium equation it was simply necessary to fix u at the mesh point x=0, i.e. $v_{0,J} = 1$ or in general a function of J.

4.4.2 Amendments to Tomoeda algorithm

As we mentioned before it was decided to modify the algorithm particularly in the way the variable time step is chosen. So instead of using the conditions (4.3.12) and (4.3.13) on K we used the variable time step:

$$K^{(n)} = \left(h^2 / a \max_i \{|\delta v_i^n|\}\right) / \alpha$$

where

$$a = \frac{m}{m-1} \quad ; \quad \delta v_i^n = v_{i+1}^n - v_i^n \quad , \quad h \in \mathbb{R}^+, (i, n \in \mathbb{Z})$$

and

$$\alpha \in \mathbb{R}^+ .$$

Essentially we now compute a sequence of numerical solutions which we expect to converge with α. This convergence is clearly shown in section 5 thus justify our amended scheme. For each value of α, μ and ν are chosen appropriately.

5. NUMERICAL EXPERIMENTS

In this section we display numerical results for problems I and II, paying particular attention to both the numerical demonstration of a waiting time for (1.4) and the large time comparison for (1.4) and (1.1).

5.1 Numerical results for problem I for the porous medium equation

To give some indication of the accuracy of each of our numerical schemes we compare the numerical solution of (1.4) with the exact Barenblatt-Pattle (B-P) solution. The easiest way to do this is to take (2.1) at t=1 as the initial condition (t=0) in our numerical solution. The results are displayed in TABLES 1 and 2 for the modified Graveleau-Jamet (G-J) and Tomoeda (T) schemes, respectively.

TABLE 1

m = 2.0, h = 0.0229

Time	Numerical solution (u(0,t))	Exact solution (u(0,t))	Numerical Interface	Exact Interface	|Error of Interface|
0.0	0.43679	0.43679	2.29	2.29	0.0
0.29525262	0.40032914	0.400701921	2.4961	2.4956	0.0005
0.99999470	0.34590521	0.346680943	2.8854	2.8845	0.0009
3.02166314	0.27366620	0.274665653	3.6411	3.6408	0.0003
6.08878660	0.22638418	0.227378266	4.3968	4.3980	0.0012
12.18109703	0.18399900	0.184908013	5.4044	5.4081	0.0037
17.25427818	0.16503856	0.165889168	6.0227	6.0281	0.0054

TABLE 2

m = 2.0, h = 0.03125

Time	Numerical solution (u(0,t))	Exact solution (u(0,t))	Numerical Interface	Exact Interface	|Error of Interface|
0.0	0.43679	0.43679	2.29	2.29	0.0
0.30302370	0.39985487	0.39990375	2.4910	2.50	0.009
0.99294132	0.34684142	0.34708945	2.8605	2.8811	0.0205
2.99454021	0.27466056	0.27528591	3.5973	3.6326	0.0353
5.99530458	0.22750115	0.22838665	4.3318	4.3785	0.0467
12.22583294	0.18364556	0.184699296	5.3546	5.4142	0.0596
17.25238800	0.16480850	0.165894894	5.9613	6.0279	0.0666

For purposes of tabulation the two solutions are compared at $x=0$ while the numerical solutions themselves are plotted in Figures 2 and 3, where the exact and numerical solutions are, on this scale, indistinguishable.

The numerical interface for the G-J scheme is shown in Figure 4 while the results of the α-convergence modified T scheme is shown in Figure 5. The convergence with α is evident up to $\alpha=7$ but for $\alpha=9$ the solution appears to be unstable at about $t=7.0$. We thus take the numerical solution for $\alpha=7$ as the converged solution.

5.2 Numerical results of problem II for the porous medium equation using the modified G-J scheme

Here we compare our numerical results with the exact similarity solution of section 2. Specifically we take (2.13)-(2.17) at $t=1$ as the initial value ($t=0$) for the numerical solution.

Table 3 compares the interface for the modified G-J scheme with the exact value. The numerical solution is shown in Figure 6 and the interface in Figure 7, which again is indistinguishable from the exact solution.

The favourable comparison of our numerical results shows the prima facie justification for extending the numerical schemes to more general initial and initial-boundary value problems for both the porous medium and reaction diffusion equations. This we do in Sections 5.3 and 5.4.

<u>TABLE 3</u>

m = 2.0, h = 0.0229

Time	Numerical Interface	Similarity Interface	|error|
0.44105482	2.7480	2.749	0.001
1.10478282	3.3205	3.3223	0.0081
2.17237568	4.0762	4.0788	0.0026
3.20831561	4.6945	4.6977	0.0032
4.57814121	5.4044	5.4085	0.0041
6.03425455	6.0685	6.0736	0.005

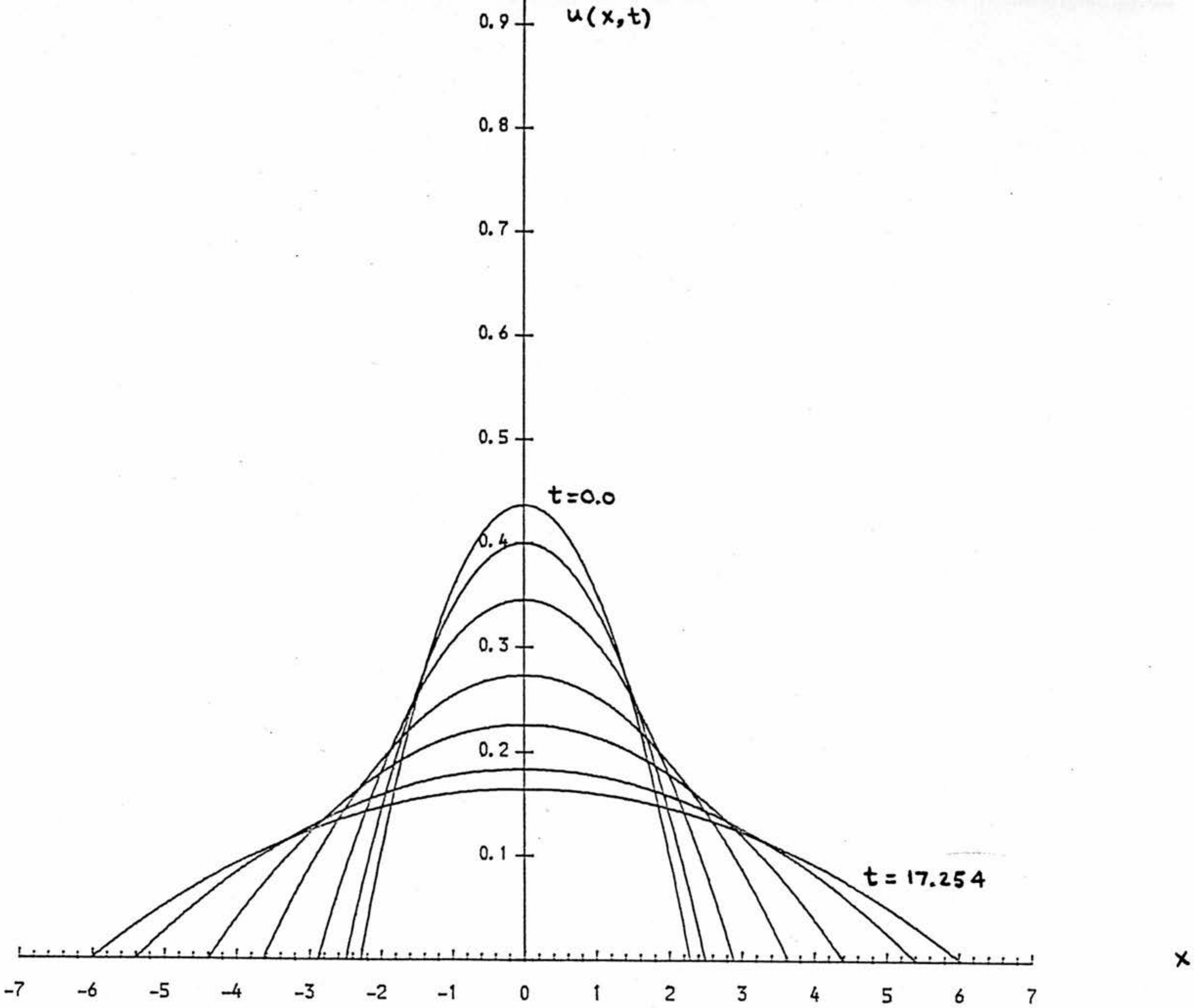


Fig.(2)

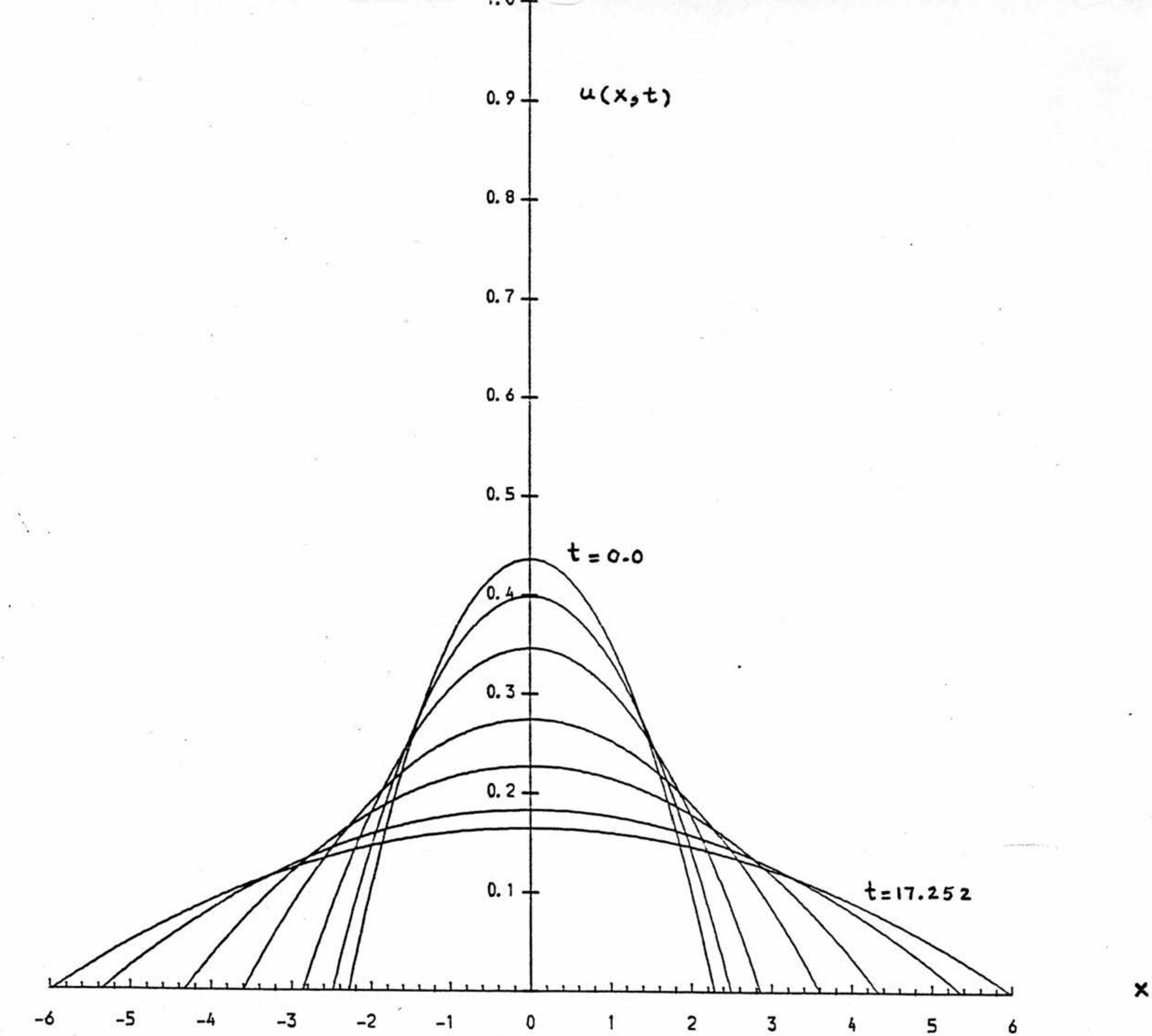


Fig.(3)

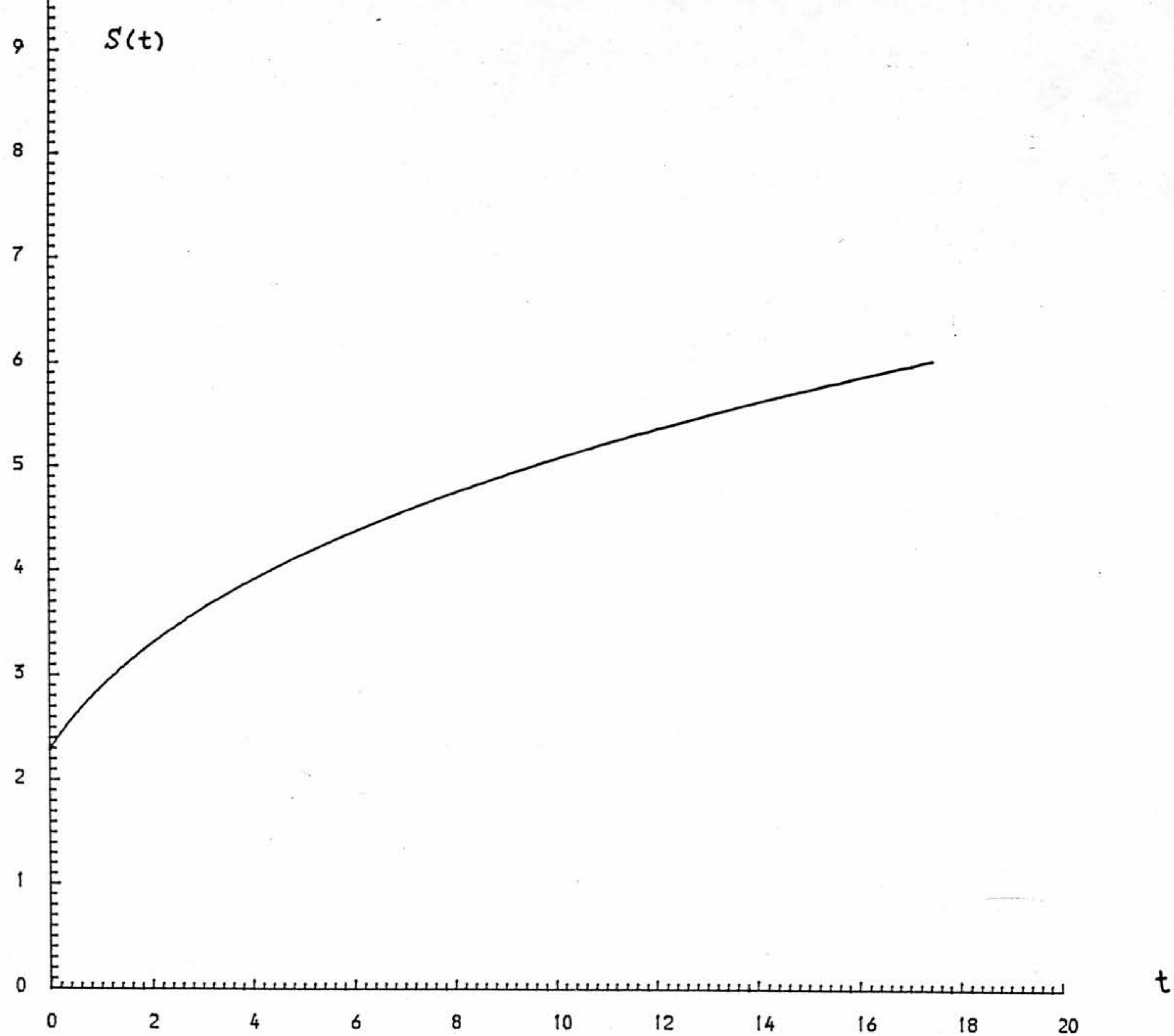


Fig.(4)

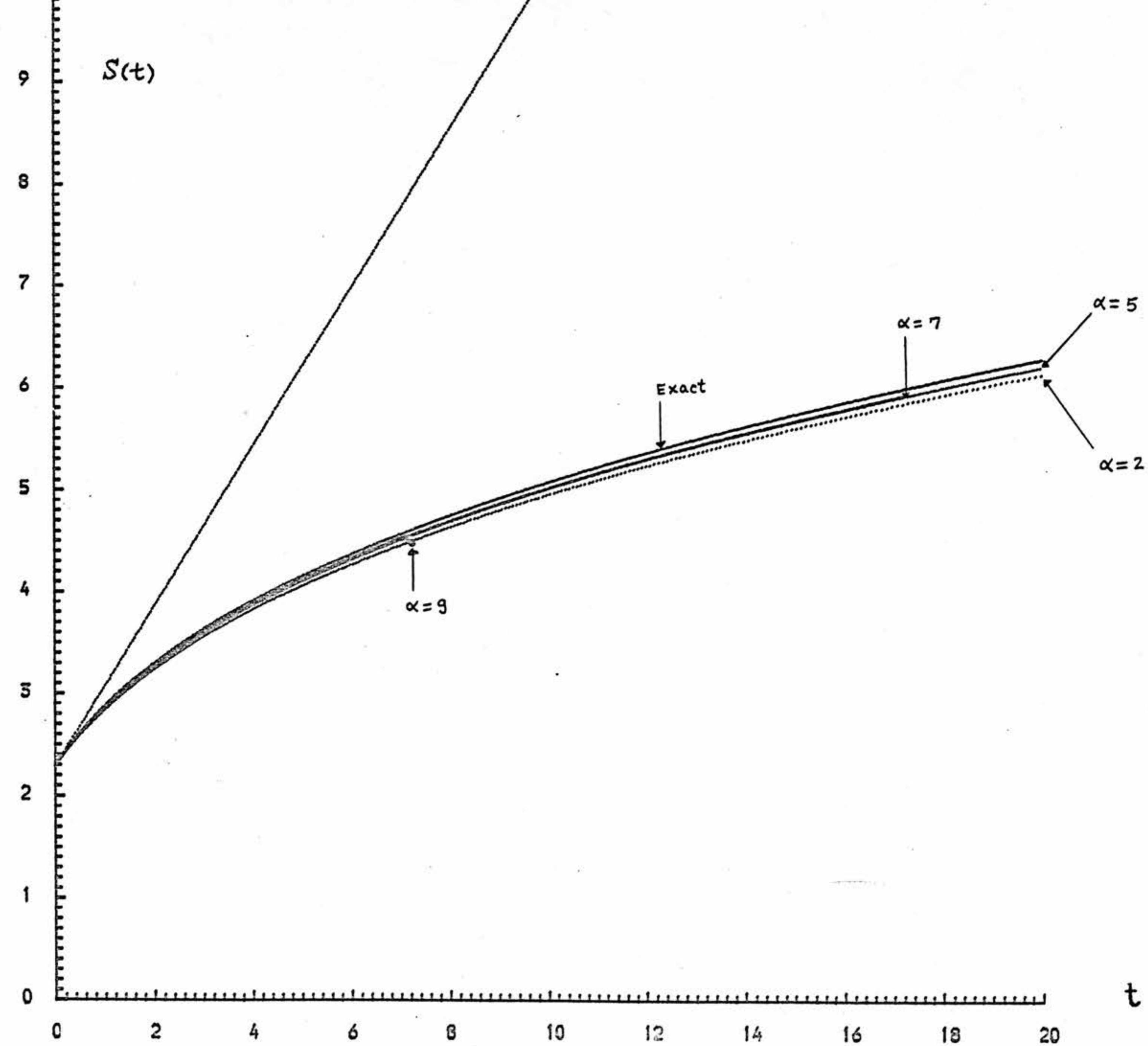


Fig.(5)

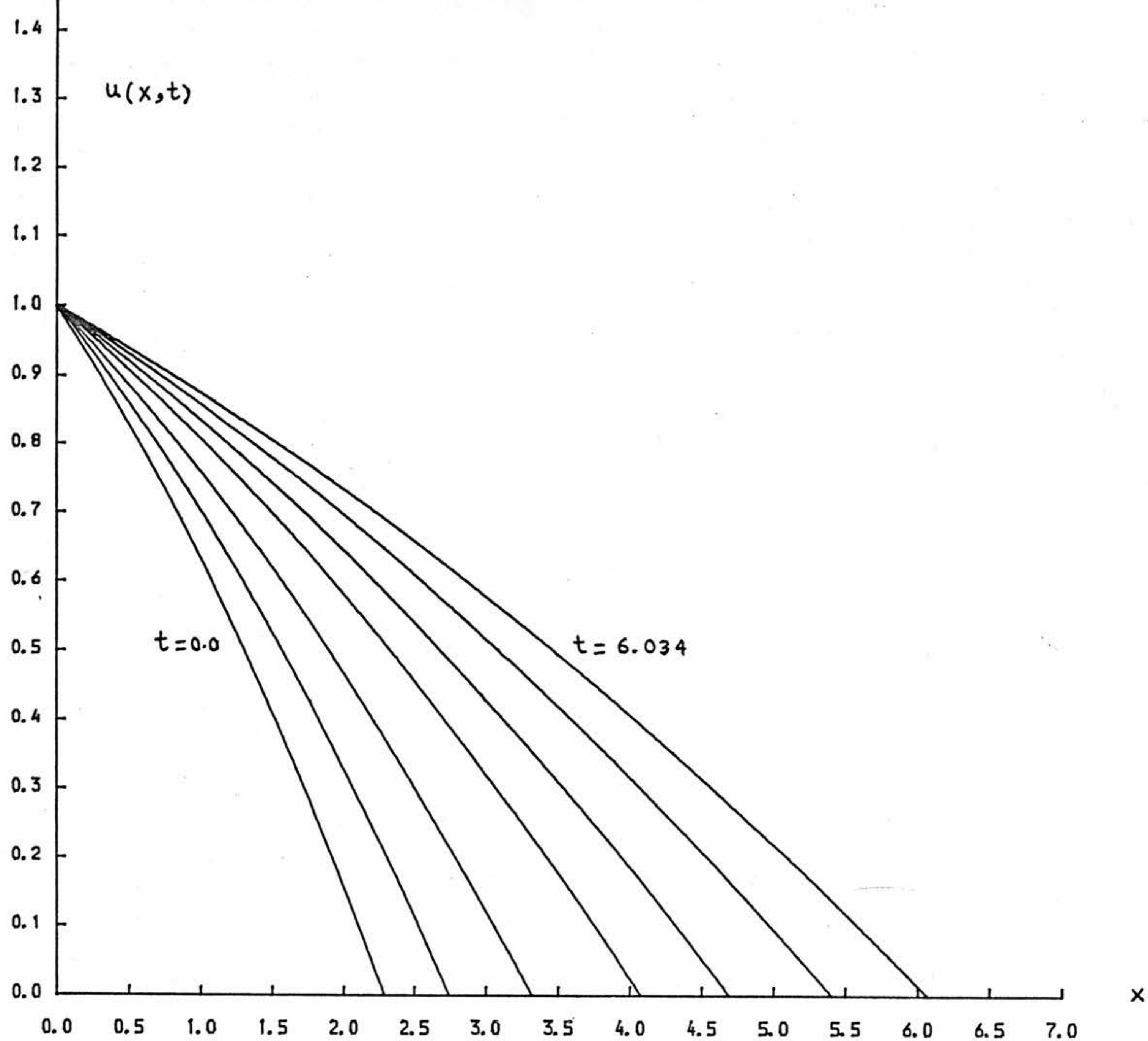

u(x,t)
t=0.0
t= 6.034
x
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0

Fig.(6)

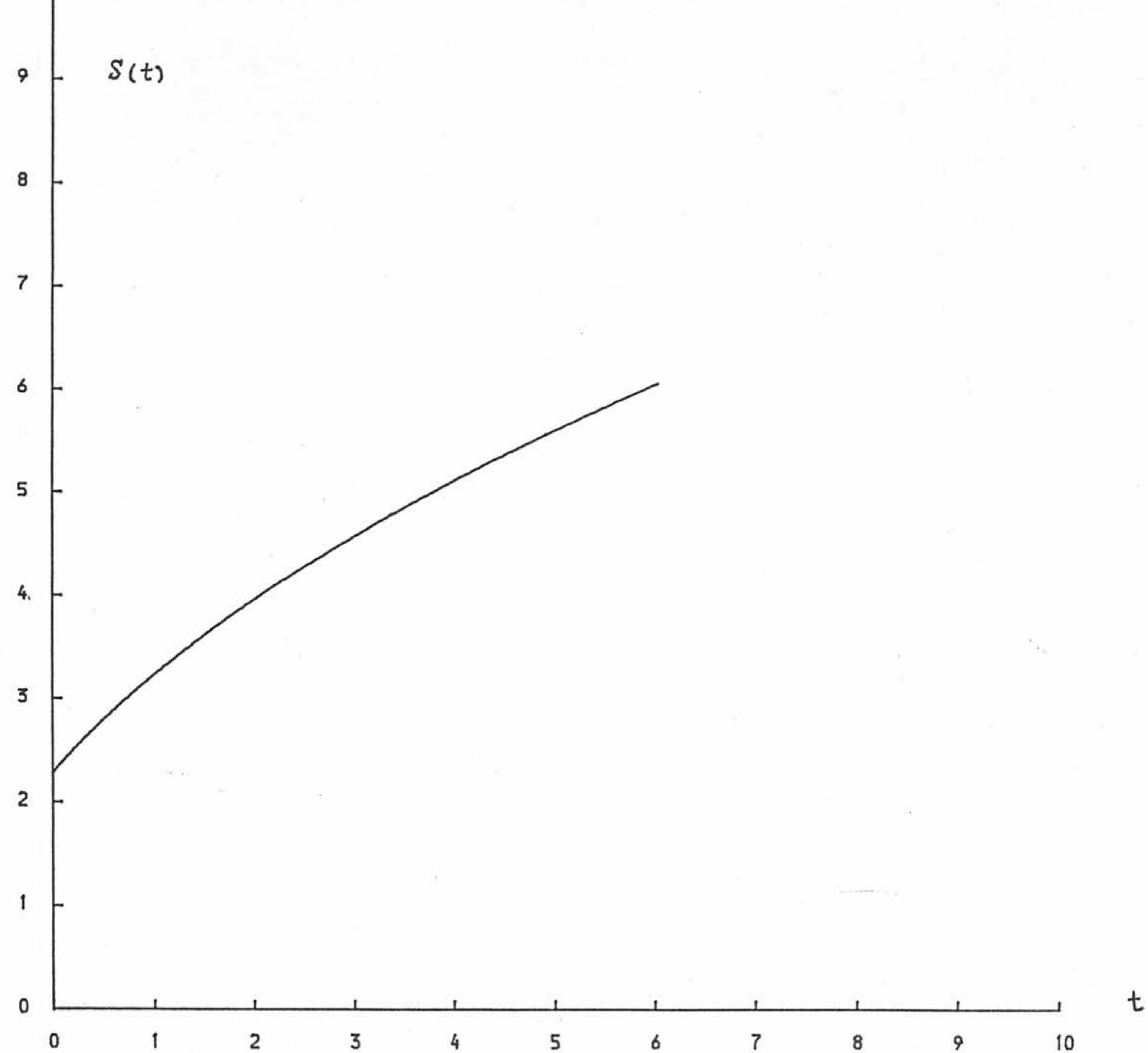


Fig.(7)

5.3 The waiting time

The most suitable algorithm for calculating waiting time is that of Tomoeda which we use here.

To demonstrate the existence of a waiting time, we take the initial data $u_0(x)$ as follows

$$u_0(x) = \begin{cases} \frac{1}{m}\left[(1-\theta)\cos^2(x) + \theta\cos^4(x)\right] & \text{for } x \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \\ 0 & \text{for } x \notin \left(-\frac{\pi}{2}, \frac{\pi}{2}\right) \end{cases} \qquad (5.3.1)$$

where $\theta \in [0,1]$. As we mentioned earlier in section 2. Aronson, Caffarelli and Kamin (1983) estimated the waiting time t^* for the above initial function. For $\theta \in [0,\frac{1}{4}]$, they found that

$$t^* = \frac{1}{2(m+1)(1-\theta)} \qquad (5.3.2)$$

while for $\theta \in (\frac{1}{4},1)$, then

$$\frac{1}{2(m+1)\beta} \leqslant t^* \leqslant \frac{1}{2(m+1)(1-\theta)} \qquad (5.3.3)$$

where β is obtained by solving the nonlinear equations

$$\beta y^2 = u_0(y) \qquad \text{and} \qquad 2\beta y = (u_0(y))'.$$

Thus in the case $\theta \in (\frac{1}{4},1)$, only bounds for t^* can be given.

The calculations of the waiting times were made for m=2 and θ = 0.0, 0.1, 0.2, 0.25, 0.5 and 1.0. The resulting motion of the interface is shown for various values of α in Figures 8-13. In each case we take α=2.0 as the converged solution since for α>2.0 certain instabilities occurrs. The results for α=2.0 are shown graphically in Figures 14-17 where they are compared, where possible, with the exact waiting times calculated from (5.3.2). The agreement in each case is satisfactory.

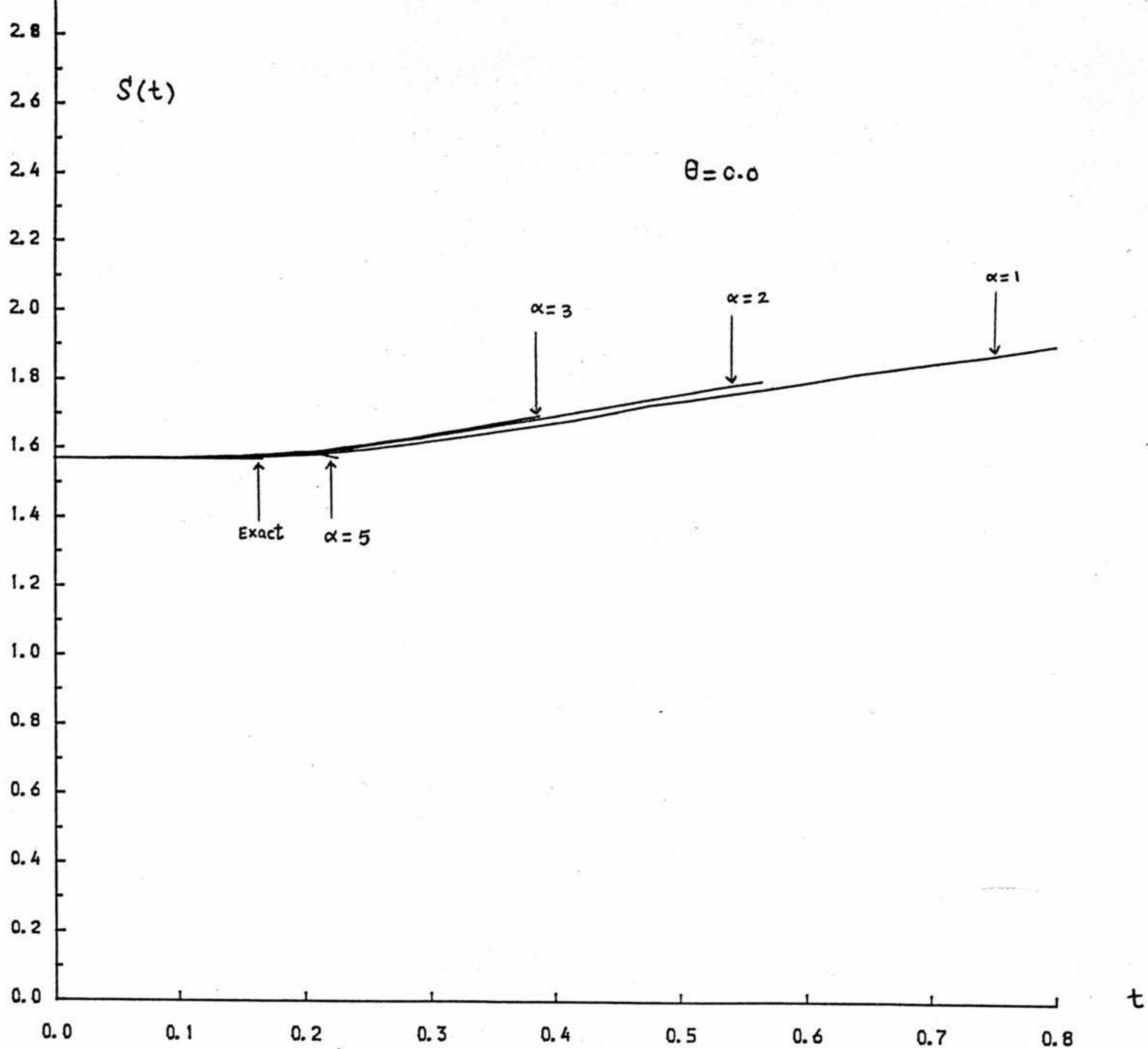

S(t)
θ=0.0
α=3
α=2
α=1
Exact
α=5
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
t

Fig.(8)

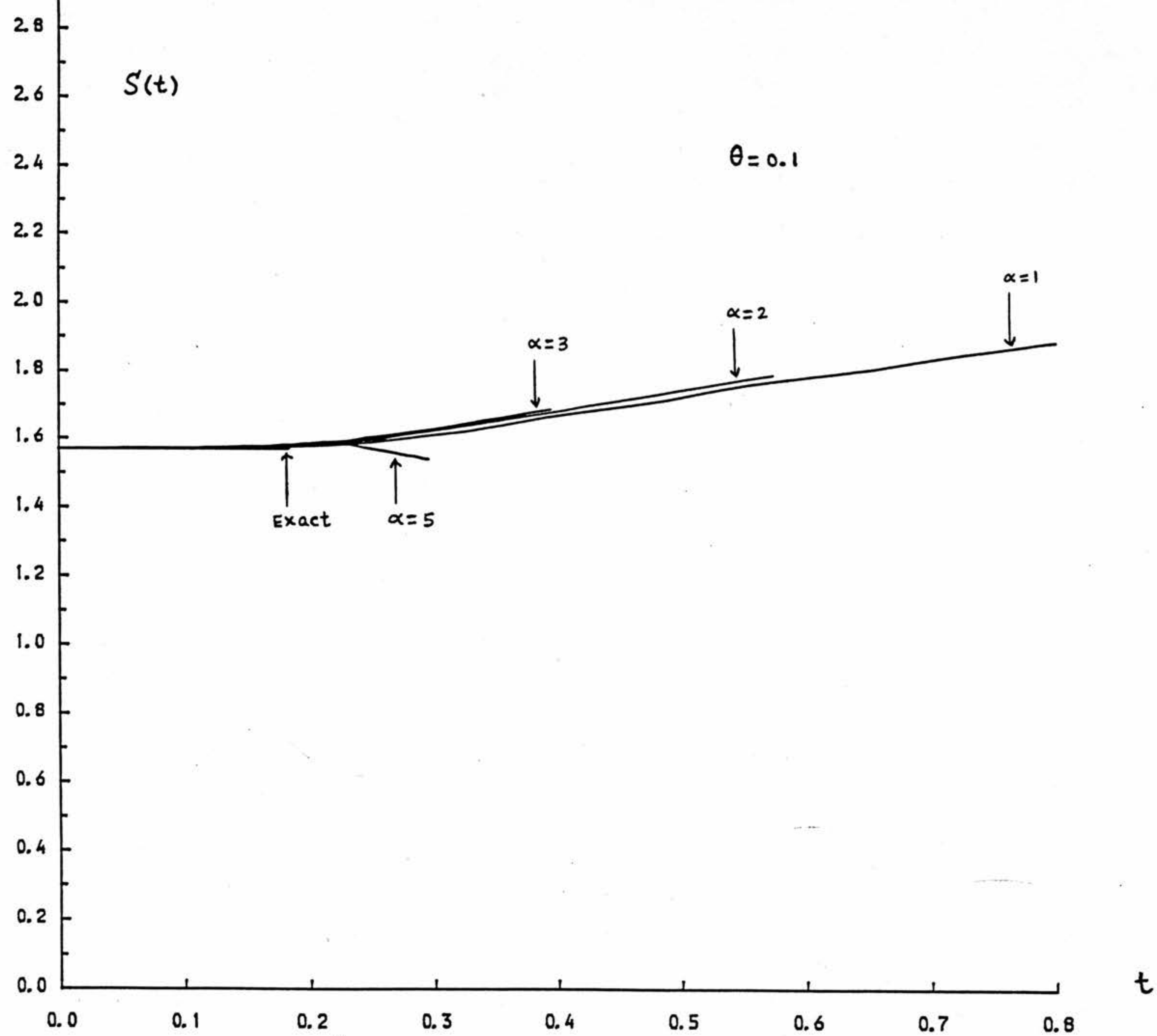
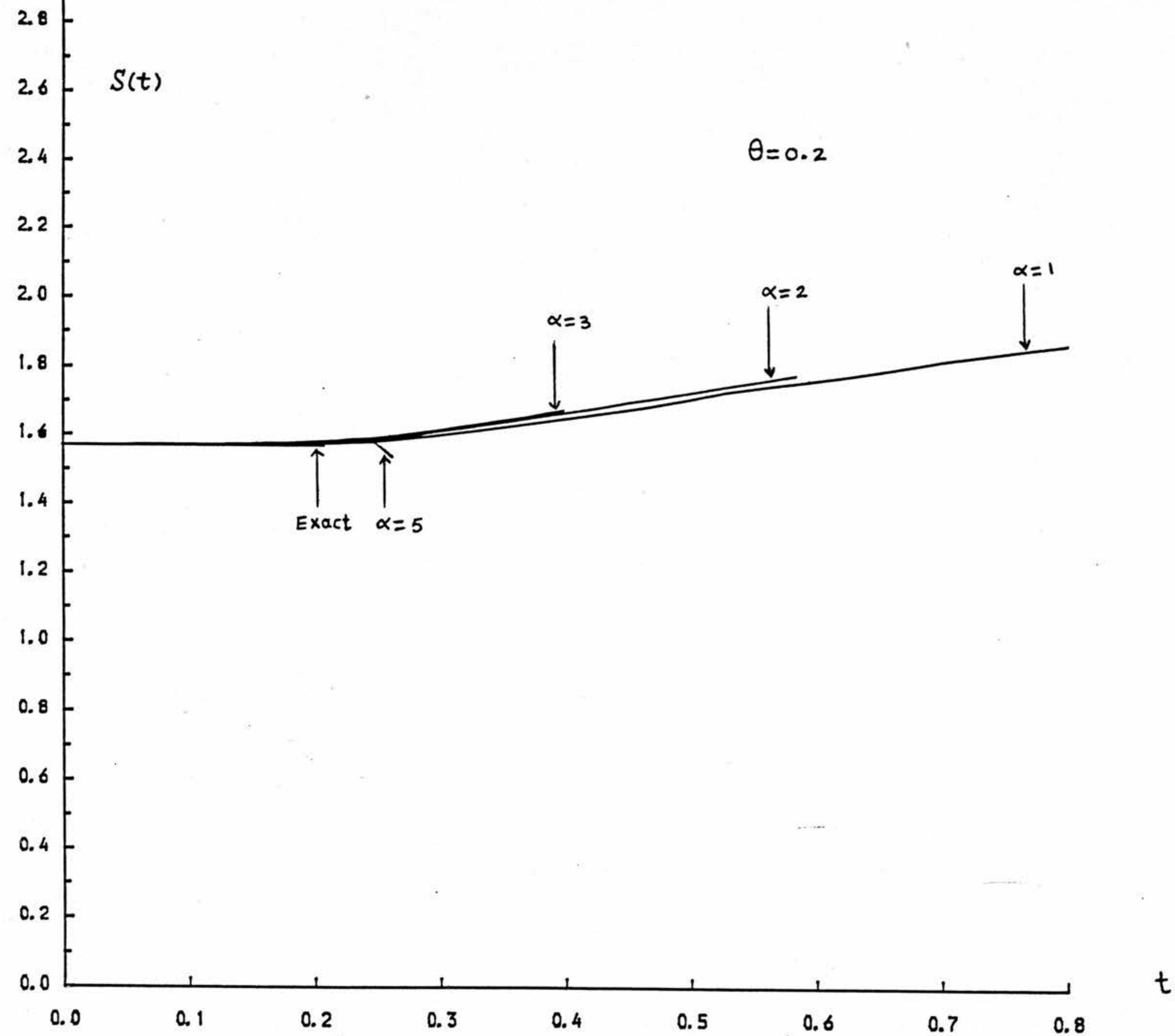

S(t)
θ= 0.1
α=1
α=2
α=3
α=5
Exact
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig.(9)



S(t)
θ=0.2
α=1
α=2
α=3
α=5
Exact
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig.(10)

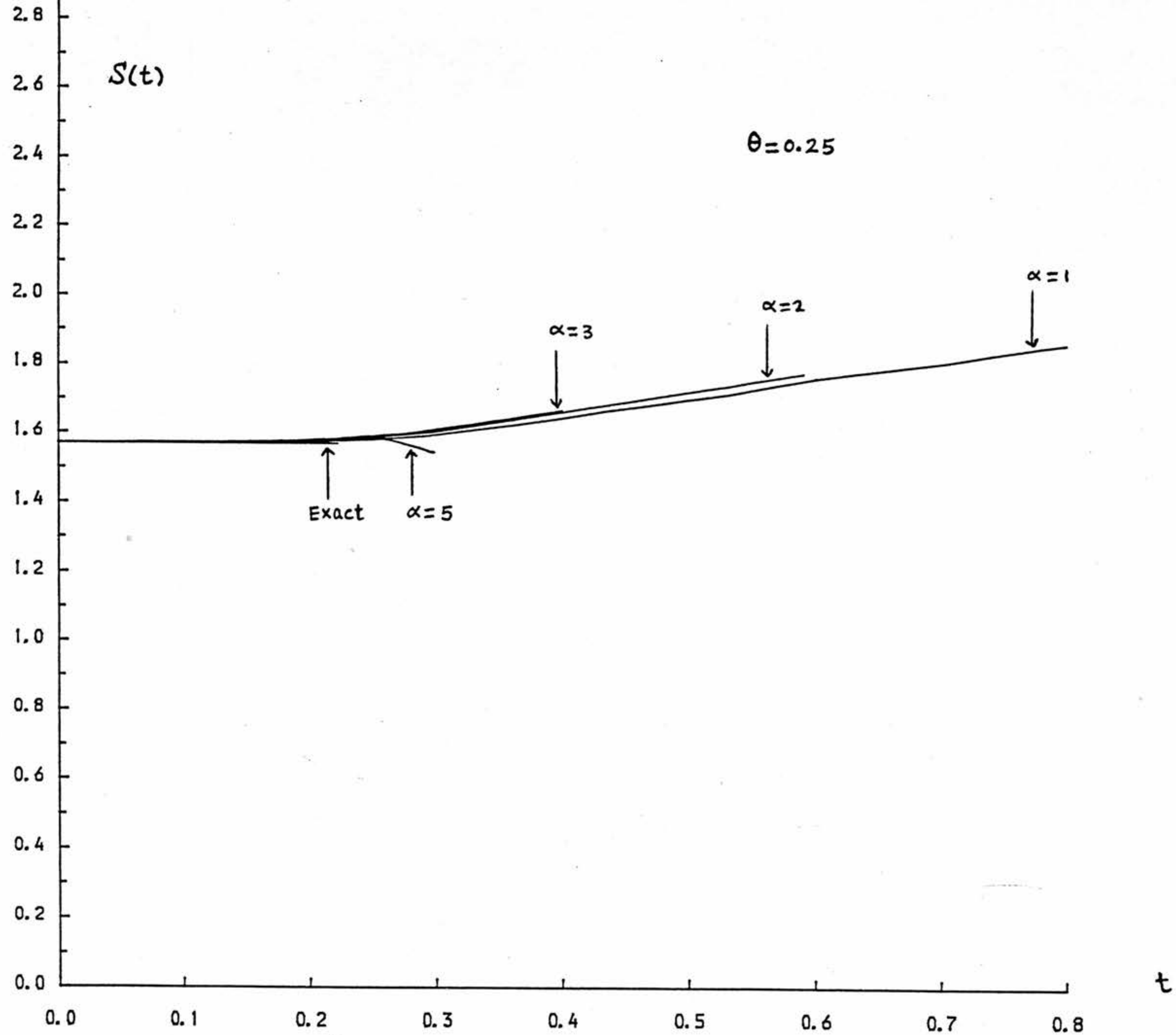

S(t)
θ=0.25
α=1
α=2
α=3
α=5
Exact
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
t

Fig. (11)

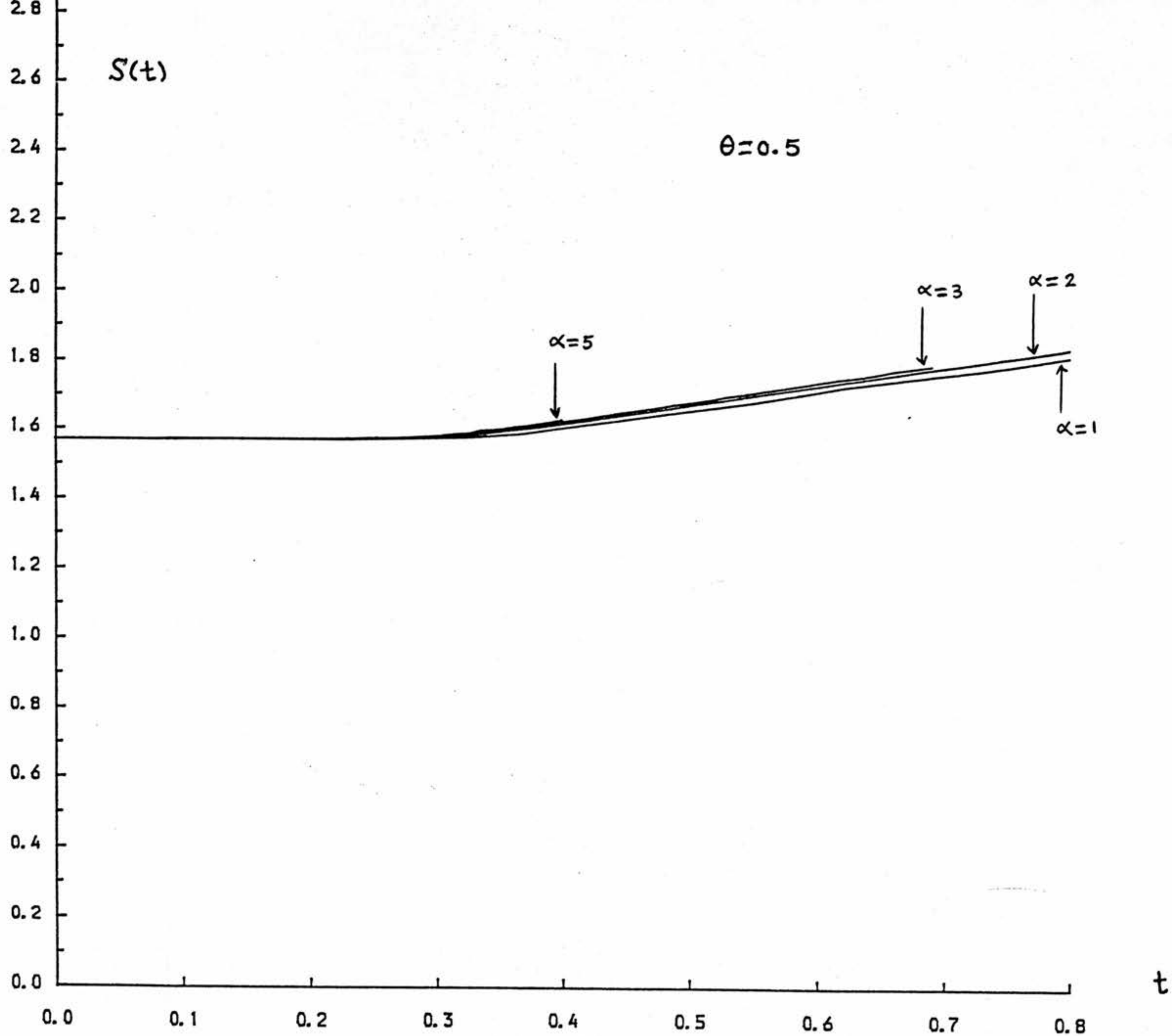

S(t)
θ=0.5
α=5
α=3
α=2
α=1
t
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
2.2
2.4
2.6
2.8
0.1
0.3
0.5
0.7

Fig. (12)

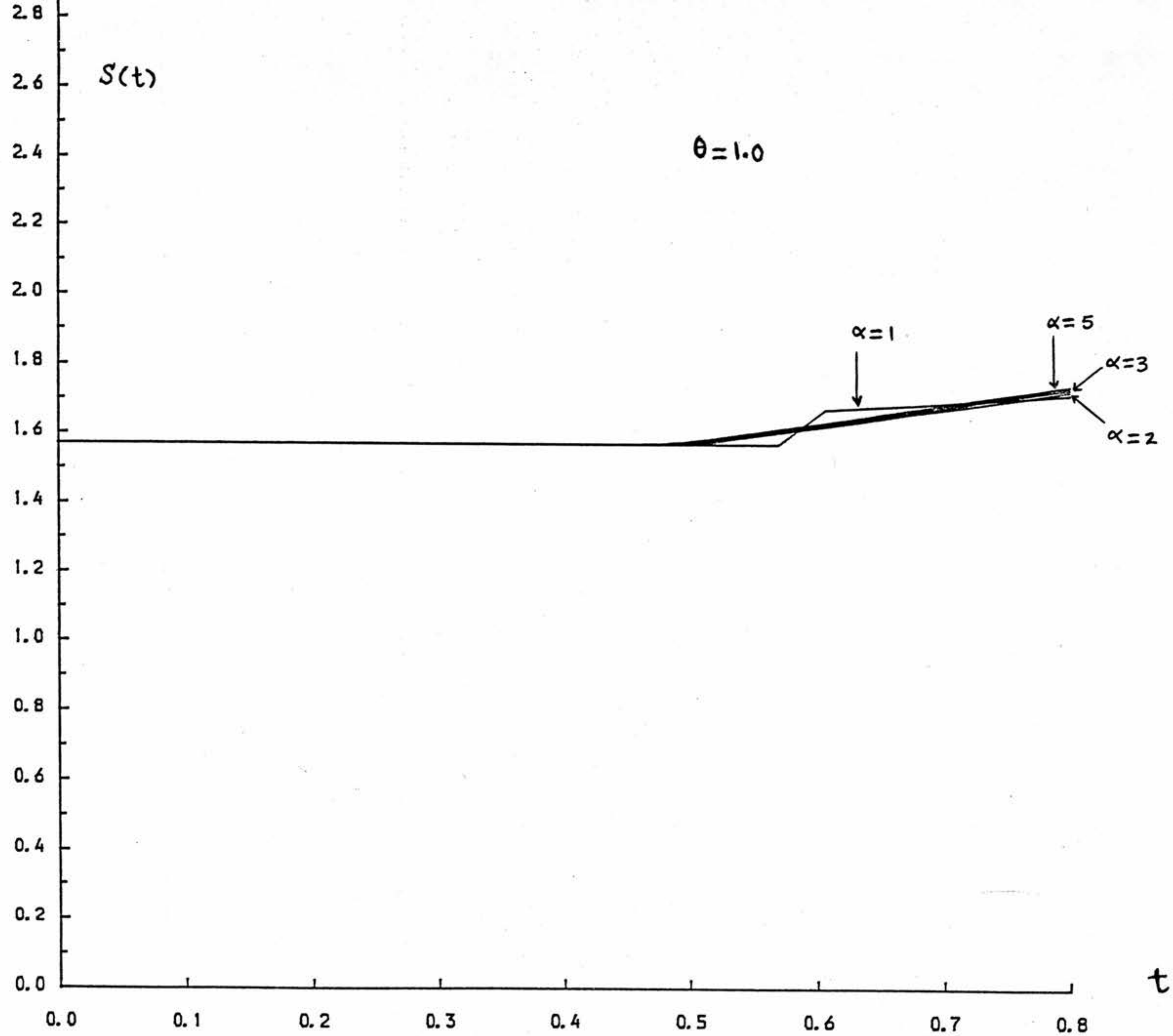
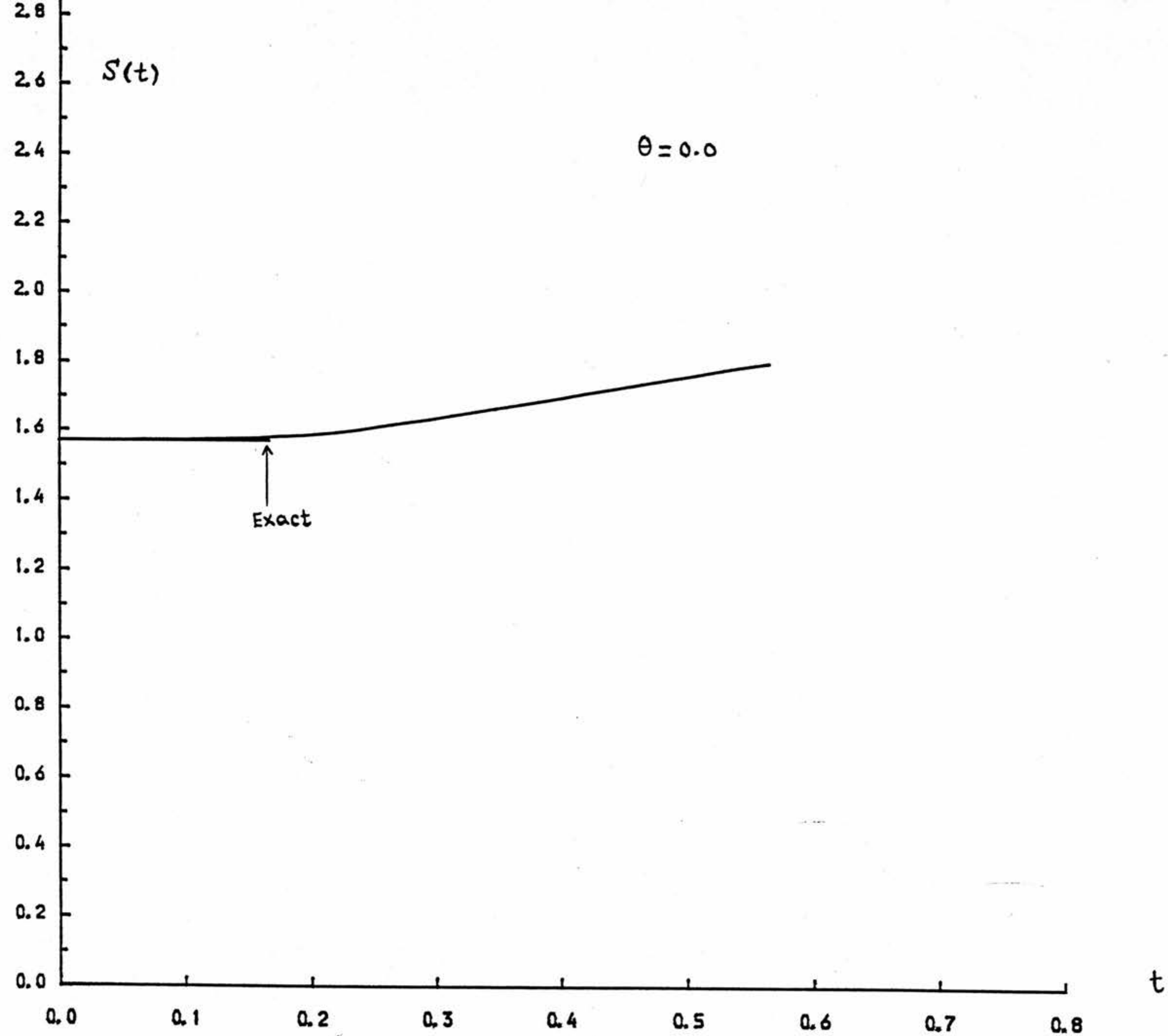

S(t)
θ=1.0
α=1
α=5
α=3
α=2
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig. (13)



S(t)
θ = 0.0
Exact
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
t

Fig. (14)

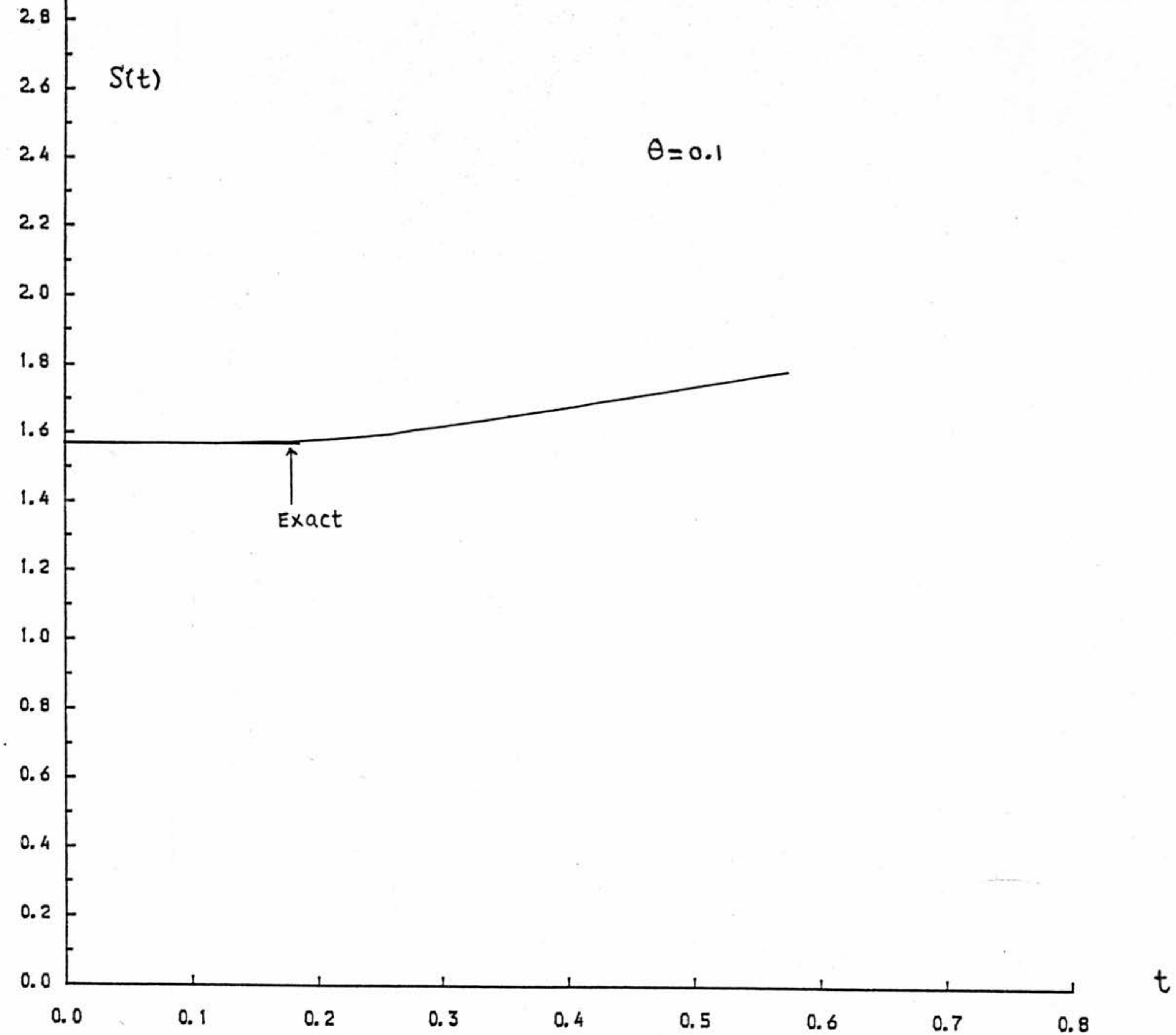

S(t)
θ=0.1
Exact
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig.(15)

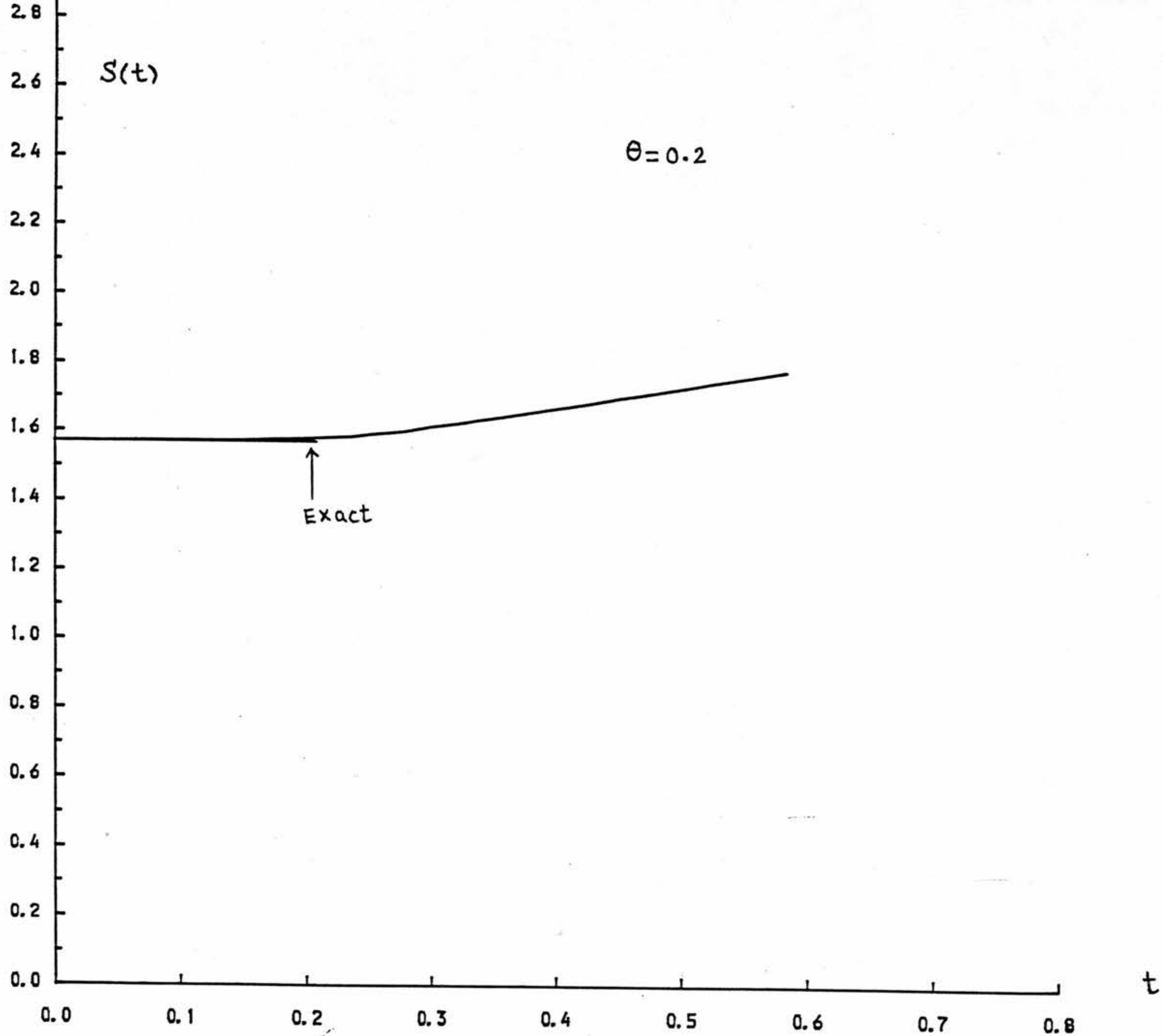

S(t)
θ=0.2
Exact
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig.(16)

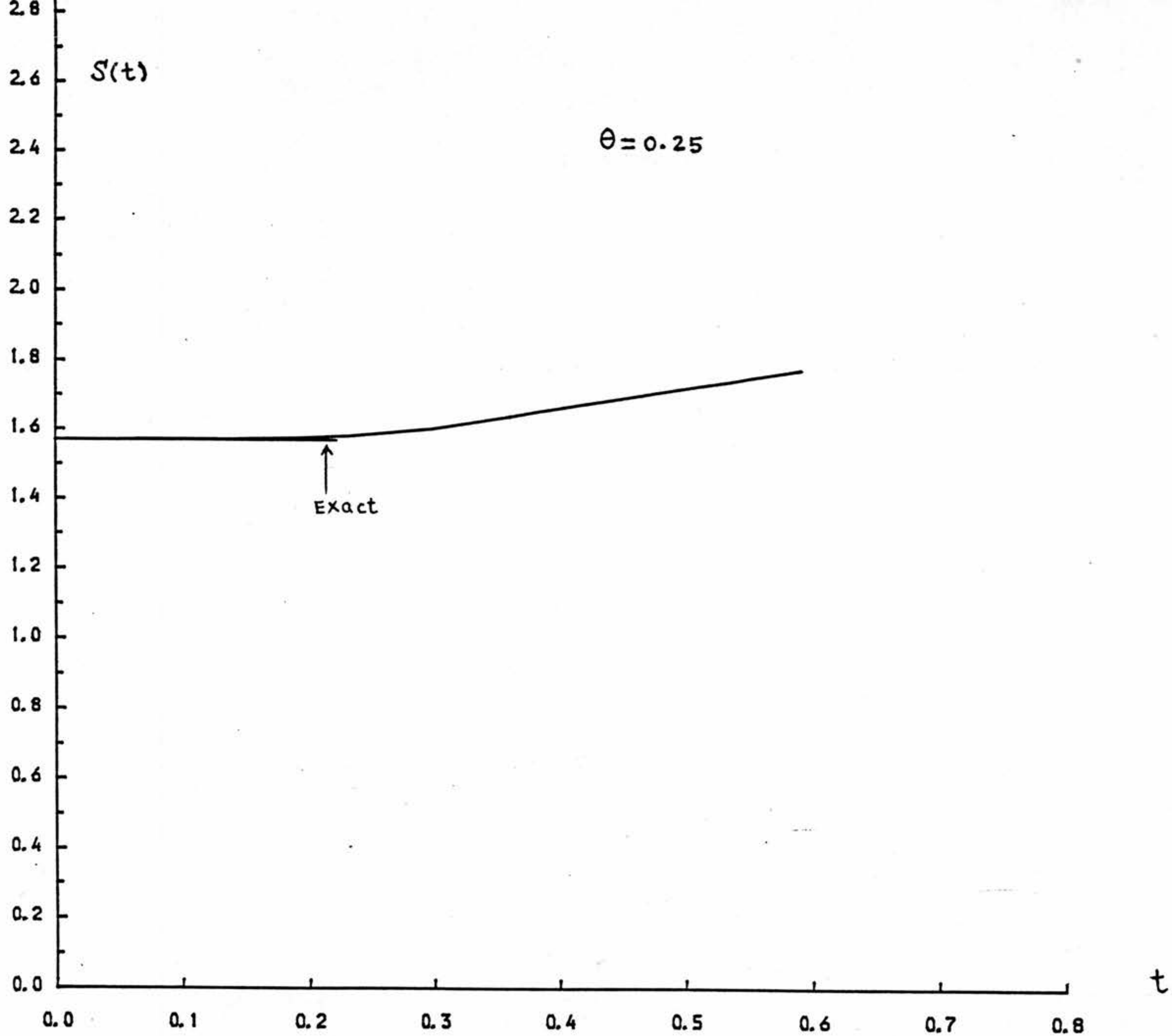

S(t)
θ=0.25
Exact
t
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Fig.(17)

5.4 Numerical results for the diffusion-reaction equation

In this subsection we shall make a comparison between numerical results obtained from implementing the modified T scheme and the asymptotic theory discussed in section 3. To do this we have taken the initial value for all regimes as

$$u_0(x) = \begin{cases} \cos(\pi x/2) & \text{for} \quad |x| < 1 \;, t=0 \\ 0 & \text{for} \quad |x| \geq 1 \;, t=0 \end{cases} \tag{5.4.1}$$

we shall discuss each of the parameter regimes separately.

(a) $p > m+2$

In this regime we have taken m=2, c=1 and p=6, as an example. The numerical right interface is shown in Figure 18, where convergence with α is evident up to α=7, for α=9 the solution appears to be unstable. We thus take the numerical solution for α=7 as the converged solution. As we proposed in section 3 the similarity interface for this regime is given by

$$s(t) = \pm \eta \; t^{1/(m+1)} \left\{ 1 + O(1) \right\} \tag{5.4.2}$$

where η is at the moment unknown and the term of O(1) represents the error, which can be shown to be $o(t^{-1/m+1})$.

To indicate a comparison with the analytic estimates we plotted the function

$$\eta(t) = s(t) \; t^{-1/(m+1)} \tag{5.4.3}$$

in Figure 19. Clearly this is converging to a finite, non-zero limit as $t \to \infty$ and agrees with the result of Section (3.1). Figure 20 shows s(t) as a function of time while Figure 21 gives the temporal evolution of the solution profile. Taking t = 69.3 in (5.4.3) we used η(69.3) as the value of η_0 in (3.1.14). The resulting Barenblatt-Pattle solution is compared with the numerical solution in Figure 22; the convergence as $t \to \infty$ is impressive.

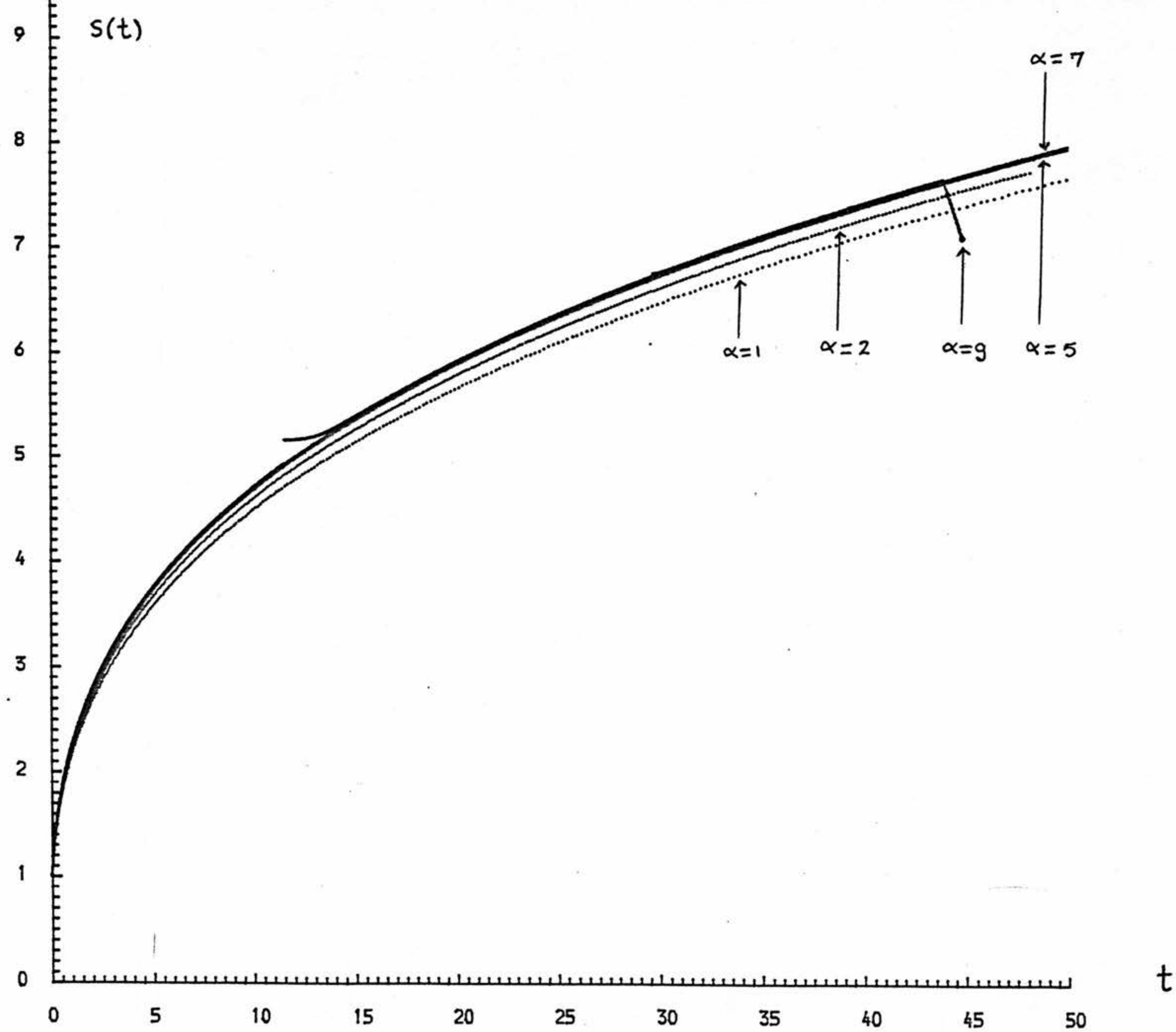


Fig.(18)

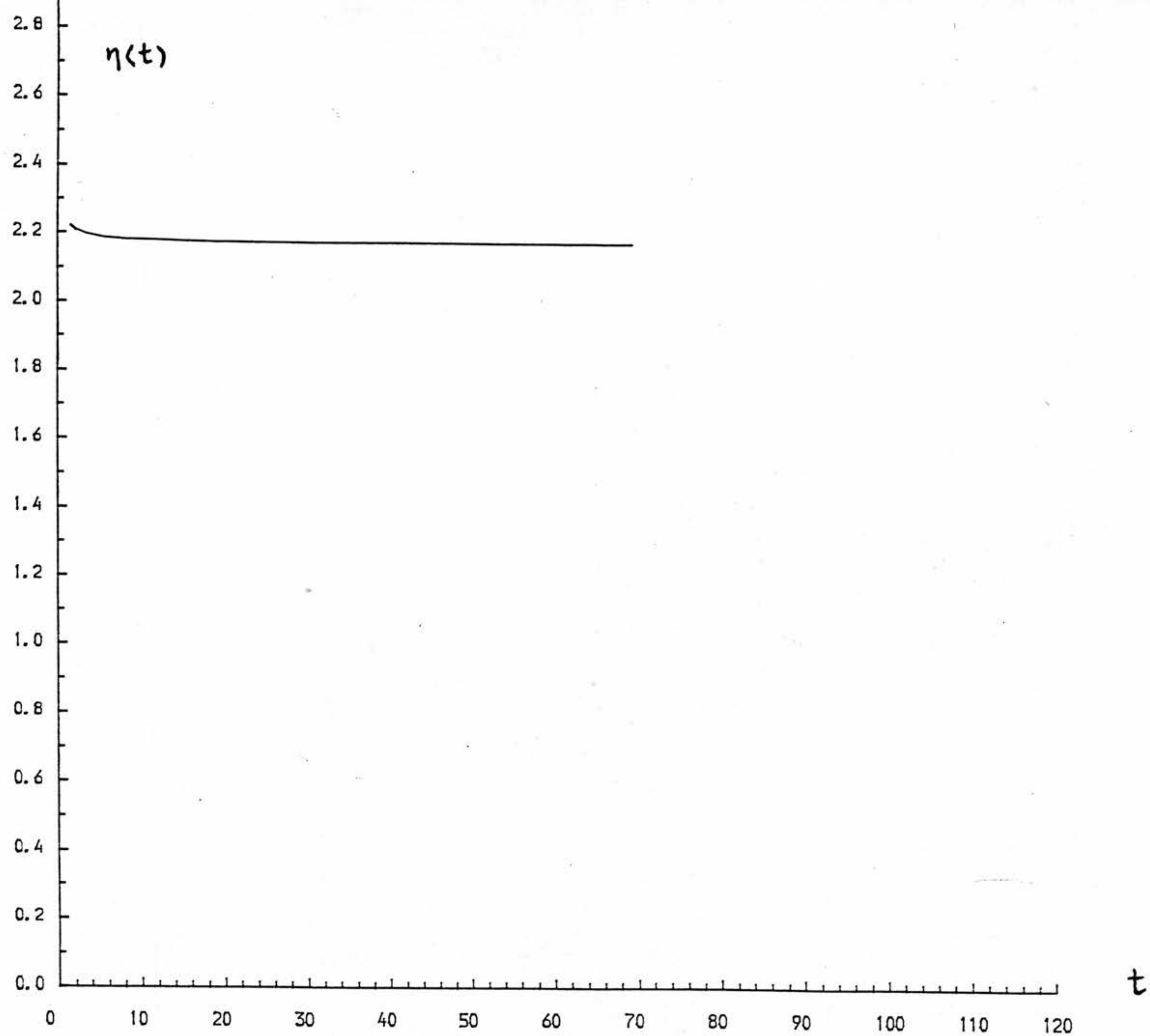

η(t)
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50
60
70
80
90
100
110
120
t

Fig.(19)

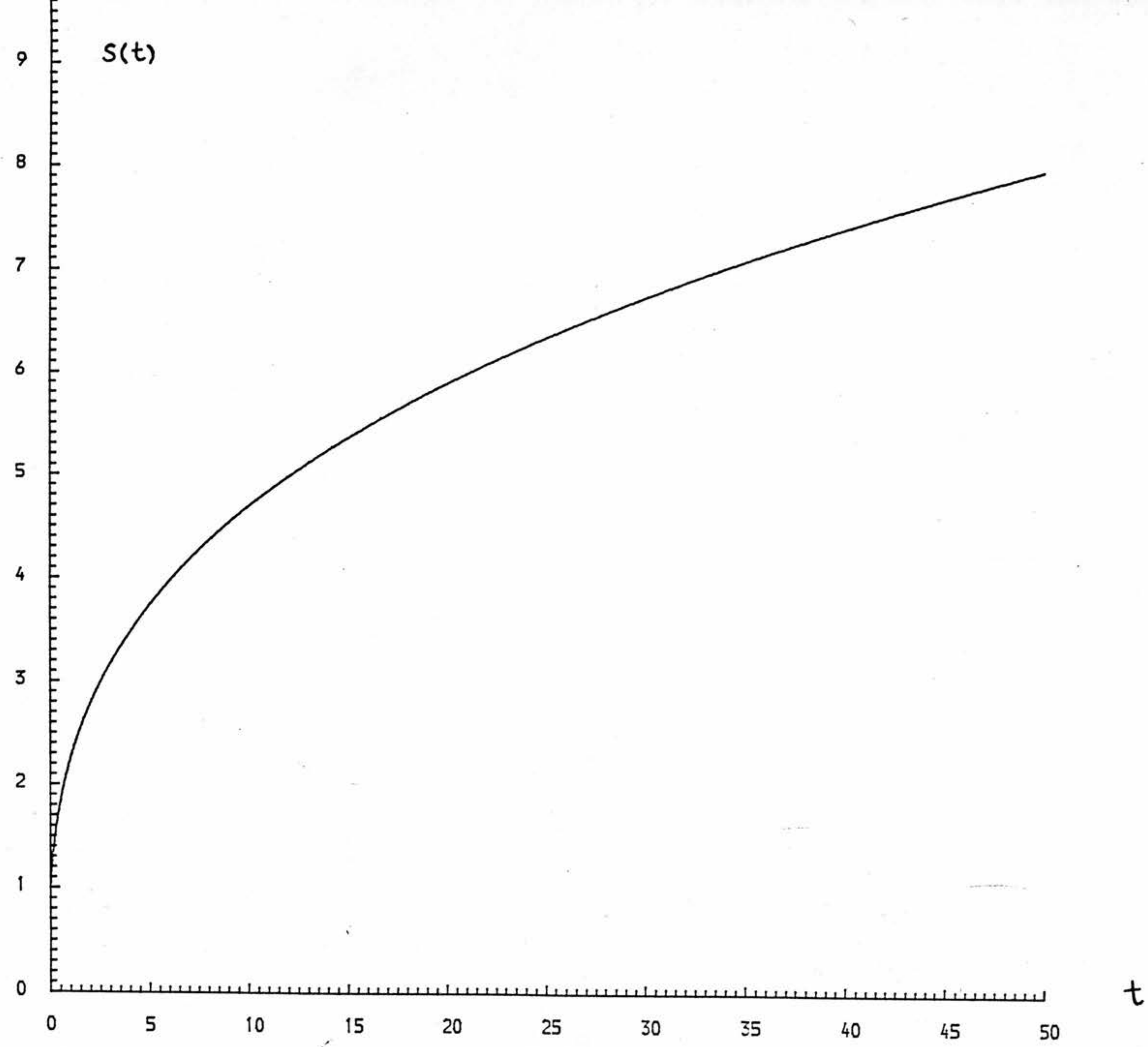


Fig.(20)

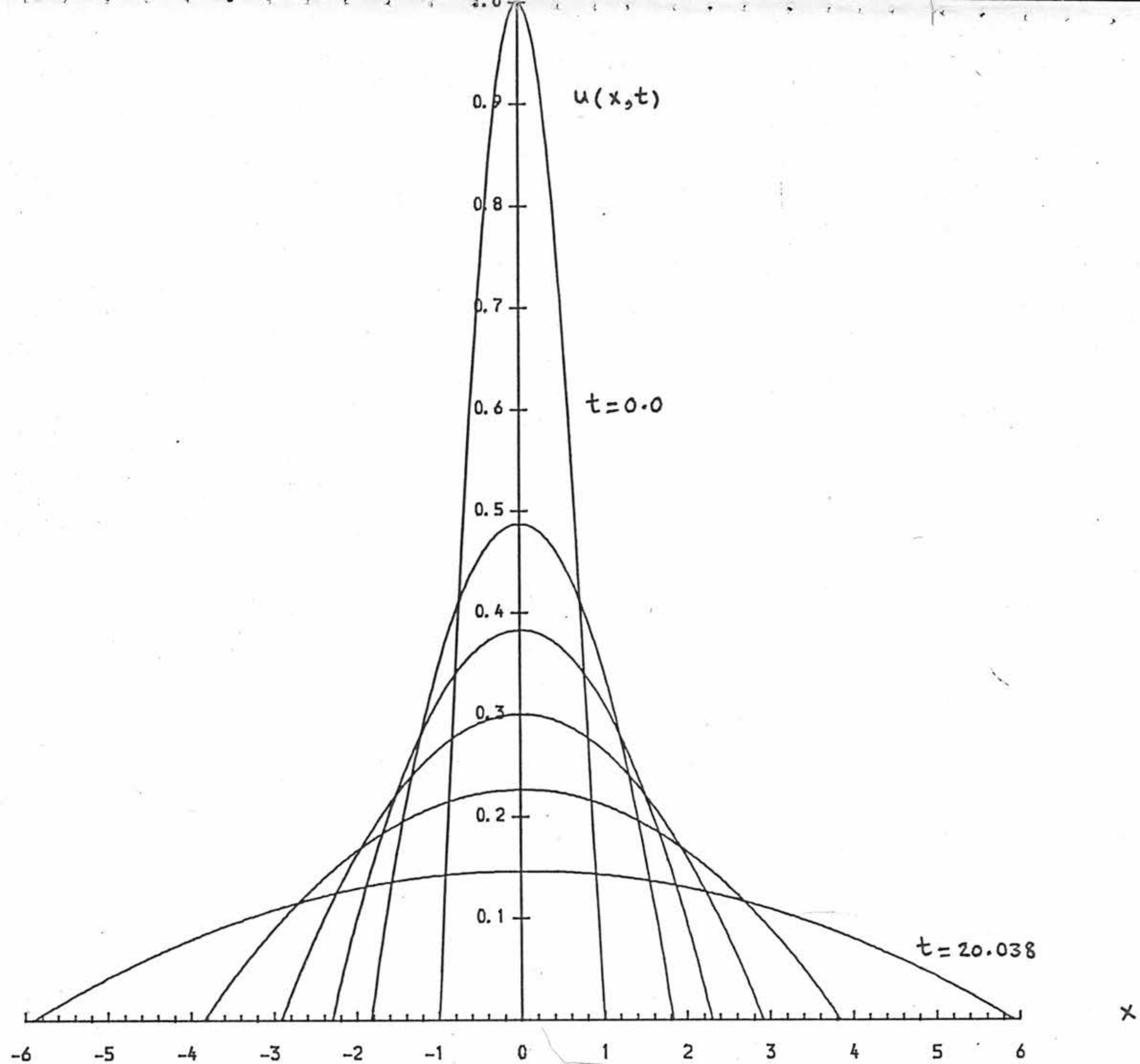


Fig. (21)

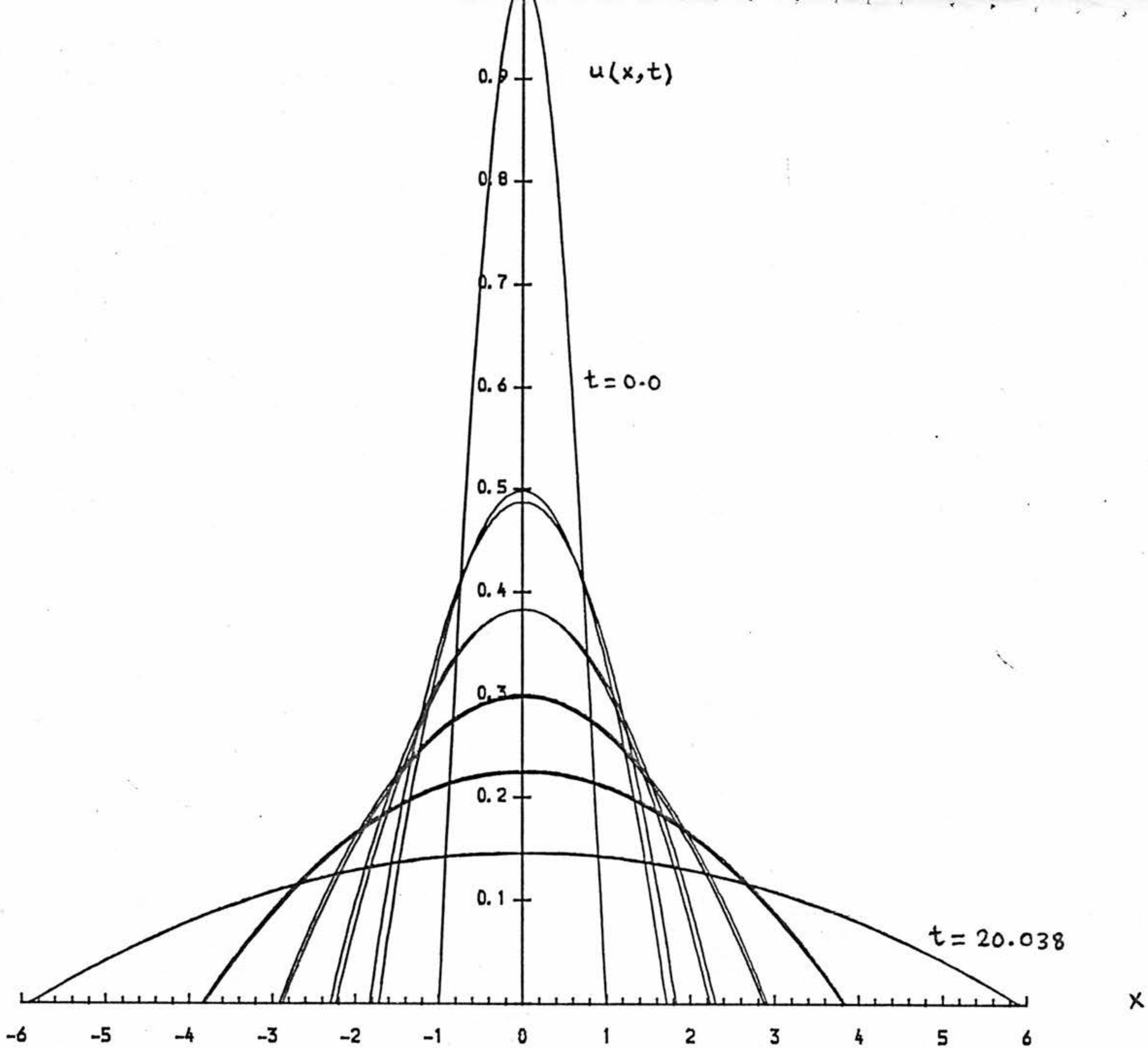


Fig.(22)

(b) $m<p\leq m+2$

In this regime we take m=2, c=1 and p=3. The same α-convergence properties apply here (Figure 23) and we take α=7.0 as the converged solution. The analytic estimate for the interface as $t\to\infty$ is given by (3.2.2) as

$$s(t) \sim \pm \eta_0 t^{\beta} \left\{ 1 + o(t^{-\beta}) \right\} \qquad (5.4.4)$$

where $\beta = \frac{1}{4}$ in this case. In section (3.2) we found that for the above values of p and m $\eta_0 = 3.4$. With this in mind $\eta(t) = s(t)\, t^{-\beta}$ was plotted against t in Figure 24. We expect comparatively slow convergence to η_0 since the error term approaches zero slowly as $t\to\infty$, certainly slower than the corresponding function in the previous regime. Looking at the numerical results however it is not inconceivable that $\eta(t) \to 3.4$ as $t\to\infty$ but it would of course be better to repeat the calculations for values of p and m which yield larger values of β. Nevertheless it is clear that s(t) does indeed have the correct temporal decay, which is somewhat of a vindication for the asymptotic theory, but solid confirmation has yet to be found.

The actual numerical solution is shown in Figure 25 for various values of time.

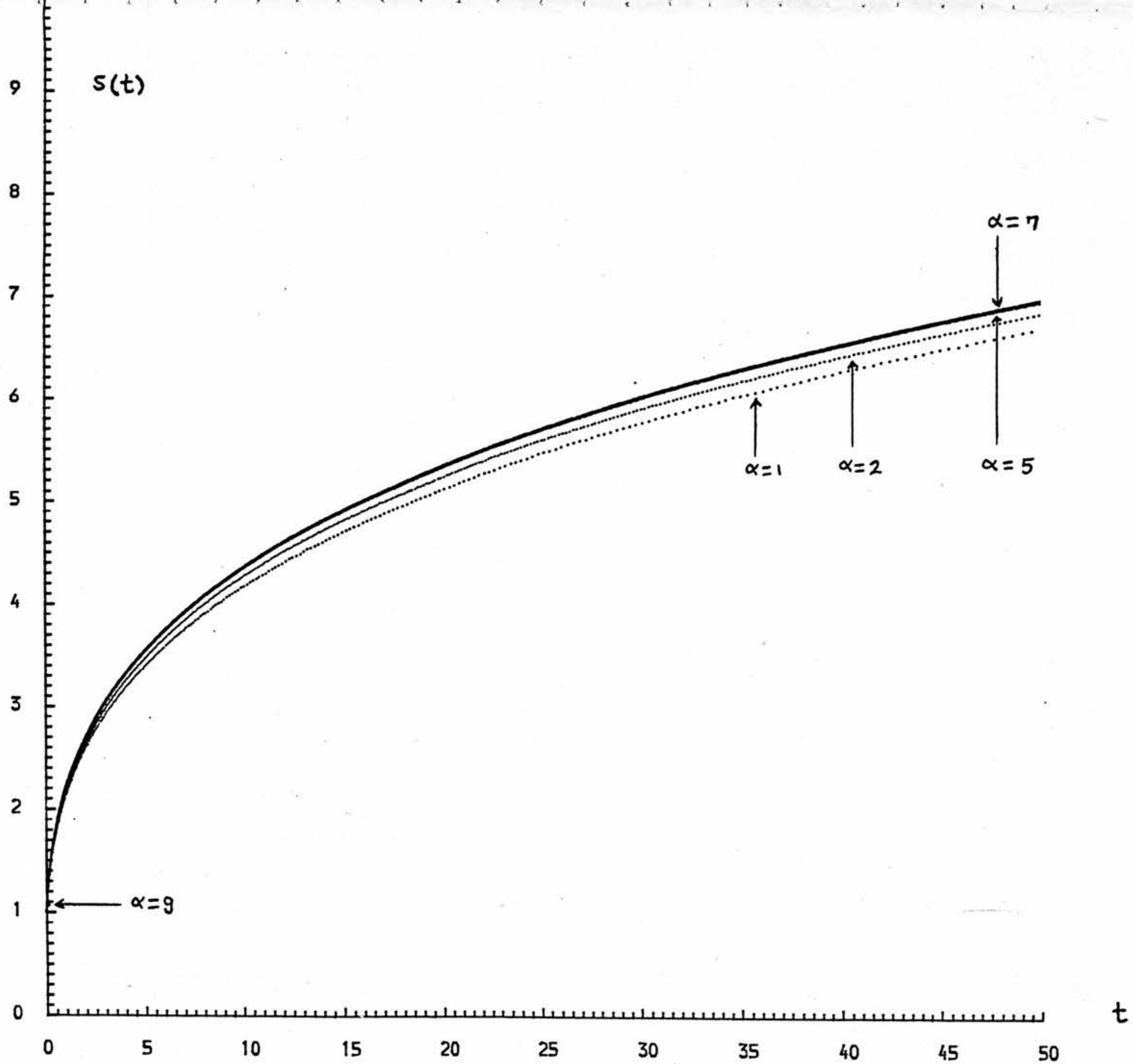


Fig. (23)

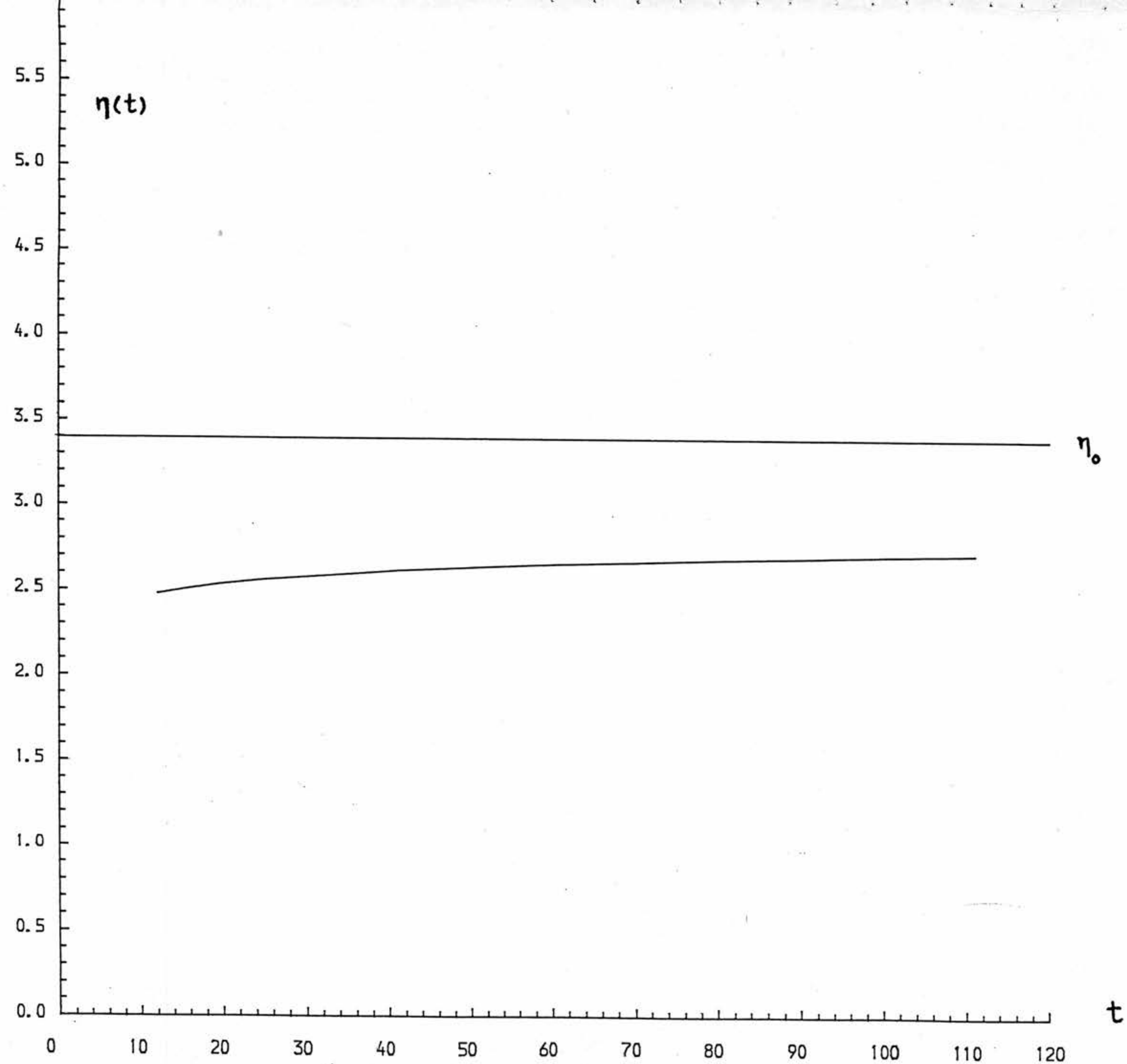

η(t)
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
η₀
0
10
20
30
40
50
60
70
80
90
100
110
120
t

Fig.(24)

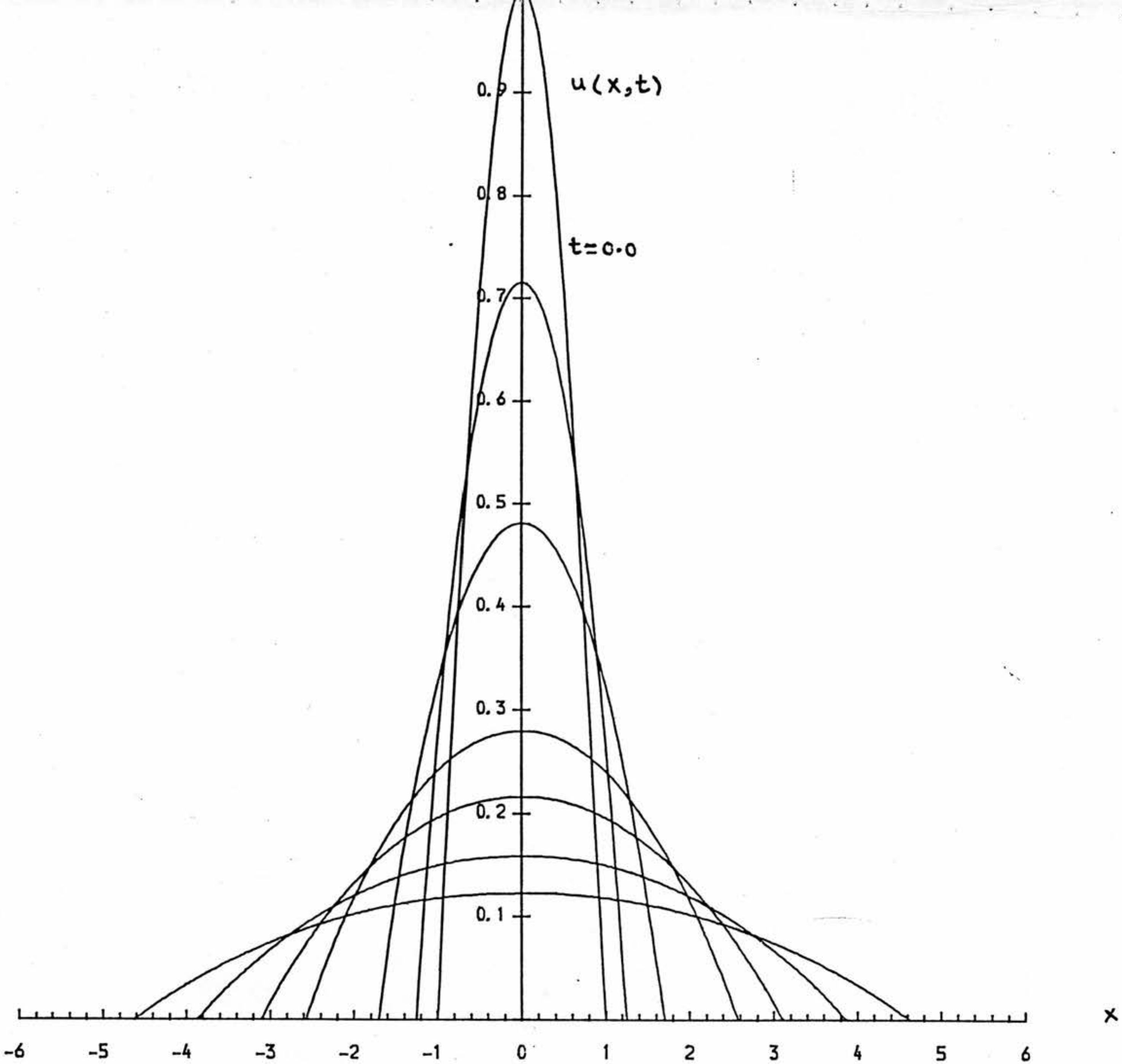


Fig.(25)

(c) $\underline{1<p<m}$

In this regime we take m=2, c=1 and p=1.5 in the numerical example. The path of the interface, for various α, is shown in Figure 26 and again we take $\alpha=7$ as the converged solution. The numerical results for the interface are clearly consistent with the analysis of (3.3), where it was shown that the interface stabilizes at some value of x ($=x_0$) which is undetermined by the asymptotic analysis. The actual numerical solution profile is plotted in Figure 27 and is consistent with the outer asymptotic estimate

$$u(x,t) \sim (p-1)^{-1/(p-1)} \quad t^{-1/(p-1)} \qquad (5.4.5)$$

as $t \longrightarrow \infty$, $|(x-x_0)| = O(1)$.

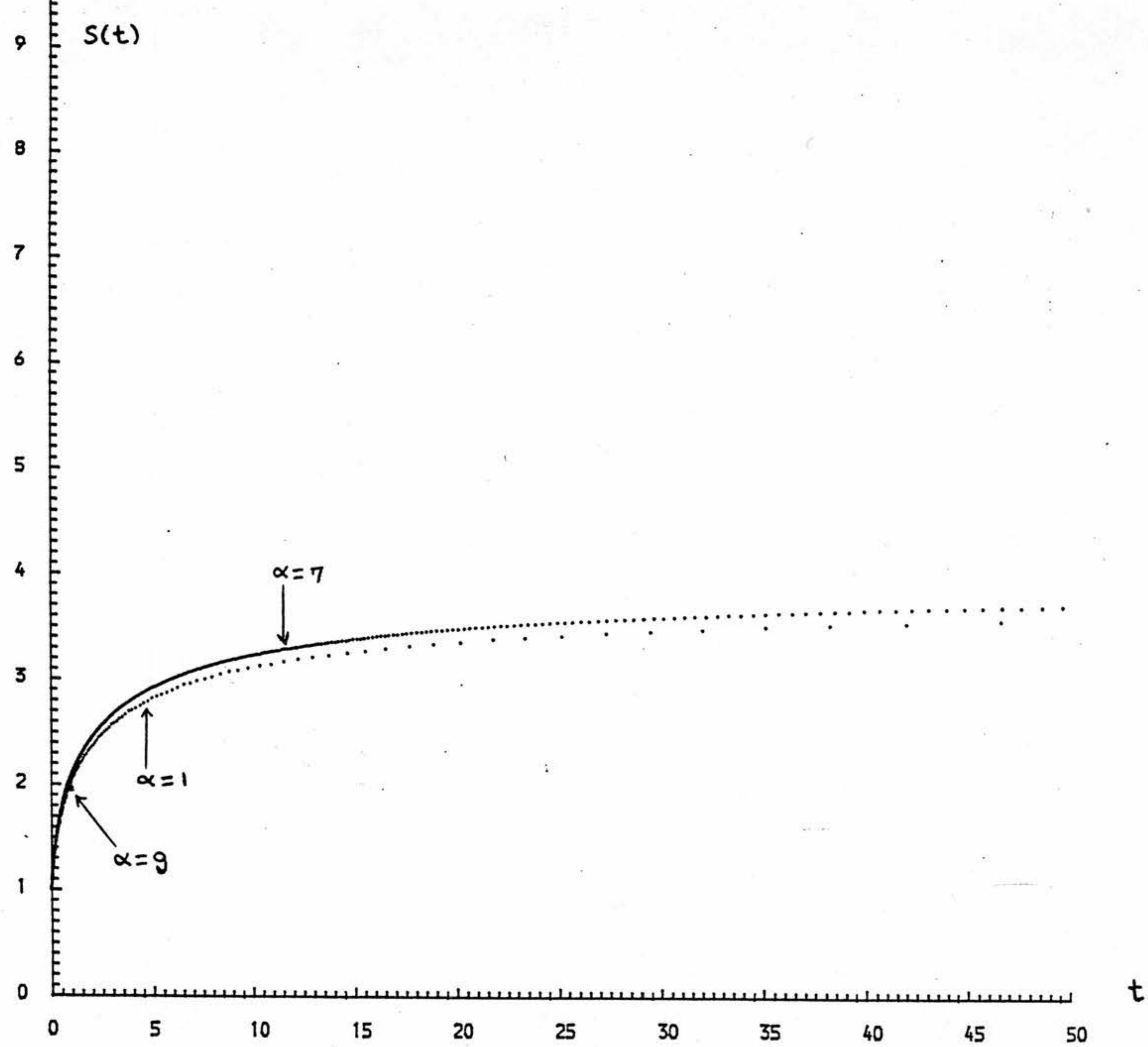


Fig.(26)

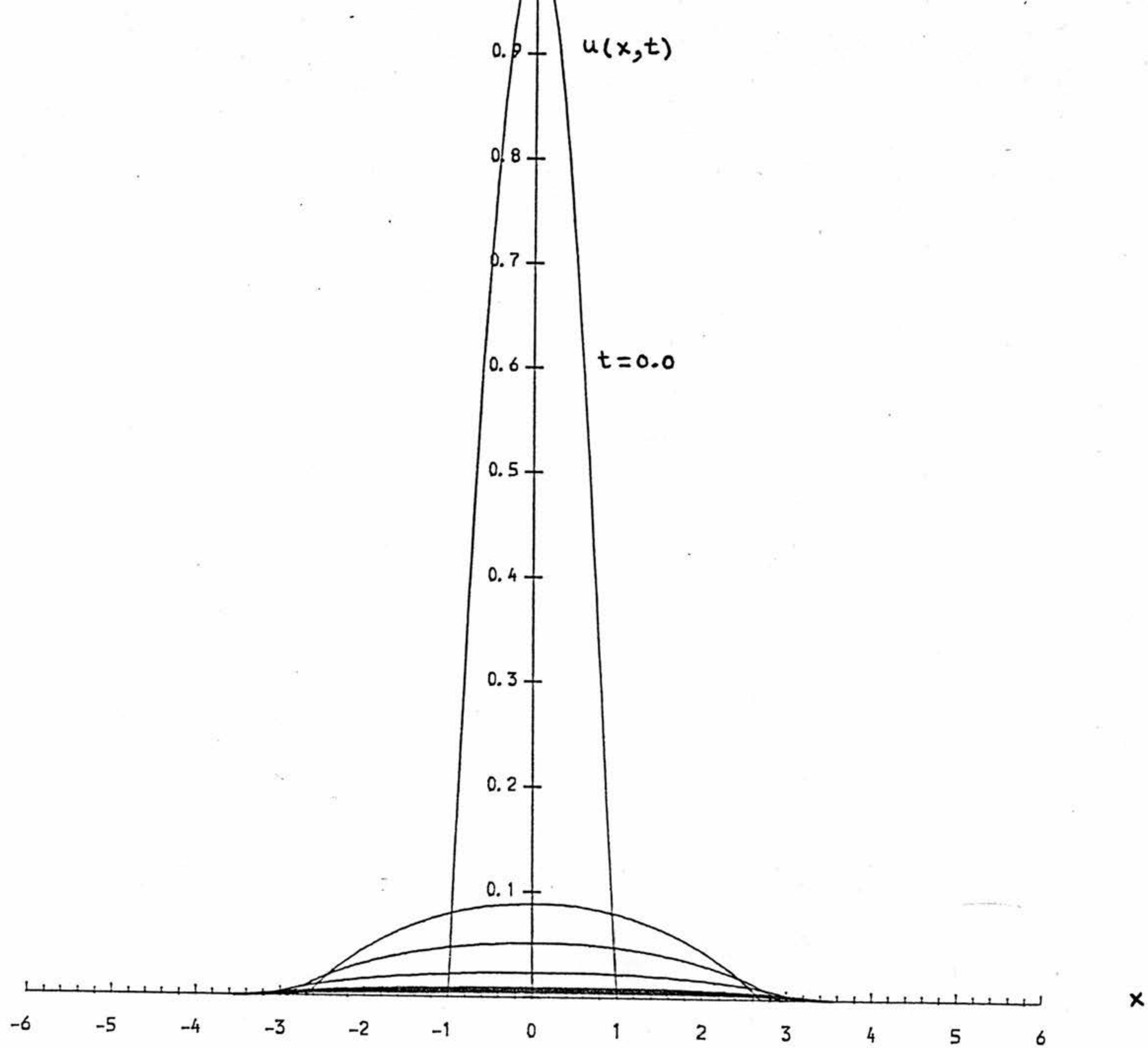


Fig. (27)

(d) p=m

We now come to the last regime where we take p=m=2, c=1. Again similar α-convergence properties hold (Figure 28) and we take α=7.

The analysis of section (3.4) proposes

$$s(t) \sim \pm (m-1) \operatorname{Log} t + \xi_0 \tag{5.4.6}$$

and so in Figure 29 we plot $\frac{s(t)}{\log t}$ against t up to t=1000 ($\log_e t = 6.9$). Convergence to the similarity form is clearly apparent, since for example when t=1000

$$\frac{S(t)}{\operatorname{Log}_e t} \sim 1 + \frac{\xi_0}{6.9}$$

which is consistent with the numerical results. Figure 30 shows a plot of the actual numerical solution for increasing t - again this is consistent with analytic result

$$u(x,t) \sim \left(\frac{1}{m-1}\right)^{1/(m-1)} t^{-1/(m-1)} . \tag{5.4.7}$$

In conclusion we have shown that, except in the case of $m<p\leq m+2$, the asymptotic theory and numerical evidence are consistent. Although inconsistency is not evident for $m<p\leq m+2$, further more detailed and perhaps more delicate computations are required in this regime before final confirmation of the analytic theory can be made.

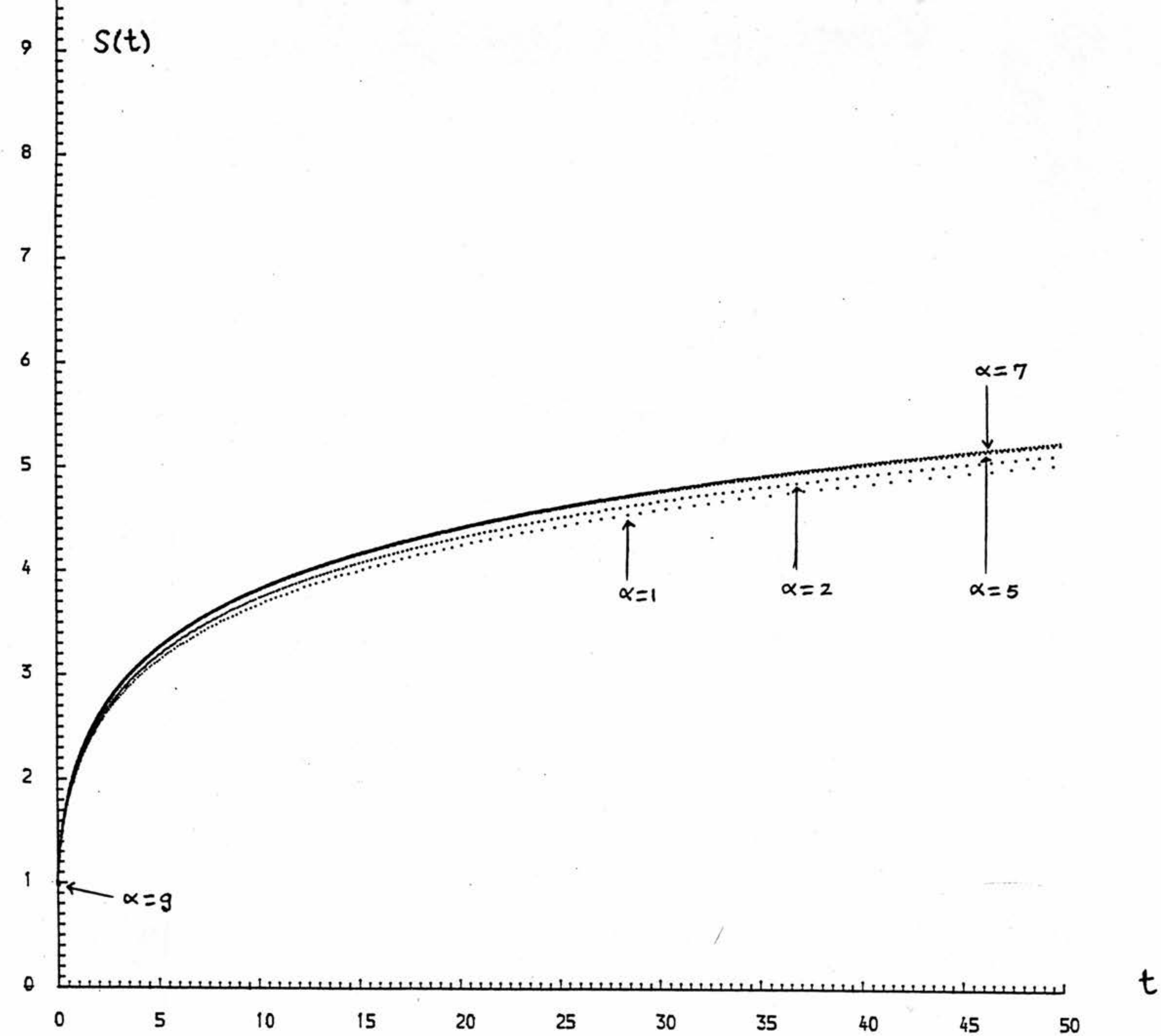


Fig.(28)

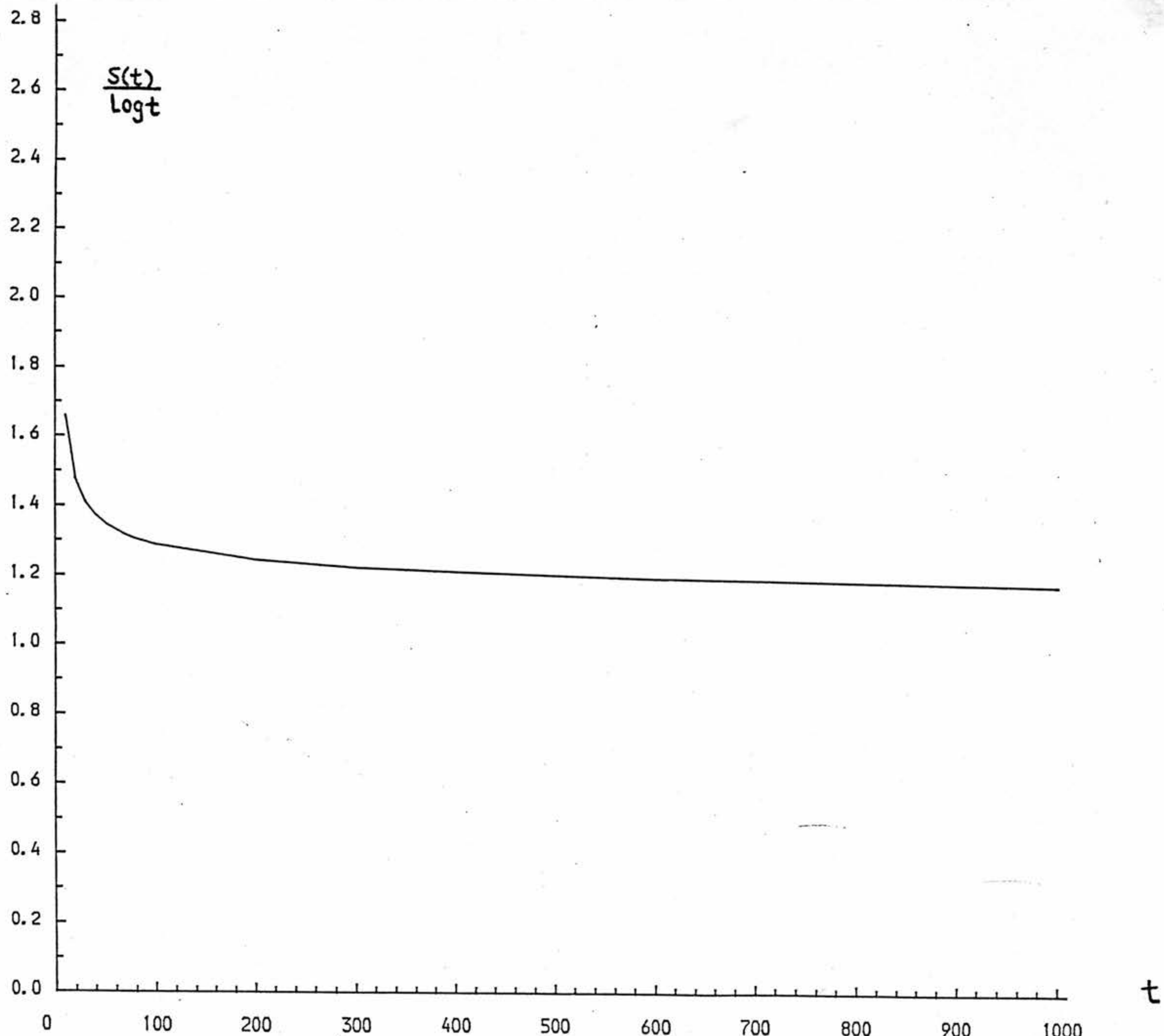

S(t)
Logt
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
600
700
800
900
1000
t

Fig.(29)

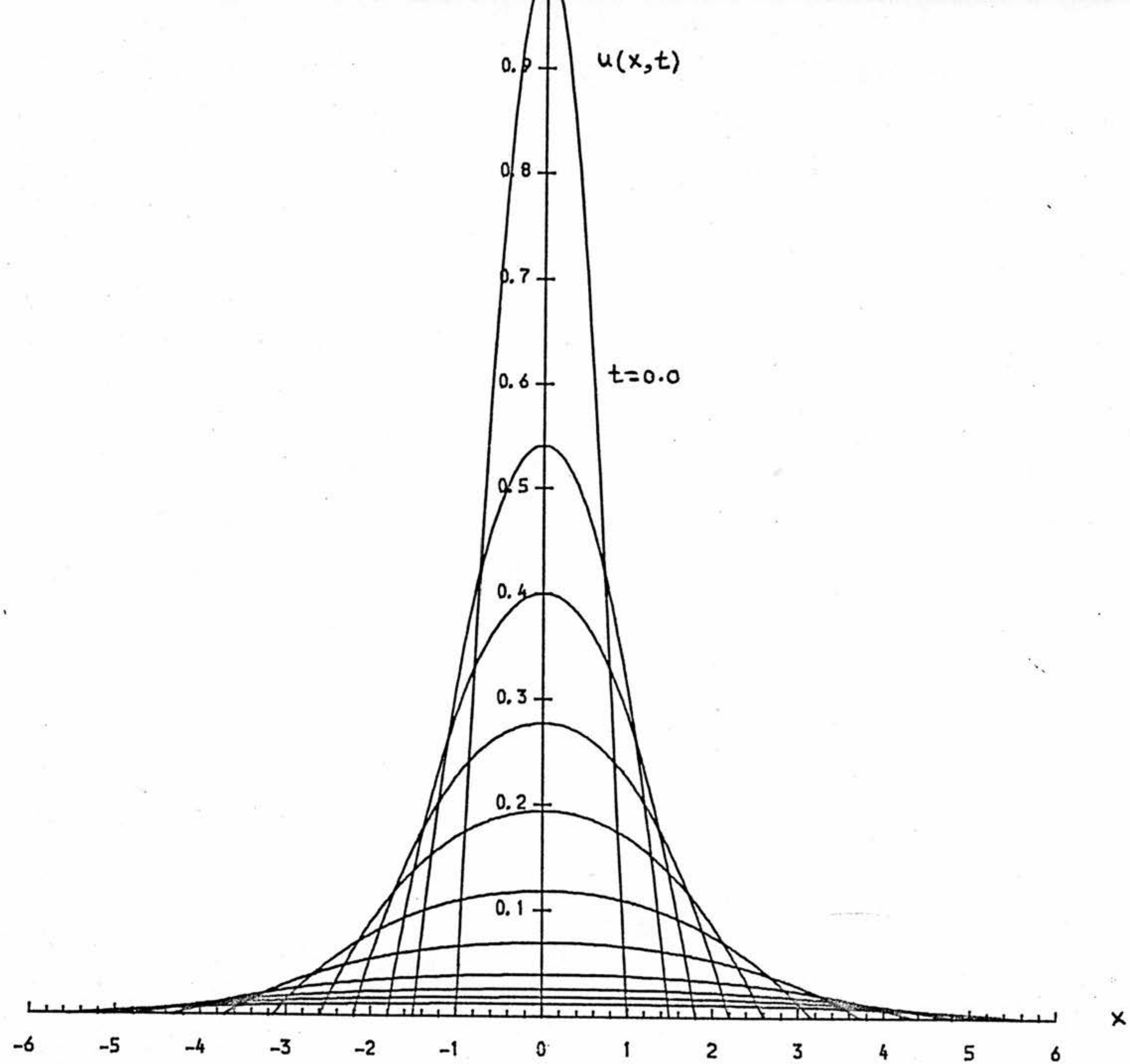


Fig. (30)

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