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A variational principle for a non-linear diffusion problem*

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NOMENCLATURE

c	reactant concentration at a point
L	biological layer thickness
t	dimensionless coordinate
x	space coordinate
y	dimensionless concentration.

Greek symbols

$\alpha, \hat{\alpha}, \beta, \hat{\beta}$	coefficients
γ	reactant concentration outside the layer.

1. INTRODUCTION

A MATHEMATICAL model describing diffusion of a chemical reactant in a bed of microorganisms has been proposed in [1] and [2]. The differential equation of the process is derived under the assumption that the rate of chemical reaction r is given by an equation of the following form

$$r = \frac{\hat{\alpha}c}{\hat{\beta}+c} \tag{1}$$

where $\hat{\alpha}$ and $\hat{\beta}$ are constants and c is the concentration of a reactant at a given point of the biological layer. Suppose that the layer of micro-organisms is positioned on the flat supporting surface, then, using (1) the following, non-linear boundary value problem for the steady-state diffusion, is obtained

$$\frac{d^2c}{dx^2} - \frac{\alpha c}{1+\beta c} = 0 \tag{2}$$

$$\frac{dc}{dx} = 0 \quad \text{at} \quad x = 0, \quad c = \gamma \quad \text{at} \quad x = L. \tag{3}$$

In (2) and (3), α, β, γ and L (the thickness of the biological layer) are known constants.

The problem (2), (3) has been treated numerically in [1], [2] and [3]. In [3] the method of invariant imbedding was used to transform (2), (3) into an initial value problem.

Our intention in this note is to construct an extremum variational principle for (2), (3) on the basis of the results given in [4]. Also, we shall use the Ritz procedure to obtain an approximate solution to (2), (3) for several choices of constants. The error of the approximate solution will be estimated by a method slighly different from methods presented in [4]. Namely, in deriving the error bound we will use an integral inequality, which although simple, seems to be new.

2. VARIATIONAL PRINCIPLE AND ERROR ESTIMATE

Following [3] we introduce new dependent and independent variables by the relations

$$y = \beta c, \quad t = \alpha^{1/2}x. \tag{4}$$

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Using (4) equations (2) and (3) become

$$y'' - y/(1+y) = 0, \quad (\cdot)' = \frac{d}{dt}(\cdot) \tag{5}$$

$$y'(0) = 0, \quad y(\hat{T}) = \hat{y}, \quad \hat{T} = L\alpha^{1/2}, \quad \hat{y} = \alpha\beta. \tag{6}$$

From the physical consideration (c is the concentration) we are interested in the positive solution of (5), (6). The question of existence of such a solution was discussed in [3]. Let y be the positive ($y > 0$) solution of (5), (6). From [4] we conclude that the functional I given by

$$I(Y) = \int_0^{\hat{T}} \left[Y'^2 + Y + \ln\frac{1}{(1+Y)(1-Y'')} - Y'' \right] dt - yY'(\hat{T}) \tag{7}$$

is stationary ($\delta I = 0$) on the solution of (5), (6). In (7) $Y(t)$ is an admissible trial function, that is a $C^2[0, \hat{T}]$ function that satisfies the boundary conditions (6) and has $Y'' < 1$. Moreover ([4], p. 206) the functional (7) has for $Y = y$ the value zero. Therefore we have

$$I(y) = 0, \quad \delta I(y, f) = 0, \quad f = Y - y. \tag{8}$$

In the analysis that follows Y will be an approximate solution to the boundary value problem (5), (6). Then, the error of the approximate solution will be expressed in terms of f. Using (8) in (7) we get

$$I(Y) = \tfrac{1}{2}\delta^2 I(\psi, f), \tag{9}$$

where $\delta^2 I(\psi, f)$ is the second variation of I calculated on the function $\psi = y + \eta f$, $0 < \eta < 1$. Note that f satisfies the homogeneous boundary conditions

$$f'(0) = 0, \quad f(\hat{T}) = 0. \tag{10}$$

Calculating the second variation of (7) and using it in (9) we have

$$2I(Y) = \int_0^{\hat{T}} [2f'^2 + f''^2(1-\psi'')^{-2} + f^2(1+\psi)^{-2}]\, dt. \tag{11}$$

It is easy to see that the positive solution of (5), (6) is convex ($y'' > 0$) and increasing ($y(t) \leqslant \hat{y}$). We shall choose trial functions $Y(t)$ so that they are (like the exact solution) convex, increasing and satisfy $Y(t) \leqslant \hat{y}$. Then,

$$\psi = y + \eta(Y - y) \leqslant \hat{y} \tag{12}$$

$$\psi'' = y'' + \eta(Y'' - y'') = (1-\eta)y'' + \eta Y'' \geqslant 0. \tag{13}$$

Note also that

$$\sup_{t\in[0,\hat{T}]} y'' = \sup_{t\in[0,\hat{T}]} \frac{y}{1+y} < 1. \tag{14}$$

From (13), (14) and the fact that $Y'' < 1$, we get

$$\sup_{t\in[0,\hat{T}]} \psi'' \leqslant \max\left\{ \sup_{t\in[0,\hat{T}]} y'', \sup_{t\in[0,\hat{T}]} Y'' \right\} < 1. \tag{15}$$

Table 1.

$\hat{y}$	C_1	C_2	C_3	I	$\|f\|_{L_\infty} \leqslant$
0.2	0.06344	0.0021	0.0005	1.7166×10^{-5}	0.002688
0.4	0.1114	0.0051	0.00006	1.009×10^{-6}	0.000657
0.8	0.1915	0.0031	0.001	1.6364×10^{-5}	0.00266

Using (14) and (15) in (11) we finally get

$$2I(Y) \geqslant \int_0^T [2f'^2 + f''^2 + Kf^2]\,dt, \tag{16}$$

where

$$K = \frac{1}{(1+\hat{y})^2}. \tag{17}$$

Let Δ be a constant such that

$$\int_0^{\hat{T}} [f''^2 + Kf^2]\,dt \geqslant \Delta \int_0^{\hat{T}} f'^2\,dt. \tag{18}$$

The value for Δ is given, for example in [5], [6] and [7]. However these values are determined either for a larger class of functions (for example, no specific boundary conditions are imposed) [5], [6] or for a more restrictive class [7] than we need. Therefore, in the Appendix, using the methods of Optimal Control Theory [8], [9] we determined the best constant in the inequality (18) for functions satisfying boundary conditions (10). The result is $\Delta = (\pi/2\hat{T})^2 + K/(\pi/2\hat{T})^2$. Using this value for Δ in (16), the inequality gives

$$\|f'\|_{L_2} \leqslant \{2I(Y)/[2 + (\pi/2T)^2 + K/(\pi/2T)^2]\}^{1/2}, \tag{19}$$

where

$$\|f'\|_{L_2} = \left(\int_0^{\hat{T}} f'^2\,dt\right)^{1/2}.$$

Also by the Cauchy–Schwarz inequality and observing (10) we finally get

$$\|f\|_{L_\infty} = \sup_{t\in[0,T]} |f| \leqslant \hat{T}^{1/2}\{2I/[2 + (\pi/2\hat{T})^2 + K/(\pi/2\hat{T})^2]\}^{1/2}. \tag{20}$$

3. NUMERICAL RESULTS

For a sample calculation we have chosen the following values for the constants

$$\hat{T} = 1, \quad \hat{y} = 0.2, 0.4, 0.8,$$

and the trial function $Y(t)$ in the form

$$Y = \hat{y} - C_1(1-t^2) - C_2(1-t^4) - C_3(1-t^6). \tag{21}$$

The constants C_i, $i = 1, 2, 3$ are determined by substituting (21) into (7) and minimizing the resulting expression with respect to C_i. The results, together with error estimates are given in Table 1.

From the results presented in the table we conclude that, although simple, the approximate solution (20) has a remarkable accuracy.

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APPENDIX

Consider the problem of determining the minimum of the functional F

$$F = \left(\int_0^{\hat{T}} [f''^2 + Kf^2]\,dt\right) \Big/ \left(\int_0^{\hat{T}} f'^2\,dt\right), \tag{A1}$$

among all functions $f \in C^2[0, \hat{T}]$ with $f'(0) = f(\hat{T}) = 0$. Following [8] and [9] we consider the optimal control problem: minimize

$$F = \left(\int_0^{\hat{T}} [u^2 + Kx_1^2]\,dt\right) \Big/ \left(\int_0^{\hat{T}} x_2^2\,dt\right) \tag{A2}$$

subject to the differential constraints

$$x_1' = x_2 \qquad x_2' = u \tag{A3}$$

and with $x_1(\hat{T}) = x_2(0) = 0$. In (A3) u is the control. The optimal control problem (A2), (A3) is, due to the form of (A2), a non-standard control problem. It was shown in [8], however, that this problem could be treated by (a version of) Pontryagin maximum principle with appropriately chosen Hamiltonian. Applying the procedure given in [9] we easily obtain that $\min F = \lambda$ is determined by the solution of the equation

$$\cos \omega_1 \hat{T} \cos \omega_2 \hat{T} = 0 \tag{A4}$$

where

$$\omega_1^2 = [\lambda - (\lambda^2 - 4K)^{1/2}]/2;$$
$$\omega_2^2 = [\lambda + (\lambda^2 - 4K)^{1/2}]/2. \tag{A5}$$

From (A4) amd (A5) we get

$$\lambda = (\pi/2\hat{T})^2 + K/(\pi/2\hat{T})^2. \tag{A6}$$