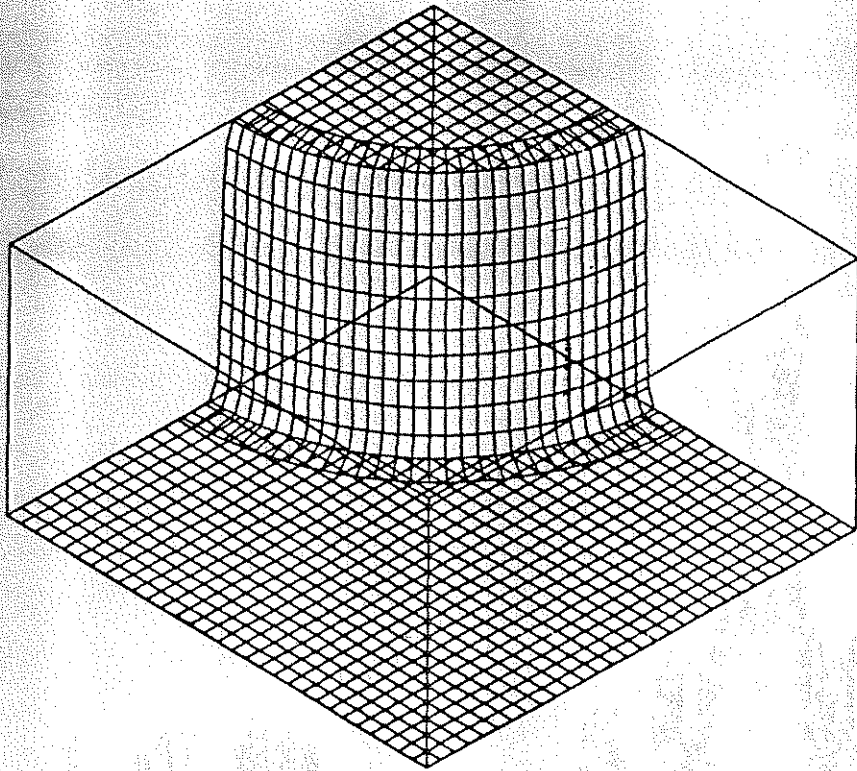


**Applications
of
Advanced Computational Methods
for
Boundary and Interior Layers**



**Edited by
J. J. H. MILLER**

NUMERICAL SOLUTION OF NON-LINEAR SINGULAR PERTURBATION PROBLEMS MODELLING CHEMICAL REACTIONS

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Abstract: A linearization method is proposed for quadratic singularly perturbed boundary value problems which model some catalytic reactions. Each of the resulting linear problems is solved numerically by using non-equidistant finite difference schemes. Numerical results confirm that the method is uniformly accurate with respect to the perturbation parameter.

1. Introduction

Singularly perturbed differential equations arise as mathematical models for various phenomena in physics, chemistry, biology and other sciences. In this paper we shall consider their application to some chemical problems. We are motivated by [2], where the following problem has been considered:

$$-\varepsilon u'' + u^r = 0, \quad x \in (0, 1), \quad (1.1)$$

$$-u'(0) = 0, \quad u(1) + \Sigma u'(1) = 1. \quad (1.2)$$

The problem arises in catalytic reaction theory: it models an isothermal reaction which is catalyzed in a pellet. Here u is the normalized concentration of the reactant, x is the dimensionless distance from the center of the pellet ($x = 0$) to the mouth ($x = 1$), $1/\sqrt{\varepsilon}$ is the so-called *Thiele modulus*, defined as K/D , where D is the diffusion coefficient and K is the reaction rate constant. Thus, when

$D \ll K$, we are dealing with a singular perturbation problem ($0 < \varepsilon \ll 1$). This is the case we shall consider in this chapter. The nonnegative integer r represents the order of the reaction, and Σ is a non-negative parameter, Σ^{-1} being called the *Sherwood number*. The Sherwood number describes the accessibility of the pellet to the bulk flow. When $\Sigma = 0$ the access is uniform, and $\Sigma > 0$ means that there is some resistance.

A more general problem, describing an isothermal reaction on a flat plate catalytic surface and involving a change of volume, is given by

$$-\varepsilon u'' + \varepsilon \theta (1 + \theta u)^{-1} u'^2 + (1 + \theta u) u^r = 0, \quad x \in (0, 1), \quad (1.3)$$

subject to the same boundary conditions as in (1.2). Note that (1.1) is a special case of (1.3) when $\theta = 0$. The parameter θ is the *volume change modulus*. There is no volume change in (1.1), while for $\theta > 0$ there is an increase in the volume due to the reaction. The case $-1 < \theta < 0$ is also possible, and it corresponds to a decrease in the volume. This case will not be considered here. The problem (1.3) has been analyzed in [2], and the following has been shown for its solution $u_\varepsilon(x)$, $x \in I := [0, 1]$:

$$\begin{aligned} 0 \leq u_\varepsilon(x) &\leq \exp[(x-1)/\mu], \quad \text{if } \Sigma = 0, \quad r = 1, \\ 0 \leq u_\varepsilon(x) &\leq [1 + \rho \frac{1-x}{\mu}]^{-1/r}, \quad \text{if } \Sigma = 0, \quad r \geq 2, \\ 0 \leq u_\varepsilon(x) &\leq \Sigma^{-1} \mu \exp[(x-1)/\mu], \quad \text{if } \Sigma > 0, \quad r = 1, \\ 0 \leq u_\varepsilon(x) &\leq \Sigma^{-1} r \sigma^{-1} \mu^{1/(r+1)} [1 + \sigma \frac{1-x}{\mu^{1/(r+1)}}]^{-1/r}, \quad \text{if } \Sigma > 0, \quad r \geq 2. \end{aligned}$$

Here, $\mu = \sqrt{\varepsilon}$ and ρ and σ are two positive constants independent of ε . Since the above estimates are sufficiently sharp, the following can be concluded. For $\Sigma > 0$ there are no boundary layers, so that these problems are easier to solve numerically. Because of this, we shall consider only the more difficult case $\Sigma = 0$. When $\Sigma = 0$, u_ε has a layer at $x = 1$. The layer is exponential when $r = 1$, while for $r \geq 2$ it is a power layer.

There is a related problem for isothermal reactions in spherical catalyst particles, considered in [13]:

$$-\varepsilon u'' + \varepsilon \theta (1 + \theta u)^{-1} u'^2 - 2\varepsilon x^{-1} u' + (1 + \theta u) u^r = 0, \quad x \in (0, 1), \quad (1.4)$$

subject to the conditions (1.2) with $\Sigma = 0$. It is concluded in [13] that the solutions of (1.3) and (1.4) are close when $\varepsilon \ll 1$.

We shall propose numerical methods for all three problems. First, we shall introduce a general linearization procedure which produces a monotonically decreasing sequence of upper solutions. Its convergence towards the exact solution

will be proved for the simplest problem, (1.1), in which case the linearization reduces to Newton's method. The convergence is uniform in ε . Each of the linear problems will be solved numerically by using finite differences on special non-uniform meshes which are dense in the layer at $x = 1$. The proof of the uniform accuracy of the numerical results will not be given, but some theoretical justification of the method will be presented. Numerical experiments will show, however, that the method is uniformly convergent for all three problems. In particular, the results for (1.4) will be compared to those from [13], and a close agreement will be found.

Note that some cases of the problems (1.1), (1.3) and (1.4) are trivial. This is so for (1.1) with $r = 0, 1$, and for (1.3) and (1.4) with $r = 0$. In these cases the exact solution can be found easily. In particular, (1.3) and (1.4) can be rewritten in the forms

$$-\varepsilon \left(\frac{u'}{1 + \theta u} \right)' + u^r = 0$$

and

$$-\varepsilon \left(\frac{x^2 u'}{1 + \theta u} \right)' + x^2 u^r = 0 \quad (1.5)$$

respectively. From this we can see that the case $r = 0$ can be solved exactly: one only has to integrate the equations from 0 to x to obtain terminal value problems which are easy to solve.

2. The Linearization

(1) A General Quadratic Problem

Consider the following quadratic singularly perturbed boundary value problem:

$$Tu := -\varepsilon u'' + a(x, u)u'^2 + b(x)u' + c(x, u) = 0, \quad x \in (0, 1), \quad (2.1)$$

$$Bu := (\alpha_0 u(0) - \beta_0 u'(0), \alpha_1 u(1) + \beta_1 u'(1)) = (\gamma_0, \gamma_1), \quad (2.2)$$

where $\varepsilon \in (0, 1]$, a , b and c are sufficiently smooth functions, and

$$\alpha_i \geq 0, \quad \beta_i \geq 0, \quad \alpha_i + \beta_i > 0, \quad i = 0, 1.$$

Moreover, we assume that there exist two constants, u_* and u^* , such that $u_* < u^*$ and

$$Tu_* \leq 0 \leq Tu^*, \quad Bu_* \leq (\gamma_0, \gamma_1) \leq Bu^*,$$

where the inequalities involving T should hold for all $x \in I$ and those with B should be understood componentwise. Thus u_* is a lower solution to (2.1-2), while u^* is an upper solution. This implies that (2.1-2) has a solution u_ε satisfying

$$u_\varepsilon(x) \in U := [u_*, u^*], \quad x \in I.$$

Note that (1.3) (which includes (1.1)) and (1.4) satisfy this with $u_* = 0$ and $u^* = 1$. Next, for $x \in I$ and $u \in U$, we assume:

$$\begin{aligned} a(x, u) &\geq 0, & c_u(x, u) &\geq 0, \\ a_u(x, u) &\leq 0, & c_{uu}(x, u) &\geq 0, \end{aligned}$$

which is also satisfied by (1.3) and (1.4). Note also that the solution u_ϵ is unique for (1.3) and (1.4), cf. [2].

We propose the following linearization of the problem (2.1-2):

$$L_k u_{k+1} = a(x, u_k) u_k'^2 + c_u(x, u_k) u_k - c(x, u_k), \quad x \in (0, 1), \tag{2.3}$$

$$B u_{k+1} = (\gamma_0, \gamma_1), \tag{2.4}$$

where

$$L_k v := -\epsilon v'' + [2a(x, u_k) u_k' + b(x)] v' + c_u(x, u_k) v, \tag{2.5}$$

(for a $C^2(0, 1)$ -function v) and $k = 0, 1, \dots$. The iterations should start with an upper solution u_0 such that:

$$T u_0 \geq 0, \quad B u_0 \geq (\gamma_0, \gamma_1). \tag{2.6}$$

This is not a Newton linearization, but reduces to it when $a(x, u) = a(x)$. For Newton's linearization as applied to boundary value problems, see for instance [1], [3], [5], [9]. Since (L_k, B) is inverse monotone, each of the linear problems (2.3-5) has a unique solution u_{k+1} .

Lemma 2.1. *The sequence defined by (2.3-6) satisfies*

$$u_k(x) \geq u_{k+1}(x) \geq u_\epsilon(x), \quad x \in I, \quad k = 0, 1, \dots$$

Proof: It is easy to see that

$$L_k(u_k - u_{k+1}) = T u_k.$$

Thus for $k = 0$ we get $L_0(u_0 - u_1) \geq 0$, and from $B u_0 \geq B u_1$ it follows that $u_0 \geq u_1$. If we show that $T u_k \geq 0$ for $k = 1, 2, \dots$, the proof will be completed, since we will have $u_k \geq u_{k+1}$ and each u_k will be an upper solution to (2.1-2). Suppose that the inductive hypothesis $u_{k-1} \geq u_k$ holds. Then from the definition of u_k we get:

$$\begin{aligned} T u_k &= a(x, u_{k-1}) u_{k-1}'^2 + c_u(x, u_{k-1}) u_{k-1} - c(x, u_{k-1}) \\ &\quad - [2a(x, u_{k-1}) u_{k-1}' + b(x)] u_k' - c_u(x, u_{k-1}) u_k + a(x, u_k) u_k'^2 + b(x) u_k' \\ &\quad + c(x, u_k) \geq a(x, u_{k-1}) (u_k' - u_{k-1}')^2 + \frac{1}{2} (u_k - u_{k-1})^2 c_{uu}(x, \eta_k), \end{aligned}$$

with some $\eta_k(x) \in (u_k(x), u_{k-1}(x))$. In the last inequality, $u_{k-1} \geq u_k$ and $a_u \leq 0$ have been used. Thus, $Tu_k \geq 0$. \square

This result does not imply convergence of $\{u_k\}$ to u_ε in the maximum $C(I)$ -norm (which we denote by $\|\cdot\|$); only weak convergence is guaranteed, cf. [5]. We shall prove convergence in the $C(I)$ -norm for the special case (1.1). Our numerical experiments will show that the convergence is present for the problems (1.3) and (1.4) as well.

(2) *The Proof of Convergence for (1.1)*

In this subsection we consider the following special case of the problem (2.1-2):

$$Tu := -\varepsilon u'' + u^r = 0, \quad x \in (0, 1), \quad (2.7)$$

$$Bu := (-u'(0), u(1)) = (0, 1). \quad (2.8)$$

This is the problem (1.1-2) with $\Sigma = 0$. As we remarked in the introduction, only the case $r \geq 2$ is interesting. In this subsection let u_ε stand for the solution of (2.7-8).

The same linearization as above will be applied. Convergence will be proved with a special initial guess u_0 which is sufficiently close to u_ε . This is not surprising for Newton's method. However, due to the structure of the problem, a special technique of proof will be applied. In some parts it is similar to that from [3].

In this special case the linearized problem (2.3-5) reduces to:

$$L_k u_{k+1} := -\varepsilon u_{k+1}'' + r u_k^{r-1} u_{k+1} = (r-1) u_k^r, \quad x \in (0, 1), \quad (2.9)$$

$$B u_{k+1} = (0, 1), \quad k = 0, 1, \dots \quad (2.10)$$

The following special initial guess u_0 will be used:

$$u_0(x) = z(x) + z'(0)(1-x), \quad z(x) = \left[1 + m \frac{1-x}{\mu}\right]^{-\alpha}, \quad (2.11)$$

where

$$\mu = \sqrt{\varepsilon}, \quad \alpha = \frac{2}{r-1}, \quad m = \frac{r-1}{\sqrt{2(r+1)}}.$$

It is easy to see that $Bu_0 = (0, 1)$, and furthermore,

$$\begin{aligned} Tu_0(x) &\geq -\varepsilon z''(x) + z(x)^r \\ &= -m^2 \alpha(\alpha+1) \left[1 + m \frac{1-x}{\mu}\right]^{-\alpha-2} + \left[1 + m \frac{1-x}{\mu}\right]^{-\alpha r} = 0, \end{aligned}$$

where it should be noted that $\alpha r = \alpha + 2$ and $m^2 \alpha(\alpha+1) = 1$. Thus u_0 is an upper solution to (2.7-8).

Theorem 2.1. *The sequence defined by (2.9-11) satisfies*

$$u_k(x) \geq u_{k+1}(x) \geq u_\epsilon(x) \geq 0, \quad x \in I, \quad k = 0, 1, \dots$$

Moreover, if $r \leq r^*$, the following holds:

$$\|u_{k+1} - u_\epsilon\| \leq \beta \|u_k - u_\epsilon\|, \quad \beta < 1. \tag{2.12}$$

Thus $\{u_k\}$ converges to u_ϵ in $\|\cdot\|$.

Proof. That the sequence $\{u_k\}$ is monotonic decreasing in k follows from Lemma 2.1. Next we shall show that γu_0 is a lower solution to (2.7-8), with

$$\gamma = (1 + \alpha)^{-1 - \alpha/2} \in (0, 1).$$

Indeed,

$$B\gamma u_0 = (0, \gamma) \leq (0, 1),$$

and

$$T\gamma u_0(x) \leq -\gamma z(x)^r + \gamma^r [z(x) + \delta]^r,$$

where

$$\delta = \alpha \left[1 + \frac{m}{\mu}\right]^{-\alpha} \geq z'(0) \geq z'(0)(1 - x).$$

Since

$$\left(\frac{z(x)}{z(x) + \delta}\right)^r \geq \left(\frac{z(0)}{z(0) + \delta}\right)^r = (1 + \alpha)^{-r} = \gamma^{r-1},$$

it follows that $T\gamma u_0 \leq 0$, and thus $\gamma u_0 \leq u_\epsilon$.

Furthermore,

$$\gamma u_k \leq u_\epsilon, \quad k = 0, 1, \dots$$

This can be proved by induction. Assume that $\gamma u_k - u_\epsilon \leq 0$. Then it follows that

$$\begin{aligned} L_k(\gamma u_{k+1} - u_\epsilon) &= \gamma(r-1)u_k^r + \epsilon u_\epsilon'' - r u_k^{r-1} u_\epsilon \\ &\leq (r-1)u_k^{r-1}(\gamma u_k - u_\epsilon) \leq 0, \end{aligned}$$

and since

$$B(\gamma u_{k+1} - u_\epsilon) = (0, \gamma - 1) \leq (0, 0),$$

we get

$$\gamma u_{k+1} \leq u_\epsilon.$$

Knowing that $u_k \geq u_\epsilon \geq \gamma u_0 > 0$, by using inverse monotonicity we can derive the following stability inequality for any $C^2(I)$ -function y satisfying $By = (0, 0)$:

$$|y(x)| \leq \max_{x \in I} \frac{|L_k y(x)|}{r u_k^{r-1}}, \quad x \in I.$$

Then for some $\zeta_k(x) \in (u_\varepsilon(x), u_k(x))$

$$L_k(u_{k+1} - u_\varepsilon) = \frac{1}{2}r(r-1)\zeta_k^{r-2}(u_k - u_\varepsilon)^2,$$

and we get

$$L_k(u_{k+1} - u_\varepsilon) \leq \frac{1}{2}r(r-1)(1-\gamma)u_k^{r-1}(u_k - u_\varepsilon).$$

Using this and the stability inequality, we obtain

$$u_{k+1}(x) - u_\varepsilon(x) \leq \frac{1}{2}(r-1)(1-\gamma)\|u_k - u_\varepsilon\|, \quad x \in I,$$

so that (2.12) holds with

$$\beta = \beta(\alpha) = \frac{1-\gamma}{\alpha}.$$

It is easy to prove that $\beta(\alpha)$ is a decreasing function, and thus

$$\beta(\alpha) \leq \beta(\alpha_*) < \beta(0) = 1,$$

where

$$\alpha \geq \alpha_* = \frac{2}{r^* - 1}. \quad \square$$

The following a-posteriori error estimate follows from (2.12):

$$\|u_{k+1} - u_\varepsilon\| \leq \beta\|u_k - \gamma u_0\|.$$

In addition, the following a-priori error estimate holds:

$$\|u_{k+1} - u_\varepsilon\| \leq \beta^{k+1}\|u_0 - u_\varepsilon\| \leq (1-\gamma)\beta^{k+1}.$$

Note that γ and β can be calculated explicitly for any given r , and also that β is independent of ε , and thus so is the convergence.

From (2.12) we can see that the rate of convergence is only 1, while for Newton's method we may expect quadratic convergence. Indeed, the following lemma shows that the sequence $\{u_k\}$ starts to converge quadratically after several iterations.

Lemma 2.2. For the sequence defined by (2.9-11) there is an index n and a constant c_2 such that

$$\|u_k - u_\varepsilon\| \leq \frac{1}{2^k c_2} (2\nu)^{2^k} \mu^\alpha \tag{2.13}$$

for all $k \geq n$ and some $\nu < \frac{1}{2}$.

Proof: The idea is similar to that from [7]. Let A be the operator from

$$S = \{u \in C^2(I) \mid -u'(0) = 0, u(1) = 1\}$$

to $C(I)$, such that

$$A(u) = -\varepsilon u'' + u^r.$$

We shall use the convergence theorem from [6] (p. 708) to prove (2.13). It can be verified that

$$\|u_0 - u_\varepsilon\| \leq \frac{2m}{(m + \mu)^{\alpha+1}} \gamma^{-(r-1)} \mu^\alpha =: c_1 \mu^\alpha. \tag{2.14}$$

Let $v_k = u_{k+n}$, $k = 0, 1, \dots$, with n yet to be determined, and let

$$\Omega = \{u \in S \mid \|u - v_0\| < c_1 \mu^\alpha\}.$$

We know that $A(u) = 0$ has a unique solution u_ε in Ω , and since $v_0 \geq v_k \geq u_\varepsilon$, we have $v_k \in \Omega$, $k = 0, 1, \dots$. Let $A'(v_k)$ be the Fréchet derivative of A at v_k . It is a mapping from

$$S_0 = \{u \in C^2(I) \mid -u'(0) = u(1) = 0\}$$

into $C(I)$. Then we have:

$$A'(v_k)(v_{k+1} - v_k) = -\varepsilon(v_{k+1} - v_k)'' + r v_k^{r-1}(v_{k+1} - v_k) = -A(v_k),$$

and

$$v_1 - v_0 = -A'(v_0)^{-1}A(v_0),$$

that is

$$\begin{aligned} \|A'(v_0)^{-1}A(v_0)\| &\leq \|v_1 - v_0\| = \|u_{n+1} - u_n\| \\ &\leq \|u_{n+1} - u_\varepsilon\| + \|u_n - u_\varepsilon\| \\ &\leq \beta^n (\beta + 1) \|u_0 - u_\varepsilon\| \leq c_1 (\beta + 1) \beta^n \mu^\alpha. \end{aligned}$$

We also have (cf.[9]):

$$A''(v) = r(r - 1)v^{r-2}E, \quad v \in \Omega,$$

where E is the identity operator. Let $V = A'(v_0)^{-1}A''(v)y$, $y \in C(I)$. Then $V \in S_0$ and $A'(v_0)V = A''(v)y$, that is:

$$-\varepsilon V'' + rv_0^{r-1}V = A''(v)y, \quad -V'(0) = 0, \quad V(1) = 0.$$

Thus for any $v \in \Omega$ we have on I :

$$\begin{aligned} |V| &\leq \max_{x \in I} \frac{|A''(v)y|}{rv_0^{r-1}} \\ &\leq \max_{x \in I} \frac{(r-1)|v|^{r-2}}{v_0^{r-1}} \|y\| \\ &\leq \max_{x \in I} \frac{(r-1)(v_0 + c_1\mu^\alpha)^{r-2}}{v_0^{r-1}} \|y\| \\ &\leq (r-1) \max_{x \in I} \frac{1}{v_0} (1 + c_1 \frac{\mu^\alpha}{v_0})^{r-2} \|y\| \\ &\leq (r-1) \frac{(m+\mu)^\alpha}{\gamma} [1 + c_1 \frac{(m+\mu)^\alpha}{\gamma}]^{r-2} \mu^{-\alpha} \|y\| \\ &\quad (\text{since } v_0 \geq \gamma u_0 \geq \frac{\gamma}{(m+\mu)^\alpha} \mu^\alpha) \\ &=: c_2 \mu^{-\alpha} \|y\|. \end{aligned}$$

Thus it follows that

$$\|A'(v_0)^{-1}A''(v)\| \leq c_2 \mu^{-\alpha}, \quad v \in \Omega.$$

Now choose n so that

$$\nu := c_1 c_2 (\beta + 1) \beta^n < \frac{1}{2}.$$

Then (2.13) follows by the theorem from [6] (p. 708). □

3. Numerical Methods for Linear Problems

(1) *The Linear Problems Arising from (1.3) and (1.4)*

The process of linearization described in subsection 2.1 gives a sequence of linear problems to be solved numerically. The linear problems derived from (1.3) and (1.4) have the following form:

$$Lu_{k+1} := -\varepsilon u_{k+1}'' + P(x)u_{k+1}' + Q(x)u_{k+1} = F(x), \quad x \in (0, 1), \quad (3.1)$$

for $k = 0, 1, \dots$. Note that P is different for (1.3) and (1.4), while Q and F are the same:

$$\begin{aligned} P(x) &= 2\varepsilon\theta(1 + \theta u_k(x))^{-1}u_k'(x) \quad \text{for (1.3),} \\ P(x) &= 2\varepsilon\theta(1 + \theta u_k(x))^{-1}u_k'(x) - 2\varepsilon x^{-1} \quad \text{for (1.4),} \\ Q(x) &= [\theta(r+1)u_k(x) + r]u_k(x)^{r-1}, \\ F(x) &= \varepsilon\theta(1 + \theta u_k(x))^{-1}u_k'^2(x) + u_k(x)^r[r\theta u_k(x) + r - 1]. \end{aligned}$$

The dependency of P , Q (and thus of L) and F on k is omitted in order to simplify the notation. The problem (3.1) is subject to the boundary conditions from (2.8):

$$Bu := (-u'(0), u(1)) = (0, 1). \tag{3.2}$$

We shall discretize (3.1-2) on a non-uniform mesh I^h with the points:

$$0 = x_0 < x_1 < \dots < x_n = 1.$$

Let

$$h_i = x_i - x_{i-1}, \quad i = 1, 2, \dots, n,$$

and let $\{w_i\}$ be a mesh function defined on I^h . The upwind finite-difference scheme to be used to discretize (3.1-2) is:

$$L^h w_0 := -D_+ w_0 = 0, \tag{3.3}$$

$$L^h w_i := -\varepsilon D'' w_i + P_i D' w_i + Q_i w_i = F_i, \quad i = 1, 2, \dots, n-1, \tag{3.4}$$

$$L^h w_n := w_n = 1, \tag{3.5}$$

where

$$D_+ w_i = \frac{w_{i+1} - w_i}{h_{i+1}}, \quad D_- w_i = \frac{w_i - w_{i-1}}{h_i},$$

$$D' w_i = \begin{cases} D_+ w_i & \text{if } P_i \leq 0, \\ D_- w_i & \text{if } P_i > 0, \end{cases}$$

$$D'' w_i = \frac{2}{h_i + h_{i+1}} \left(\frac{w_{i-1} - w_i}{h_i} + \frac{w_{i+1} - w_i}{h_{i+1}} \right).$$

Thus w_i is the numerical approximation to $u_{k+1}(x_i)$. Let v_i denote the previously obtained approximation to $u_k(x_i)$ (when $k = 0$, $v_i = u_0(x_i)$). Then

$$P_i = 2\varepsilon\theta(1 + \theta v_i)^{-1} D_- v_i \quad \text{for (1.3),}$$

and analogous expressions hold for P_i for (1.4), Q_i and F_i .

Lemma 3.1. *The discrete problem (3.3-5) has a unique solution. Moreover, the following stability inequality holds for any mesh function $\{y_i\}$:*

$$|y_i| \leq |D_+ y_0| + |y_n| + \max_{1 \leq i \leq n-1} \frac{|L^h y_i|}{Q_i}, \quad i = 0, 1, \dots, n. \tag{3.6}$$

Proof: We wish to show that $w_i > 0$ and $Q_i > 0$ for all i and all k . We proceed by induction. It is clear that $v_i > 0$, for $k = 0$, since we can take $v_0 \equiv u_0 \equiv 1$. Consider the $(k+1)$ -st iteration. Assume now that the solution of the k -th iteration

v_i satisfies $v_i \geq v_* > 0$ and that the corresponding $Q_i = Q_i(v) > 0$, whence L^h is inverse monotone. Choose κ to be a positive constant, $\kappa \leq 1$, such that

$$L^h \kappa = Q_i \kappa \leq F_i = L^h w_i, \quad i = 1, 2, \dots, n-1.$$

Now $w_i \geq \kappa > 0$ follows from $L^h(w_i - \kappa) \geq 0$ and the inverse monotonicity of L^h . It also follows from the form of Q_i that $Q_i = Q_i(w) > 0$. By induction, therefore, $w_i > 0$ and $Q_i > 0$ for all i and all k . Thus (3.3-5) represents a non-singular linear system. Next let

$$\omega_i = |D_+ y_0|(1 - x_i) + |y_n| + \max_{1 \leq i \leq n-1} \frac{|L^h y_i|}{Q_i}.$$

Then

$$\begin{aligned} -D_+ \omega_0 &\geq -D_+(\pm y_0), \quad \omega_n \geq \pm y_n, \\ L^h \omega_i &\geq L^h(\pm y_i), \quad i = 1, 2, \dots, n-1, \end{aligned}$$

and this implies (3.6). □

Let us now consider the discretization meshes. It is easy to check that $g(x) = \exp[(1 + \theta)(x - 1)/\mu]$ is a lower solution to both (1.3), (3.2) and (1.4), (3.2). Since $g(1) = u_\varepsilon(1) = u_k(1) = 1$, it follows that

$$u'_k(1) \leq u'_\varepsilon(1) \leq g'(1) = \frac{1 + \theta}{\mu}.$$

This indicates that $P(x)$ behaves like $const.\mu$ when x is close to 1, meaning that we are dealing with two-parameter problems. Such problems have been considered in [11] in the case which corresponds to $r = 1$. Because of that the linearizations of the quadratic problems (1.3) and (1.4) with $r = 1$ will be solved numerically on a mesh similar to that from [11]. When $r \geq 2$, however, we are dealing with a power layer near $x = 1$, and a mesh similar to that from [12] should be used. Both kinds of meshes are generated by suitable functions and are dense near $x = 1$. They can be expressed in the following way:

$$x_i = \lambda(ih), \quad i = 0, 1, \dots, n, \quad h = \frac{1}{n}, \quad (3.7)$$

$$\lambda(t) = \begin{cases} \varphi'(\tau)t & \text{if } t \in [0, \tau], \\ \varphi(t) := 1 - s\mu \left[\left(\frac{1-q}{t-q} \right)^p - 1 \right] & \text{if } t \in [\tau, 1]. \end{cases} \quad (3.8)$$

Here q is a parameter to be chosen from $(0, 1/2]$, and τ is the solution to

$$\varphi'(\tau)\tau = \varphi(\tau), \quad \tau \in (q, 1). \quad (3.9)$$

For such a τ to exist, the following condition has to be satisfied:

$$\varphi'(1) \leq 1, \text{ i.e. } s\mu p \leq 1 - q.$$

This is always true if μ is sufficiently small. If the condition is violated, however, we may safely use an equidistant mesh. When $r = 1$ it is sufficient to use $p = 1$. Then (3.9) reduces to a quadratic equation and τ is easy to find:

$$\tau = (1 + s\mu)^{-1} [q + s\mu + \sqrt{s\mu(q + s\mu)(1 - q)}]. \quad (3.10)$$

For $r = 1$ there is no restriction on s , and we shall use $s = 1$. However, for $r \geq 2$ we have to use:

$$s \geq \frac{1}{m}, \quad p \geq \frac{1}{\alpha} = \frac{r-1}{2}, \quad (3.11)$$

where m and α are as in (2.11). Thus for $r = 2, 3$ we can choose $p = 1$ and τ can be expressed as in (3.10).

Mesh generating functions of the type λ have been used very often, cf. [8], [10], [12] and the references therein. Numerical results will show that the difference schemes (3.3-5) on these meshes are uniformly accurate for the linearizations of problems (1.1), (1.3) and (1.4) respectively.

(2) *The Linear Problem Arising from (1.1)*

If we take the problem (2.7-8), the discretization (3.4) reduces to

$$L^h w_i := -\varepsilon D'' w_i + r v_i^{r-1} w_i = (r-1) v_i^r, \quad i = 1, 2, \dots, n-1, \quad (3.12)$$

where, as before, w_i and v_i correspond to $u_{k+1}(x_i)$ and $u_k(x_i)$ respectively. Note that this is a second-order central discretization, corresponding to (2.9). The discrete problem (3.3), (3.12), (3.5) is considered on the mesh (3.7-9), (3.11). Although numerical results are in practice quite satisfactory, there are some technical difficulties in proving this analytically. We shall illustrate the feasibility of the method by considering the following discrete problem instead:

$$\begin{aligned} \tilde{L}^h w_i &:= -\varepsilon D'' w_i + r u_k(x_{i+1})^{r-1} w_i = (r-1) u_k(x_i)^r, \\ &i = 1, 2, \dots, n-1. \end{aligned} \quad (3.13)$$

The boundary conditions and the mesh remain the same. Note the use of $u_k(x_{i+1})$ instead of $u_k(x_i)$, which is necessary for technical reasons. It is clear that (3.13) is a discretization of (2.9), where we retain the coefficients as known functions. In practice, the coefficients are approximated by using $\{v_i\}$, and the analysis of the discretization (3.12) is much more complicated. When $k = 0$, we assume that u_0 is the same as in (2.11).

Theorem 3.1. *The discrete problem (3.3), (3.13), (3.5) has a unique solution $\{w_i\}$, and on the mesh (3.7-9), (3.11)*

$$|w_i - u_{k+1}(x_i)| \leq Mh, \quad i = 0, 1, \dots, n. \tag{3.14}$$

Here M denotes a constant which is independent of h and ε .

Proof: The following stability inequality, analogous to (3.6), holds:

$$|y_i| \leq |D_+ y_0| + |y_n| + \max_{1 \leq i \leq n-1} \frac{|\tilde{L}^h y_i|}{ru_k(x_{i+1})^{r-1}}, \quad i = 0, 1, \dots, n.$$

From this we get

$$|w_i - u(x_i)| \leq |D_+ u(x_0)| + \max_{1 \leq i \leq n-1} \frac{|R_i|}{ru_k(x_{i+1})^{r-1}}, \quad i = 0, 1, \dots, n, \tag{3.15}$$

where u stands for u_{k+1} and

$$R_i = \tilde{L}^h u(x_i) - (r - 1)u_k(x_i)^r.$$

Let M be a positive generic constant independent of h and ε . We shall prove that

$$\frac{|R_i|}{u_k(x_{i+1})^{r-1}} \leq Mh, \tag{3.16}$$

for $i = 1, 2, \dots, n - 1$. In a similar way, we can prove that

$$|D_+ u(x_0)| = |D_+ u(x_0) - u'(0)| \leq Mh,$$

and this, (3.16) and (3.15) imply (3.14).

The properties of the special mesh will be used in the proof of (3.16). This is a well-known technique from [8], [10], [12] and many other papers. Let $t_i = ih$. The proof will be divided into the following three steps:

1. $t_{i+1} \leq \tau$.
2. $t_{i+1} > \tau$ and $t_{i+1} \geq q + 3h$.
3. $\tau < t_{i+1} < q + 3h$.

In the first two cases the following estimate of R_i will be used:

$$|R_i| \leq M\mu^{-1} \left[1 + m \frac{1 - x_{i+1}}{\mu} \right]^{-\alpha-1} h_i z(x_{i+1})^{r-1}, \tag{3.17}$$

where z is as in (2.11). First let us prove (3.17). Using (2.9) we get:

$$|R_i| \leq Mh_i \varepsilon \max_{x_{i-1} \leq x \leq x_{i+1}} |u'''(x)| + ru(x_i) |u_k(x_{i+1})^{r-1} - u_k(x_i)^{r-1}|.$$

On differentiating (2.9), we obtain

$$\varepsilon|u'''(x)| \leq Mu_k(x)^{r-1}[|u'(x)| + |u'_k(x)|].$$

Then from

$$u(x) \leq u_k(x) \leq u_0(x) \leq (1 + \alpha)z(x) \leq Mz(x_{i+1}), \quad x \leq x_{i+1},$$

we conclude that

$$|R_i| \leq Mh_i z(x_{i+1})^{r-1} \max_{x_{i-1} \leq x \leq x_{i+1}} [|u'(x)| + |u'_k(x)|].$$

Finally, to show that (3.17) holds, we require

$$|u'_k(x)| \leq M\mu^{-1} \left[1 + m \frac{1-x}{\mu} \right]^{-\alpha-1}, \quad k = 0, 1, \dots \quad (3.18)$$

This follows immediately for $k = 0$:

$$0 \leq u'_0(x) = z'(x) - z'(0) \leq z'(x).$$

For $k = 1, 2, \dots$, (3.18) follows after integration of (2.9):

$$\begin{aligned} |u'_{k+1}(x)| &\leq M\varepsilon^{-1} \int_0^x u_k(s)^r ds \leq M\varepsilon^{-1} \int_0^x u_0(s)^r ds \\ &\leq M\mu^{-1} \left[1 + m \frac{1-x}{\mu} \right]^{-\alpha-1}. \end{aligned}$$

Now recall that

$$u_k(x) \geq \gamma u_0(x) \geq \gamma z(x).$$

From this and (3.17) we see that to prove (3.16) it suffices to show that

$$h_i \mu^{-1} \left[1 + m \frac{1-x_{i+1}}{\mu} \right]^{-\alpha-1} \leq Mh.$$

Turning to the special mesh, we conclude that the above inequality holds if we prove

$$S := \lambda'(t_{i-1}) \mu^{-1} \left[1 + m \frac{1-\lambda(t_{i+1})}{\mu} \right]^{-\alpha-1} \leq M. \quad (3.19)$$

In case 1 this follows from

$$\lambda'(t_{i-1}) \leq M,$$

and

$$1 + m \frac{1 - \lambda(t_{i+1})}{\mu} \geq 1 + m \frac{1 - \lambda(r)}{\mu} \geq M \mu^{-p/(p+1)},$$

on noting that by the choice of p in (3.11)

$$\frac{p}{p+1}(\alpha+1) \geq 1.$$

In case 2,

$$t_{i-1} - q \geq \frac{1}{3}(t_{i+1} - q) \geq h,$$

and

$$\lambda'(t_{i-1}) \leq \varphi'(t_{i-1}) \leq M \mu (t_{i+1} - q)^{-p-1}.$$

Using this and $\lambda(t_{i+1}) = \varphi(t_{i+1})$ with $ms \geq 1$, we get

$$S \leq M(t_{i+1} - q)^{-p-1+p(\alpha+1)} \leq M,$$

and (3.19) is proved in this case too.

We shall use a different expression for R_i in case 3:

$$|R_i| \leq 2\varepsilon \max_{x_{i-1} \leq x \leq x_{i+1}} |u''(x)| + rz(x_{i+1})^r.$$

Then using (2.9) we get

$$|R_i| \leq Mz(x_{i+1})^r,$$

so that to prove (3.16) we must show that

$$z(x_{i+1}) = z(\lambda(t_{i+1})) \leq Mh. \quad (3.20)$$

But in case 3 we have

$$\lambda(t_{i+1}) \leq \lambda(q + 3h) = \varphi(q + 3h),$$

and it follows that

$$z(x_{i+1}) \leq Mh^{p\alpha} \leq Mh,$$

from which (3.20) is proved. Thus in all three cases (3.16) holds, and as indicated earlier (3.14) follows. \square

This result justifies our method. Moreover, from (2.14) we see that u_0 is a good approximation to u_ε when ε is small. There is thus no need to seek a numerical approximation, unless its error is smaller than $O(\mu^\alpha)$. We consider this case in the next theorem.

Theorem 3.2. Let $\{w_i\}$ be the unique solution to the discrete problem

$$\begin{aligned}
 -\varepsilon D'' w_i + r u_k(x_i)^{r-1} w_i &= (r-1) u_k(x_i)^r, \\
 i = 1, 2, \dots, n-1, \quad -D_+ w_0 &= 0, \quad w_n = 1,
 \end{aligned}$$

on the mesh (3.7-9) with

$$s \geq \frac{1}{m}, \quad p \geq \frac{3}{\alpha},$$

and with

$$h \leq c_3 \mu^\alpha, \tag{3.21}$$

where c_3 is a constant independent of h and ε . Then

$$|w_i - u_{k+1}(x_i)| \leq Mh, \quad i = 0, 1, \dots, n.$$

The proof will be omitted since its technique is the same as that of Theorem 3.1. However, some comments are due. When (3.21) is not satisfied, then u_0 is a $O(h)$ approximation to u_ε . But on the other hand, (3.21) implies that only cases 1 and 2 from the proof of Theorem 3.1 are possible. We can handle these cases without the artificial shift from (3.13), provided $p \geq 3/\alpha$. Since there is no shift, we can even expect accuracy of second order. The first order discretization of the left boundary condition, however, appears, in practice, to decrease that accuracy to first order, particularly for large ε .

4. Numerical Results

In this section we present numerical results for problems (1.3) and (1.4). In all cases, the linearization is performed as indicated in section 2. The linearized equations are then solved using upwinded differences, as given in the equations (3.3-5). Our numerical experiments show that in practice it is not necessary to take u_0 very close to u_ε , as we did in the theoretical analysis when we chose u_0 satisfying (2.11) for the problem (2.7-8). Thus the initial guess in all cases is $u_0(x) \equiv 1$. The non-equidistant mesh described in section 3 was used except as indicated below. The values chosen for the parameters of the mesh were $p = 1$; $q = 0.5$; for the case $r = 1$, $s = 1$, and for $r > 1$, $s = 1/m$, where m is as in (2.11). Finally the parameter τ is determined from (3.10). In order for τ to exist the condition

$$\frac{s\mu}{q-1} \leq 1,$$

given in section 3.1, must be satisfied. For large ε , that is for values of $\varepsilon > 1/2$ or $\varepsilon > 1/64$, depending on r , this condition is violated. In these cases a standard equidistant mesh was employed.

Table 4.1

| ε | Number of Mesh Points n | | | | | | Average |
|---------------|---------------------------|------|------|------|------|------|---------|
| | 8 | 16 | 32 | 64 | 128 | 256 | |
| 1/2 | 1.16 | 1.08 | 1.04 | 1.02 | 1.01 | 1.01 | 1.05 |
| 1/4 | 1.22 | 1.11 | 1.06 | 1.03 | 1.01 | 1.01 | 1.07 |
| 1/8 | 1.31 | 1.17 | 1.08 | 1.04 | 1.02 | 1.01 | 1.11 |
| 1/16 | 1.44 | 1.24 | 1.12 | 1.06 | 1.03 | 1.02 | 1.15 |
| 1/32 | 1.82 | 1.70 | 1.19 | 1.10 | 1.05 | 1.03 | 1.31 |
| 1/64 | 1.64 | 1.99 | 2.00 | 2.00 | 2.00 | 1.80 | 1.91 |
| 1/128 | 1.92 | 1.94 | 1.98 | 2.00 | 2.00 | 2.00 | 1.97 |
| 1/256 | 2.05 | 1.97 | 1.97 | 2.00 | 2.00 | 2.00 | 2.00 |
| 1/512 | 1.98 | 1.94 | 1.97 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/1024 | 1.86 | 1.90 | 2.00 | 2.00 | 2.00 | 2.00 | 1.96 |
| 1/2048 | 1.75 | 1.98 | 1.99 | 2.00 | 2.00 | 2.00 | 1.95 |
| 1/4096 | 1.70 | 2.04 | 2.00 | 2.00 | 2.00 | 2.00 | 1.96 |
| 1/8192 | 1.71 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.96 |
| 1/16384 | 1.74 | 2.05 | 2.00 | 2.00 | 2.00 | 2.00 | 1.97 |
| 1/32768 | 1.76 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.97 |
| 1/65536 | 1.78 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.97 |
| 1/131072 | 1.79 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/262144 | 1.81 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/524288 | 1.82 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/1048576 | 1.82 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/2097152 | 1.83 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/4194304 | 1.84 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/8388608 | 1.84 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| 1/16777216 | 1.84 | 2.05 | 2.01 | 2.00 | 2.00 | 2.00 | 1.98 |
| p_d^n | 1.66 | 1.08 | 1.04 | 1.02 | 1.01 | 1.01 | |

Uniform Rate p_d^+ : 1.14

Double Mesh Rates of Convergence for Problem (1.3) with $r = 1, \theta = 1$

The uniform rate of convergence was determined using a variation of the double mesh method described in [4]. This involves calculating the double mesh error

$$e_{de}^n = \max_{0 \leq i \leq n} |u_i^n - \bar{u}^{2n}|,$$

which is the difference between the values of the solution on a mesh of n points and the interpolated value for the solution at the same point on a mesh of $2n$

points. The uniform rate of convergence is then given by

$$p_d = \text{average}_n p_d^n$$

where

$$p_d^n = (\ln e_d^n - \ln e_d^{2n}) / \ln(2)$$

and

$$e_d^n = \max_{\epsilon} e_{d\epsilon}^n.$$

Some cautions on the interpretation of uniform rates of convergence derived in this way are also given in [4].

Table 4.1 gives in tabular form the values of the local rates of convergence, for a range of n and ϵ , for the problem (1.3) with $r = 1$ and $\theta = 1$. These are given by

$$p_{d\epsilon}^n = (\ln e_{d\epsilon}^n - \ln e_{d\epsilon}^{2n}) / \ln(2).$$

The rightmost column contains the average rate of convergence for the row, that is for a fixed value of ϵ , given by $\text{average}_n p_{d\epsilon}^n$. The bottom row contains the values of p_d^n . This indicates a uniform rate of convergence $p_d = 1.14$, although it should be noted that examination of the p_d^n indicates that this is unduly influenced by the rate for $n = 8$ and a better estimate would be 1.01.

Although the derivation of the difference schemes (3.3-5) in section 3 employed an upwinded difference scheme, we remark that uniform convergence can be achieved with a scheme which uses centered difference approximations to the first derivatives throughout. This is what is presented in Table 4.1. We emphasize that we use the centered difference approximation instead of D' in (3.4), as well as $u'_k(x_i)$ appearing in P and F . We still use the directed difference approximation $-D_+ w_0 = 0$, however, for the boundary condition at $x = 0$. This appears to degrade the performance of the centered difference scheme to first order when ϵ is of order 1. For small ϵ , however, the convergence is classically $O(h^2)$. It should be remarked that for problem (1.4) this effect does not occur. This may perhaps be explained by considering that for problem (1.3), with small ϵ , and for problem (1.4) the solution is almost constant near $x = 0$, and hence the upwind approximation $D_+ w_0$ attains second order accuracy.

Tables 4.2 and 4.3 give the uniform rates of convergence, calculated using the double mesh method, for problems (1.3) and (1.4) respectively.

Table 4.2

| θ | Scheme | r | | |
|----------|-----------|------|------|------|
| | | 1 | 2 | 3 |
| 0.0 | Upwinding | 1.20 | 1.25 | 1.59 |
| | Centered | 1.20 | 1.25 | 1.59 |
| 0.5 | Upwinding | 1.11 | 1.21 | 1.55 |
| | Centered | 1.16 | 1.24 | 1.57 |
| 1.0 | Upwinding | .99 | 1.08 | 1.52 |
| | Centered | 1.14 | 1.23 | 1.56 |
| 2.0 | Upwinding | .85 | .92 | 1.37 |
| | Centered | 1.10 | 1.22 | 1.54 |
| 3.0 | Upwinding | .77 | .87 | 1.29 |
| | Centered | 1.07 | 1.21 | 1.52 |

Uniform Rates of Convergence for Problem (1.3)

Table 4.3

| θ | Scheme | r | | |
|----------|-----------|------|------|------|
| | | 1 | 2 | 3 |
| 0.0 | Upwinding | 1.14 | 1.18 | 1.52 |
| | Centered | 1.94 | 2.10 | 1.69 |
| 0.5 | Upwinding | .84 | 1.00 | 1.38 |
| | Centered | 1.96 | 2.09 | 1.67 |
| 1.0 | Upwinding | .64 | .74 | 1.20 |
| | Centered | 1.98 | 2.08 | 1.66 |
| 2.0 | Upwinding | .67 | .67 | 1.00 |
| | Centered | 1.99 | 2.04 | 1.65 |
| 3.0 | Upwinding | .64 | .61 | .89 |
| | Centered | 2.00 | 1.96 | 1.64 |

Uniform Rates of Convergence for Problem (1.4)

It is clear that both schemes are uniformly convergent for both problems. Further, it should be noted that the centered difference approximation shows second-order convergence for problem (1.4), in contrast to the case for problem (1.3).

To compare our results with those given in [13], we calculate the *Effectiveness Factor*. This represents the actual reaction rate divided by the rate which would occur if the intra-particle reactant concentration were everywhere identical to that at the pellet surface. The effectiveness factor, for an r -th order reaction with volume change in a spherical catalyst pellet such as that treated by equation (1.4) is given by

$$\eta = \frac{3\varepsilon(du/dx)|_{x=1}}{1 + \theta}$$

It is clear that this value can be calculated from the numerical solution of problem (1.4). The most direct way would be to estimate the derivative $(du/dx)|_{x=1}$ by the directed difference $D_- w_n$ at the boundary point $x_n = 1$. This is presumably a similar procedure to that used in [13], although no details are given there. Table 4.4 gives the effectiveness factors calculated on a mesh of 256 points using this method.

Table 4.4

| θ | ε | | | | |
|----------|---------------|-------|-------|-------|-------|
| | 4 | 1 | 1/9 | 1/36 | 1/100 |
| | $r = 0$ | | | | |
| 1.0 | .9979 | .9974 | .9946 | .9870 | .9308 |
| 2.0 | .9977 | .9967 | .9892 | .9594 | .7666 |
| 3.0 | .9976 | .9961 | .9837 | .9083 | .6608 |
| | $r = 1$ | | | | |
| 1.0 | .9663 | .8885 | .5627 | .3342 | .2135 |
| 2.0 | .9518 | .8488 | .5000 | .2903 | .1841 |
| 3.0 | .9382 | .8153 | .4565 | .2613 | .1649 |
| | $r = 2$ | | | | |
| 0.0 | .9664 | .8891 | .5667 | .3397 | .2189 |
| 1.0 | .9385 | .8165 | .4599 | .2643 | .1679 |
| 2.0 | .9137 | .7626 | .4007 | .2251 | .1420 |
| 3.0 | .8913 | .7201 | .3610 | .1998 | .1254 |

Effectiveness Factors for (1.4) using Differences

With the exception of the case $r = 0$ our results are in agreement with those in [13] to within 0.3%. To examine this discrepancy further, one should note that the case $r = 0$ has an exponential layer as opposed to a power layer for $r > 1$. Thus it might be expected that a classical shooting based method such as that used in [13] might fare badly. As remarked in section 1, equation (1.4) can be rewritten in the form (1.5), and in the case of $r = 0$ becomes

$$-\varepsilon \left(\frac{x^2 u'}{1 + \theta u} \right)' + x^2 = 0.$$

This may be solved exactly for $u'(1)$ and gives $u'(1) = (1 + \theta)/3\varepsilon$. Thus the effectiveness factor $\eta \equiv 1$, independently of ε and θ . Our results are significantly closer to this than the results in [13]. It is clear that the inaccuracies in our case are a result of using a difference approximation to the derivative at a boundary with an exponential layer. To avoid this we may make use of equation (1.5) to rewrite the derivative as an integral from 0 to 1 and then employ quadrature:

$$\frac{x^2 u'}{1 + \theta u} \Big|_{x=1} - \frac{x^2 u'}{1 + \theta u} \Big|_{x=0} = \frac{1}{\varepsilon} \int_0^1 x^2 u''(x) dx.$$

Using the facts that $u'(0) = 0$ and $u(1) = 1$ we get the following expression for the effectiveness factor:

$$\eta = 3 \int_0^1 x^2 u'(x) dx.$$

Table 4.5 gives the effectiveness factor calculated using this formula with the integrals being evaluated using the trapezoidal rule. In this case the result is exact for the case with $r = 0$.

Table 4.5

| θ | ε | | | | |
|----------|---------------|--------|--------|--------|--------|
| | 4 | 1 | 1/9 | 1/36 | 1/100 |
| $r = 0$ | | | | | |
| 1.0 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 2.0 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| 3.0 | 1.0000 | 1.0000 | 1.0000 | 1.0000 | 1.0000 |
| $r = 1$ | | | | | |
| 1.0 | .9685 | .8914 | .5664 | .3366 | .2151 |
| 2.0 | .9543 | .8523 | .5046 | .2933 | .1861 |
| 3.0 | .9409 | .8193 | .4617 | .2645 | .1671 |
| $r = 2$ | | | | | |
| 0.0 | .9685 | .8915 | .5703 | .3434 | .2213 |
| 1.0 | .9409 | .8196 | .4652 | .2696 | .1714 |
| 2.0 | .9162 | .7662 | .4069 | .2312 | .1460 |
| 3.0 | .8940 | .7241 | .3678 | .2063 | .1296 |

Effectiveness Factors for (1.4) using Quadrature

Thus to summarize, the method described in this paper is in practice uniformly convergent for both problem (1.3) and problem (1.4). The paper also introduces a more accurate method for calculating the effectiveness factor numerically.

5. References

- [1] R.E. Bellman and R.E. Kalaba *Quasilinearization and Non-Linear Boundary Value Problems*, Elsevier Publishing Company, New York (1965)
- [2] K.W. Chang and F.A. Howes *Non-Linear Singular Perturbation Phenomena: Theory and Applications*, Springer-Verlag, New York (1984)
- [3] E.P. Doolan, J.J.H. Miller and W.H.A. Schilders *Uniform Numerical Methods for Problems with Initial and Boundary Layers*, Boole Press, Dublin (1980)
- [4] P.A. Farrell and A. Hegarty "On the determination of the order of uniform convergence," in *Proc. of 13th IMACS World Congress (J.J.H. Miller, R. Vichnevetsky, eds.)*, Dublin (1991), 501-502

- [5] **V. Hutson and J.S. Pym** *Applications of Functional Analysis and Operator Theory*, Academic Press, London (1980)
- [6] **L.V. Kantorovich and G.P. Akilov** *Functional Analysis in Normed Spaces*, Pergamon Press, New York (1964)
- [7] **P. Lin** "A numerical method for a quasilinear singular perturbation problem with turning points," *Computing* 46 (1991), 155-164
- [8] **V.D. Liseikin and V.E. Petrenko** "On the Numerical Solution of Non-Linear Singularly Perturbed Problems," (Russian), Preprint 687, SO AN SSSR, Novosibirsk (1987)
- [9] **L.B. Rall** *Computational Solution of Non-Linear Operator Equations*, Wiley, New York (1969)
- [10] **R. Vulcanović** "On a numerical solution of a type of singularly perturbed boundary value problem by using a special discretization mesh," *Univ. u Novom Sadu Zb. Rad. Prirod.-Mat. Fak. Ser. Mat.* 13 (1983), 187-201
- [11] **R. Vulcanović** "On the numerical solution of a singularly perturbed boundary value problem with two small parameters," in *Numerical Methods and Approximation Theory II* (D. Herceg, ed.), Institute of Mathematics, Novi Sad (1985), 65-71
- [12] **R. Vulcanović** "On a numerical solution of a power layer problem," in *Numerical Methods and Approximation Theory III* (G.V. Milovanović, ed.), University of Niš, Niš (1988), 423-431
- [13] **V.W. Weekman Jr and R.L. Goring** "Influence of volume change on gas-phase reactions in porous catalysts," *J. Catalysis* 4 (1965), 260-270