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NOTE ON A THREE-POINT EXTRAPOLATION FORMULA

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Differential equations which describe several chemical engineering processes when written in cylindrical polar co-ordinates are very often amenable to numerical integration on a high-speed digital computer. This is expecially true of differential equations of "parabolic" form, which suggests the use of the well-known four-point forward-difference integration method. In all these numerical integration methods, modifications of the calculation methods are required at the axis of the cylinder (or at a boundary) since a singularity in finite-difference approximation exists there. This singularity necessitates an assumption of the value of the function at these points. Hence it is desirable to extrapolate the value at the axis of the cylinder from the known values of the function in the vicinity of the axis. Very often a linear extrapolation of the functional form is chosen but this can lead to serious errors. Also in such cases one often has the condition that the gradient of the function vanishes at the axis (or at the boundary).

In this note we present a three-point extrapolation formula from which the value of the function at point s can be calculated from the known values at the points $(s - 1)$, $(s - 2)$, and $(s - 3)$ together with the condition that the gradient of the function vanishes at point s.

We express function f at a point s in the Taylor series form as

$$f_s = f_{s-1} + \left(\frac{\partial f}{\partial r}\right)_{s-1} \Delta r + \frac{1}{2!} \left(\frac{\partial^2 f}{\partial r^2}\right)_{s-1} (\Delta r)^2 + \frac{1}{3!} \left(\frac{\partial^3 f}{\partial r^3}\right)_{s-1} (\Delta r)^3 + \dots \quad . \tag{1}$$

Also we write the first derivative in the following form

$$\left(\frac{\partial f}{\partial r}\right)_s = \left(\frac{\partial f}{\partial r}\right)_{s-1} + \left(\frac{\partial^2 f}{\partial r^2}\right)_{s-1} \Delta r + \frac{1}{2!} \left(\frac{\partial^3 f}{\partial r^3}\right)_{s-1} (\Delta r)^2 + \dots , \qquad (2)$$

where r is the radial distance.

Now, using the boundary condition $\left(\frac{\partial f}{\partial r}\right)_s = 0$, and after combining Equations (1) and (2), we have

$$f_s = f_{s-1} - \frac{1}{2!} \left(\frac{\partial^2 f}{\partial r^2}\right)_{s-1} (\Delta r)^2 - \frac{1}{3!} \left(\frac{\partial^3 f}{\partial r^3}\right)_{s-1} (\Delta r)^3 + \dots . \qquad (3)$$

The second and third derivatives of the function f with respect to the distance r can be replaced by finite-difference forms as follows:

$$\left(\frac{\partial^2 f}{\partial r^2}\right)_{s-1} \approx \frac{f_s - 2f_{s-1} + f_{s-2}}{(\Delta r)^2} . \qquad (4)$$

and

$$\left(\frac{\partial^3 f}{\partial r^3}\right)_{s-1} \approx \frac{f_s - 3f_{s-1} + 3f_{s-2} - f_{s-3}}{(\Delta r)^3} . \qquad (5)$$

Substituting the relationships (4) and (5) into (3) and after simplifying, we obtain

$$f_s = \frac{18}{11} f_{s-1} - \frac{9}{11} f_{s-2} + \frac{2}{11} f_{s-3} . \qquad (6)$$

Equation (6) enables us to extrapolate the value of the function f at point s from the known values at points $(s-1)$, $(s-2)$, and $(s-3)$.

The usefulness of the proposed extrapolation formula was discovered by the author in numerical integration of the diffusion-convection equation for cylindrical tubes by using the high speed digital computer (IBM 7090).

It is noted that in an analogous manner one can develop a four-point (or more accurate) extrapolation formula. The formula given by equation (6) was found to be quite adequate in the present calculation method described in Ref. (1) and probably should find a wider use in solving several chemical engineering problems with the help of high speed machines.

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References

1. Wasan, D. T., Ph. D. thesis under preparation in Chemical Engineering Department of University of California.