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Letters to the Editors

Solution of a non-linear equation

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Dear Sirs,

In a recent paper, Shacham and Kehat[1] discuss the problem of solving a single non-linear algebraic equation. They present the following convergence criteria (their notation and equation numbers)—

$$|x_{i+1} - x_i| < \epsilon \tag{7}$$

$$f(x_{i+1}) \times f(x_i) < 0. \tag{15}$$

Thus convergence is deemed to have occurred when two successive iterates are close together and bound the root. The authors state that criterion (15) is not used in the chemical engineering literature. It would appear that they may have overlooked two algorithms which make use of (15), namely the Rule of False Position[2] and Cox's method[3], both of which exhibit superlinear convergence[4] and have been successfully applied to chemical engineering problems[5, 6].

If the comparison of algorithms had included these two techniques the advantages of the authors' novel algorithms might have been demonstrated more clearly.

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Non-iterative solution of a boundary value problem in reactor design by parameter differentiation

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In this letter the method of parameter differentiation is applied to the solution of the nonlinear, two-point boundary value problem governing the concentration of reactant in an isothermal tubular flow reactor. Starting from a given set of solutions of the differential equation for a particular value of the reaction parameter R, solutions for a range of values of R can be obtained by this method noniteratively. Although the method has been discussed in general form in Ref. [1], it is felt that its usefulness has not been emphasized; especially its application to other engineering problems has already established that it is as convenient and simple as the method of transformation groups of Ref. [2].

Consider the isothermal packed-bed reactor in which a chemical reaction of the form

$$A + A \rightarrow B \tag{1}$$

takes place. Assuming negligible influence of the packing on the reaction except for its contribution to the axial mixing, the nondimensional differential equation for the fraction, y, of the reactant A remaining is of the form:

$$\frac{1}{N_{pe}} \frac{d^2y}{ds^2} + \frac{dy}{ds} - Ry^n = 0 \tag{2}$$

subject to the boundary conditions:

$$s = 0: \frac{dy(0)}{ds} = 0 \tag{3a}$$

$$s = 1: 1 = y(1) + \frac{1}{N_{pe}} \frac{dy(1)}{ds} \tag{3b}$$

To apply the method of parameter differentiation, we have to identify initially the parameter to be differentiated. For the problem under consideration, we are looking for solutions of Eq. (2), subjected to the boundary conditions (3), corresponding to a given value of N_{pe} and a given order of reaction, n, for a *range* of values of R. The parameter is therefore identified as R.

Differentiating Eq. (2) and its boundary conditions (3) with respect to R, we get:

$$\frac{d^2f}{ds^2} + N_{pe}\frac{df}{ds} - N_{pe}Rny^{n-1}f = N_{pe}y^n \tag{4}$$

and the boundary conditions:

$$\frac{df(0)}{ds} = 0, \quad f(1) + \frac{1}{N_{pe}} \frac{df(1)}{ds} = 0 \tag{5}$$

where f is defined as:

$$f = \frac{dy}{dR} \tag{6}$$

Equation (4) is now linear and can be separated into two initial value problems as follows: Let

$$f = F + \lambda G \tag{7}$$

If we identify

$$\lambda = f(0) \tag{8}$$

then Eq. (4) can be separated into the following equations:

$$\frac{d^2F}{ds^2} + N_{pe}\frac{dF}{ds} - N_{pe}Rny^{n-1}F = N_{pe}y^n \tag{9}$$

$$F(0) = 0, \quad \frac{dF(0)}{ds} = 0$$

$$\frac{d^2G}{ds^2} + N_{pe}\frac{dF}{ds} - N_{pe}Rny^{n-1}G = 0 \tag{10}$$

$$G(0) = 1, \quad \frac{dG(0)}{ds} = 0$$

The value of λ can be evaluated by using the boundary condition at $s = 1$, which gives:

$$-\lambda = \frac{N_{pe}F(1) + dF(1)/ds}{N_{pe}G(1) + dG(1)/ds} \tag{11}$$

The solution procedure can be illustrated by an example. Consider the solutions of Eq. (2) for $N_{pe} = 1$ and $n = 3$ and a range of R from $R = 0{\cdot}1219$ to $2{\cdot}5$, with the solutions of Eq. (2) for $R = 0{\cdot}1219$ given as:

$$R = 0{\cdot}1219, \quad y(0) = 0{\cdot}9058$$

It should be noted that, in applying this method, the solutions for *one* value of the parameter is needed as a starting solution. With this in mind and with the function $y(S)$ in Eqs. (9) and (10) known, Eqs. (9) and (10) can now be integrated for $R = 0{\cdot}1219 + \Delta R$ to give F and G along with their derivatives. These values can then be used to evaluate λ from Eq. (11) and subsequently f from Eq. (7). As a final step, integration of Eq. (6) yields the solution of Eq. (2) for $R = 0{\cdot}1219 + \Delta R$ as follows:

$$y(s)\Big|_{R = 0{\cdot}1219 + \Delta R} = y(s)\Big|_{R = 0{\cdot}1219} + f(s)\Big|_{\text{from Eq. (7)}} \cdot \Delta R$$

This procedure can be repeated to calculate the solutions of Eq. (2) for $R = 0{\cdot}1219 + 2\Delta R$, $0{\cdot}1219 + 3\Delta R, \ldots$, *etc.*

Based on our experience in this method, we found that a high degree of accuracy can be obtained using this method when ΔR does not exceed a one percent of the range of R being studied. In our case we investigated a range of R from $0{\cdot}1219$ to $3{\cdot}9128$ for $n = 3, 2, \frac{1}{4}$, and $N_{pe} = 1$, 2, and 5 and found that our results are essentially the same as those obtained from the transformation group method. The choice of $R = 0{\cdot}1219$ as our starting solution was made simply because such a solution was available to us. Other starting solutions can be used including the one with $R = 0$.

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