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VARIATIONAL SOLUTIONS FOR TWO NONLINEAR BOUNDARY-VALUE PROBLEMS FOR DIFFUSION WITH CONCENTRATION-DEPENDENT COEFFICIENTS*

BY R. I. REEVES (*University of York, England*)

Abstract. The theory of complementary variational principles is used to obtain variational solutions for two nonlinear boundary-value problems which arise in the theory of diffusion with concentration-dependent coefficients.

In many practical diffusion problems the coefficient D depends upon the concentration of the diffusion substance. The one-dimensional case for a semi-infinite medium is described by the partial differential equation

$$\frac{\partial}{\partial z}\left(D(C)\frac{\partial C}{\partial z}\right) = \frac{\partial C}{\partial t} \tag{1}$$

subject to the conditions

$$\begin{aligned} C &= C_0 \quad \text{for} \quad z > 0, \qquad t = 0, \\ C &= C_1 \quad \text{for} \quad z = 0, \qquad t > 0. \end{aligned} \tag{2}$$

Lee [1] and Shampine [2, 3] have recently considered this problem, and several examples of the diffusion coefficient can be found in Crank [4].

We consider here the following two forms of $D(C)$ when the initial and boundary conditions are those of desorption from the semi-infinite medium:

(i) $D(C) = D_0 \exp [kC/C_0]$ where $k \geq 0$, (3)

(ii) $D(C) = D_0/(1 - \lambda C)^2$ where $\lambda > 0$ and $0 < \lambda C_0 < 1$. (4)

D_0 denotes the value of D when $C = 0$, and in both cases the initial and boundary conditions are

$$\begin{aligned} C &= C_0 \quad \text{for} \quad z > 0, \qquad t = 0, \\ C &= 0 \quad\ \ \text{for} \quad z = 0, \qquad t > 0, \end{aligned} \tag{5}$$

where it is assumed that C_0 is a constant.

On changing the variables by introducing

$$c = C/C_0\,, \qquad K(c) = D(C)/D_0\,, \qquad x = \tfrac{1}{2}z/(D_0 t)^{1/2} \tag{6}$$

and using the transformation ([4] eq. (9.35))

$$\psi = \int_0^c K(b)\, db \Big/ \int_0^1 K(b)\, db, \tag{7}$$

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the following boundary-value problems for the two cases are obtained:

(i)
$$-\frac{d^2\psi}{dx^2} = \frac{2x}{(1+\alpha\psi)}\frac{d\psi}{dx} \tag{8}$$

with

$$\psi(0) = 0, \qquad \psi(\infty) = 1, \tag{9}$$

where $\alpha = (e^k - 1)$, and

(ii)
$$-\frac{d^2\psi}{dx^2} = \frac{2x}{(1+\beta\psi)^2}\frac{d\psi}{dx} \tag{10}$$

with

$$\psi(0) = 0, \qquad \psi(\infty) = 1, \tag{11}$$

where $\beta = \lambda C_0/(1 - \lambda C_0)$.

It can be shown [2] that these problems possess unique solutions.

We use the theory of complementary variational principles [5, 6] to find maximum and minimum principles associated with these boundary-value problems, and to obtain simple variational solutions.

For problem (i) we use the theory of Anderson and Arthurs [6] to define the functionals

$$J(\Phi) = \int_0^\infty \{\Phi' \log \Phi' - \Phi' - 2x[\log(1+\alpha\Phi) - k]/\alpha\}\, dx \tag{12}$$

with boundary conditions $\Phi(0) = 0$, $\Phi(\infty) = 1$, and

$$G(U) = (1/\alpha)\int_0^\infty \{U' - \alpha \exp[U] + 2x[\log(-U'/2x) + k + 1]\}\, dx + U(\infty). \tag{13}$$

It can readily be shown that these functionals are stationary at

$$\Phi = \psi \text{ and } U = \log(d\psi/dx) \tag{14}$$

where ψ is the exact solution of (8) and (9).

Also, for trial functions Φ which satisfy

$$d\Phi/dx \geq 0 \tag{15}$$

the extremum principles

$$G(U) \leq J(\psi) \leq J(\Phi) \tag{16}$$

hold, equality occurring when the conditions in (14) are satisfied.

The values of the complementary functionals were calculated using trial functions

$$\Phi = 1 - [1 - \operatorname{erf}(\gamma_1 x)]^{\gamma_2}, \tag{17}$$

$$U = -x^2 \exp[-k] + \mu_1 + \mu_2 \exp[-\mu_3 x^2] \tag{18}$$

where

$$\operatorname{erf}(x) = 2\pi^{-1/2}\int_0^x \exp[-t^2]\, dt,$$

and γ_1, γ_2, μ_1, μ_2 and μ_3 are variational parameters which were found by performing the optimisation.

For $k = 5.3$ the values were found to be

$$J = -3.399 \quad \text{at} \quad \gamma_1 = 3.6(-2), \qquad \gamma_2 = 2.9, \tag{19}$$

$$G = -3.410 \quad \text{at} \quad \mu_1 = -2.80, \qquad \mu_2 = 5.62(-1), \qquad \mu_3 = 1.96(-2). \tag{20}$$

Here $m(-n)$ means $m \times 10^{-n}$.

For problem (ii) the functionals are now

$$J(\Phi) = \int_0^\infty \{\Phi' \log \Phi' - \Phi' + 2x[1/(1 + \beta\Phi) - 1/(1 + \beta)]/\beta\}\, dx \tag{21}$$

with

$$\Phi(0) = 0, \qquad \Phi(\infty) = 1,$$

$$G(U) = (1/\beta) \int_0^\infty \{2(-2xU')^{1/2} + U' - \beta \exp[U] - 2x/(1 + \beta)\}\, dx + U(\infty). \tag{22}$$

TABLE I

Comparison of variational and iterative solutions of Eqs. (8) *and* (9) *with* $k = 5.3$.

x	S(x)	Φ(x)
0.0	0.0	0.0
1.0	0.113	0.113
2.0	0.216	0.218
3.0	0.311	0.313
4.0	0.397	0.400
6.0	0.544	0.549
8.0	0.663	0.668
10.0	0.756	0.760
12.0	0.828	0.831
16.0	0.921	0.922
20.0	0.968	0.967
24.0	0.989	0.987
28.0	0.997	0.996
32.0	0.999	0.999
36.0	1.000	1.000

These functionals are stationary at

$$\Phi = \psi, \qquad U = \log (d\psi/dx) \tag{23}$$

where ψ is the exact solution of (10) and (11).

For functions Φ which satisfy

$$\Phi \geq 0, \qquad d\Phi/dx \geq 0, \tag{24}$$

we have the extremum principles

$$G(U) \leq J(\psi) \leq J(\Phi) \tag{25}$$

with the equality arising when the conditions in (23) are satisfied.

If we take trial functions of the form

$$\Phi = 1 - [1 - \operatorname{erf}(\gamma_1 x)]^{\gamma_2}, \tag{26}$$

$$U = -x^2/(1+\beta)^2 + \mu_1 + \mu_2 \exp[-\mu_3 x^2], \tag{27}$$

the optimum functional and parameter values for $\lambda C_0 = 0.6838$ are

$$J = -1.870 \quad \text{at} \quad \gamma_1 = 1.6\,(-1), \qquad \gamma_2 = 3.0, \tag{28}$$

$$G = -1.880 \quad \text{at} \quad \mu_1 = -1.38, \qquad \mu_2 = 6.89\,(-1), \qquad \mu_3 = 3.67\,(-1). \tag{29}$$

The closeness of the bounds J and G in each problem indicates that the variational solutions Φ given by (17) and (26) are reasonable approximations to the exact solutions ψ of the problems described by (8), (9) and (10), (11) respectively. This is borne out by comparing the variational solutions Φ with iterative solutions $S(x)$ described by Crank [4]. The comparisons are given in Tables I and II.

TABLE II

Comparison of variational and iterative solutions of Eqs. (10) *and* (11) *with* $\lambda C_0 = 0.6838$.

x	S(x)	Φ(x)
0.0	0.0	0.0
0.5	0.248	0.247
1.0	0.450	0.447
1.5	0.608	0.604
2.0	0.726	0.723
3.0	0.878	0.876
4.0	0.952	0.951
5.0	0.984	0.983
6.0	0.995	0.995
7.0	0.999	0.999
8.0	1.000	1.000

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