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THE TREATMENT OF BOUNDARY
SINGULARITIES IN AXIALLY SYMMETRIC
PROBLEMS CONTAINING DISCS

by

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<u>ABSTRACT</u>

Axially symmetric problems (e.g. Laplace's equation in cylindrical
co-ordinates) containing discs possess boundary singularities
arising from the mixed boundary conditions that occur across the
disc edge.   A modified finite-difference method is presented which
effectively eliminates the inaccuracies that occur in the standard
numerical solution near such singularities.   Techniques   for
developing the analytical forms of such singularities   are given
and modified finite-difference approximations   are obtained.   The
steady-state diffusion of oxygen around a circular electrode is
taken as the model problem and a modified quadrature method is
presented for the calculation of the oxygen flux through the
electrode.

1. Introduction

The generalised axially symmetric problem is to solve

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{k}{x}\frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad, \qquad x \neq 0 \ , \ k>0 \ \text{and known}, \tag{1.1}$$

for the unknown function $\phi(x,y)$. The commonest form of (1.1) is Laplace's equation in cylindrical co-ordinates which occurs when $k = 1$ and when the co-ordinates (x,y) are replaced by the cylindrical co-ordinates (r,z), where $r = 0$ is the axis of symmetry and lies along the vertical axis of the cylinder (Fig.1), viz.

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = 0 \quad, \ r \neq 0. \tag{1.2}$$
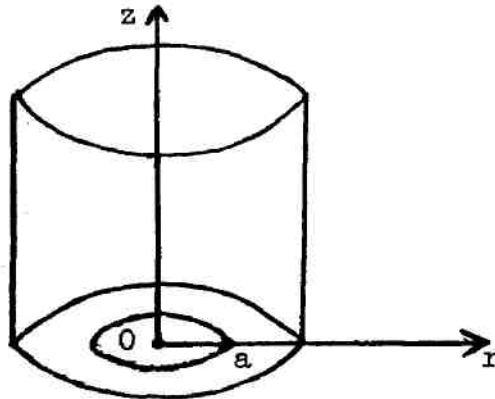

FIG.1. Cylindrical region containing a disc on $z = 0$.

Of particular interest are problems of the above type where there is a disc lying on the top or bottom surface of the cylinder, e.g. a disc of radius a, centre z - axis, lying on $z = 0$ (Fig.1). Such problems are characterised by the singularity that occurs in $\partial\phi/\partial z$ on the disc edge. The singularity arises from the mixed boundary conditions that occur across the disc edge, typically

$$\phi = 0 \quad, \quad 0 \leq r \leq a \quad; \quad \frac{\partial \phi}{\partial z} = 0 \quad, \ r > a \ \text{ on } \ z = 0 \ . \tag{1.3}$$

Physical applications of (1.2) and (1.3) are, in the steady-state, the heat flow around a disc-shaped heat source, Grigull (1961), or around a disc-shaped crack, Parton (1972); the diffusion of

oxygen around an electrode, Saito (1968), Evans and Gourlay (1976), or the diffusion of vapours through a membrane clamped between two annular plates, Barrer et al (1962); the electrostatic potential around an electrified disc, Sneddon (1966); the elastic stress distribution in a cylinder, Zak (1972). Further applications occur when k is other than unity. For example, the case k = 3 represents the problem of stream functions for incompressible three-dimensional flow, Payne (1952), and the case k = 5 describes the torsion of shafts, Weinstein (1952). Tricomi's equation, with suitable change of co-ordinates, see Weinstein (1951), is the case $k = \frac{1}{3}$.

Analytical solutions based on dual integral or dualseries techniques have long been available for such mixed boundary value problems, Sneddon (1966). For more general cases numerical techniques are needed to solve the dual integral equations. Also, dual series solutions have been shown to converge slowly in the neighbourhood of the singularity, Whiteman (1970). This paper presents a general numerical method based on finite—difference approximations which is capable of extension to problems involving more than one disc or to time-dependent situations. The method employs modified approximations near the singularity which take into account the nature of the singularity. The modified approximations are developed from a local truncated series form of the solution, centred on the singularity, as suggested by Motz (1946). The development of such a local series form is complicated by the presence of the $\frac{k}{x}\frac{\partial\phi}{\partial x}$ term in (1.1) and so, for convenience, a transformation of (1.1) to the self-adjoint form used by Fox and Sankar (1969) is introduced. The method differs from that of Motz in that the modified approximations are developed from the derivatives in the governing equation rather than from the algebraic equations for the solution values. The method also differs in the set of neighbouring points used to approximate the unknown coefficients in the truncated series approximations for the derivatives. The model problem treated is the steady-state diffusion of oxygen around a circular electrode, Saito (1968), and a modified quadrature method is given for the calculation of the oxygen flux diffusing through the electrode surface.

2.   Numerical Treatment of Boundary Singularities

The majority of numerical treatments for boundary singularities
of the infinite derivative type have been for steady-state, linear
problems, usually Laplace's equation, formulated in terms of
rectangular Cartesian co-ordinates (x,y).   For such problems, a
series form of the solution near the singularity can be found by
converting the co-ordinates (x,y) to local polar co-ordinates
centred on the singularity,   followed by application of the standard
separable-variable techniques, Fox and Sankar (1969), or asymptotic
expansion techniques, Wigley (1969). For example, for the mixed
boundary condition

$$\frac{\partial \phi}{\partial n} = 0 \ \text{ on } \ \theta = 0 \ ; \quad \o = 0 \ \text{ on} = \ \theta = \omega \quad , \qquad (2.1)$$

where $\theta = 0$ represents one arm of the boundary at the singularity
at 0, and $\theta = \omega$ represents the other arm (Fig.2), then the series
form of the solution of Laplace's equation, valid near the singularity
at 0, is

$$\phi \ \sum_{k=0}^{\infty} c_k \rho^{(k+\frac{1}{2})\frac{\pi}{\omega}} \cos(k+\frac{1}{2})\frac{\pi}{\omega}\theta \quad . \qquad (2.2)$$

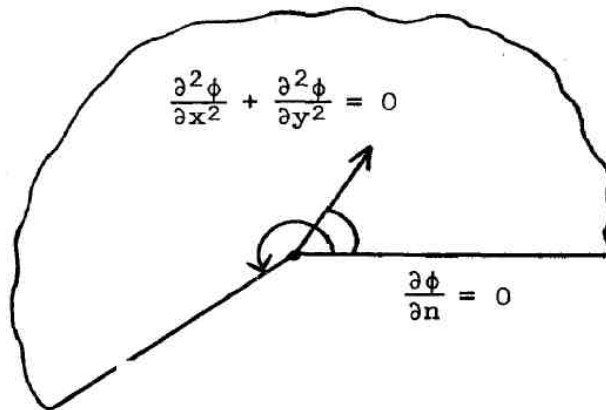(The c_k are constants to be found.)

FIG.2.   Typical singularity.

It will be seen later that such orms are harder to obtain for Laplace's
equation in cylindrical co-ordinates.

From (2.2), it is evident that $\partial\phi/\partial\rho$ becomes unbounded as $\rho\to0$ if $\omega > \pi/2$. It is well-known that standard finite—difference or finite element approximations using a uniform mesh prove to be highly inaccurate near such singularities unless a relatively fine mesh is used, and that a 'pollution effect' occurs since the inaccuracies spread throughout the entire region, Babuska and Aziz (1972). Local mesh refinement has been used successfully to neutralise the singularity errors by Webb and Whiteman (1970), Whiteman (1974), Thatcher (1975).

The main alternative is the method of Motz (1946) mentioned earlier. The method has been extended, in the finite-difference context, by Whiteman (1967), Fox and Sankar (1969), Bell and Crank (1973,1975), Crank and Furzeland (1976), and, in the finite element context, by Wait and Mitchell (1971), Barnhill and Whiteman (1973). A slightly different approach was given by Woods (1953), and extended by Emery and Segedin (1973), Emery (1973), Benzley (1974). The Motz and Woods methods tend to be computationally more efficient than mesh refinement but do require special knowledge about the form of the singularity. However, they have the disadvantage that any banding or symmetry present in the global matrix is destroyed.

Conformal transformation methods have been proposed by Papamichael and Whiteman (1973) and have proved to be highly accurate and efficient for the solution of elliptic problems in simply-connected polygonal regions with general mixed boundary conditions. The methods rely on the fact that equations such as Laplace's equation in Cartesian co-ordinates are invariant under conformal transformations, but this is not true for equations of the form (1.1). Other methods are reviewed in Crank (1973).

3.   Model Problem

The steady-state, diffusion problem of determining the axially
symmetric oxygen concentration distribution around a circular
disc—shaped electrode surface (centre origin, radius a, see Fig.3)
in an electrolytic solution is taken as the model problem.
Saito (1968), using the dual integral equation method, developed
an exact analytical solution for the above problem in a semi—infinite
region and this will be used for purposes of comparison.   Saito's
form of the problem was to solve

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = 0 \quad , \ 0 < r < \infty \ , \ 0 \le z < \infty \ , \qquad (3.1)$$

where $\phi(r,z)$ denotes the oxygen concentration, subject to

$$\phi = 0 \qquad\qquad 0 \le r \le a \left.\begin{array}{c}\\[2ex]\end{array}\right\} \text{ on } z = 0 , \qquad\begin{array}{c}(3.2)\\[2ex](3.3)\end{array}$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad\qquad r > a$$

$$\frac{\partial \phi}{\partial z} = 0 \qquad\qquad r = 0 \ , \quad z > 0 \ , \qquad (3.4)$$

$$\phi = C_0 \qquad\qquad r \to \infty \ , \quad z \ge 0 \ , \qquad (3.5)$$

$$\phi = C_0 \qquad\qquad z \to \infty \ , \quad r \ge 0 \ . \qquad (3.6)$$

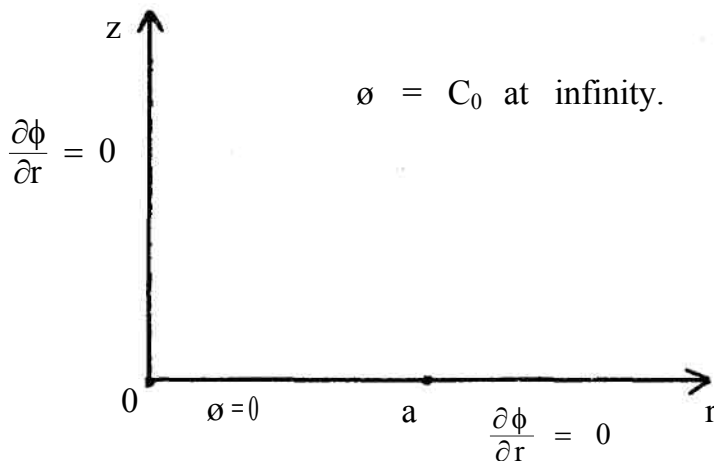C_0 is a constant denoting the oxygen concentration in the bulk of
the solution.

FIG. 3.   Semi-infinite region.

Also of interest in such, problems is the oxygen flux, Q say, diffusing through the electrode surface.   This is determined from

$$Q = 2\pi D \int_0^a r \frac{\partial \phi}{\partial z}\bigg|_{z=0} dr \ , \tag{3.7}$$

where D denotes the diffusion coefficient. The flux can he measured experimentally as an electrical current. The same problem, but in a time-dependent, finite region, has an important medical application, viz. the diffusion with absorption problem of Evans and Gourlay (1976).

Saito found the following exact form for the concentration distribution

$$\phi = C_0 - \frac{2C_0}{\pi} \int_0^\infty \frac{\sin (am)}{m} J_0 (rm) \ e^{-zm} \ dm \ . \tag{3.8}$$

Using standard integral results, Gradshteyn and Ryzhik (1965), (3.8) becomes

$$\phi = C_0 - \frac{2C_0}{\pi} \arcsin \frac{2a}{\sqrt{z^2+(a+r)^2} + \sqrt{z^2+(a-r)^2}} \ , \ z > 0 \ , \tag{3.9}$$

and

$$\phi = 0 \ , \ 0 \le r \le a \ ; \ \phi = C_0 - \frac{2C_0}{\pi} \arcsin \frac{a}{r} \ , \ r > a \ \text{for} \ z = 0 \ . \tag{3.10}$$

Differentiating (3.8) and using standard integral results gives

$$\frac{\partial \phi}{\partial z}\bigg|_{z=0} = \frac{2C_0}{\pi} \frac{1}{\sqrt{a^2-r^2}} \ , \qquad 0 \le r \le a \qquad , \tag{3.11}$$

and so

$$Q = 4DC_0 \int_0^a \frac{r}{\sqrt{a^2-r^2}} \ dr = 4aDC_0 \quad . \tag{3.12}$$

From (3.11), it is clear that $\partial\phi/\partial z$ becomes unbounded on $z = 0$ as $r \to a$. This means that a standard numerical solution of (3.1) - (3.6), and a standard numerical quadrature of (3.7), will produce highly inaccurate results near $(a,0)$. In the following sections, modified methods are developed which take into account the behaviour of the singularity at $(a, 0)$.

4. Finite-Difference Approximations away from (a,0)

Let N[a] denote the neighbourhood around $(a,0)$ such that the error in the finite-difference approximations at points outside N[a] is less than some specified precision. In this section, standard finite-difference approximations are used for points outside N[a] and, in the following sections, modified approximations are developed and used for points inside N[a].

In the model problem, the semi-infinite region $\{0<r<\infty, 0\leq z<\infty \}$ of Fig.3 is replaced by the finite region $\{0<r<r_L ,0<z<z_L \}$, where $r_L, >>a$, and the boundary conditions (3.5), (3.6) are replaced by

$$\phi = g_1(z) \quad \text{on} \quad r = r_L \quad , \quad 0 < z < z_L \quad , \tag{4.1}$$

$$\phi = g_2(r) \quad \text{on} \quad z = z_L \quad , \quad 0 < r < r_L \quad , \tag{4.2}$$

where the exact form (3.8) of ϕ is used to find g_1 and g_2 .

The finite region is discretised so that $r = 0$ and $r = a$ do not lie on mesh lines by choosing a uniform mesh size δr in the r direction such that $r = a$ lies midway between two mesh points and is an integer multiple of δr from $r = 0$. A uniform mesh size z is chosen in the z direction and $z = 0$ is a mesh line. For convenience, r_L and z_L are chosen such that they lie on mesh lines (Fig.4). i.e. the mesh lines are

$$r = (i + \frac{1}{2}) \delta r \qquad i = 0, \ 1,2, \ ... \quad , \tag{4.3}$$

$$r = j \delta z \qquad j = 0, \ 1, \ 2 .... \tag{4.4}$$

This discretisation was used by Evans and Gourlay and is chosen here in order to facilitate comparisons with their results.
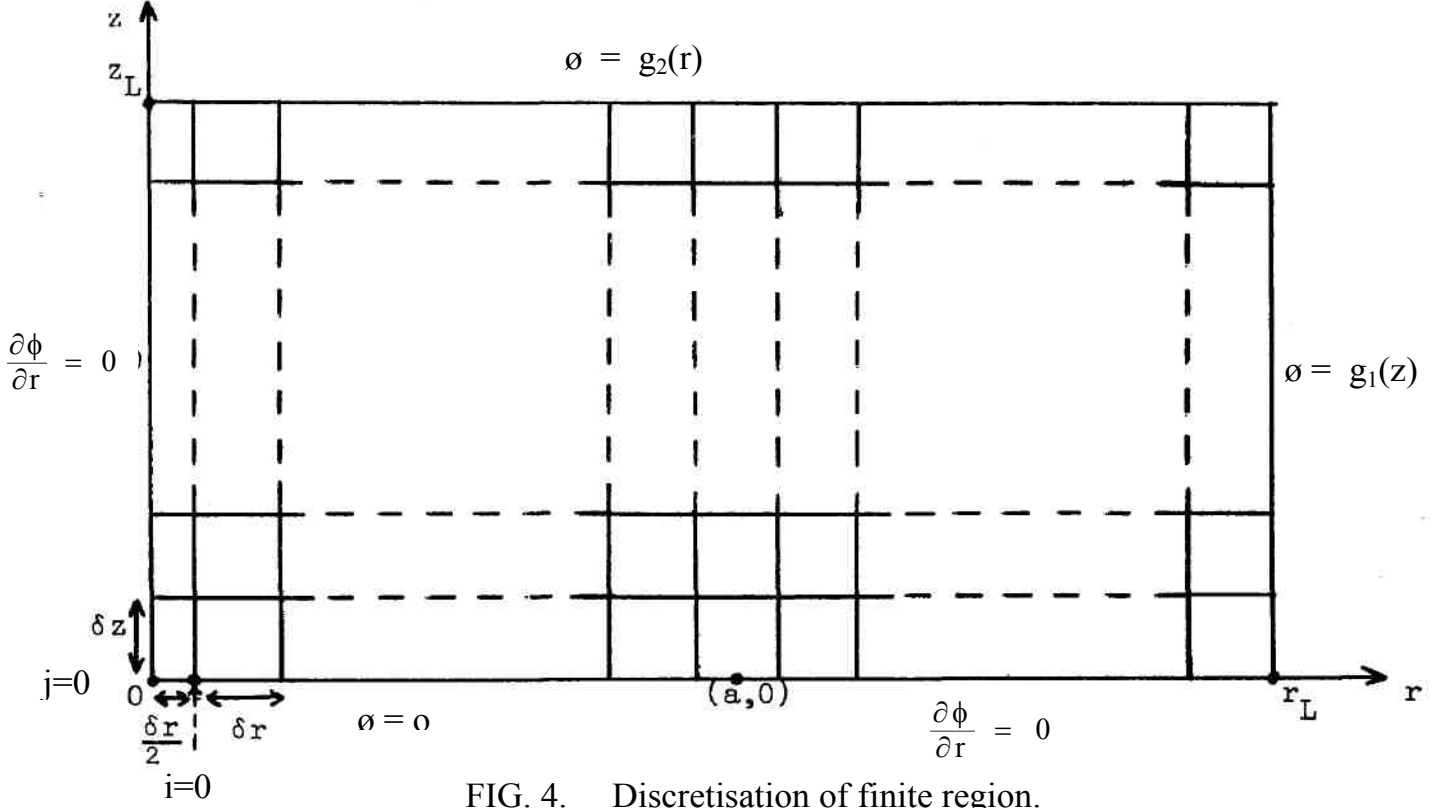

FIG. 4.   Discretisation of finite region.

Using central difference approximations, the standard finite-difference replacement of (3.1) is

$$\frac{1}{(\delta R)^2}\left\{1-\frac{1}{(2i+1)}\right\}\phi_{i-\frac{1}{2},j} + \frac{1}{(\delta r)^2}\left\{i+\frac{1}{(2i+1)}\right\}\phi_{i+\frac{3}{2},j} + \frac{1}{(\delta z)^2}\phi_{i+\frac{1}{2},j-1} + \frac{1}{(\delta z)^2}\phi_{i+\frac{1}{2},j+1}$$

$$-2\left\{\frac{1}{(\delta r)^2}+\frac{1}{(\delta z)^2}\right\}\phi_{i+\frac{1}{2},j} = 0 \quad , \tag{4.5}$$

for points $(i+\frac{1}{2},j)$ outside N[a] and not involving the boundary.

For points which do involve the boundary, the following are used:

   (i)   on $z=0$, $0 < r < a$, $\phi = 0$ (known) ,

   (ii) on $z=0$, $a < r < r_L$, $\phi_{i+\frac{1}{2},j-1} = \phi_{i+\frac{1}{2},j+1}$,

   (iii) on $r = r_L$, $0 < z < z_L$, $\phi = g_1(z)$ (known) ,

(iv)   on $z - z_L$, $0 < r < r_L$, $\o = g_2(r)$ (known)   ,

(v)   on $r = \dfrac{\delta r}{2}$ (i.e. $i = 0$) , $\o_{-\frac{1}{2},j} = \o_{\frac{1}{2},j}$,

(vi)   on $r = 0$,   (3.1)   becomes

$$2 \frac{\partial^2 \phi}{\partial r^2} + \frac{\partial^2 \phi}{\partial z^2} = 0 \quad , \tag{4.6}$$

and this is used in conjunction with $\o_{-\frac{1}{2},j}$, $= \o_{\frac{1}{2},j}$.

5.   Truncated Series Form near (a,0)

The presence of the $\frac{1}{r}$ coefficient of $\frac{\partial \phi}{\partial r}$ in (3.1) means that, after shifting the origin to the singularity (a,0) and converting to polar co-ordinates centred on (a,0), the resulting equation contains complicated non-constant coefficients which need series expansions, Zak (1972). A more convenient way of proceeding is to transform the problem to the self-adjoint form

$$\frac{\partial^2 u}{\partial \xi^2} + \frac{\partial^2 u}{\partial \eta^2} + g(\xi, \eta) u = 0, \tag{5.1}$$

by suitable transformations of the co-ordinates (r,z) to (ξ, η) and, if necessary, of the unknown function $\o$ to u . Once the problem is in this form it can be written in terms of local polar co-ordinates and readily solved by standard separable-variables or asymptotic expansion techniques. The above idea was suggested and used by Fox and Sankar (1969).

For the problem (3.1) - (3.6) the simple transformation   (5.2)

$$u(r,z) = r^{\frac{1}{2}} \, \o(r,z) \quad ,$$

leads to the self-adjoint form. Using (5.2) equation (3.1) becomes

$$\frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial z^2} + \frac{u}{4r^2} = 0 \quad , \tag{5.3}$$

and (3.2), (3.3) become

$$\left. \begin{array}{ll} u = 0 & 0 = r = a \\[2ex] \dfrac{\partial u}{\partial z} = 0 & r > a \end{array} \right\} \quad \text{on } z = 0 \quad . \tag{5.4}$$
$$\tag{5.5}$$

The transformation (5.2) results in the cancellation of first derivative terms and the introduction of a 'heat source' term. For the general axisymmetric problem (1.1) the corresponding transformation is

$$u(x,y) = x^{\frac{k}{2}} \, \phi(x,y) \quad , \tag{5.6}$$

which gives the self-adjoint form

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{k}{2}\left(1 - \frac{k}{2}\right)\frac{u}{x^2} = 0 \quad . \tag{5.7}$$

No change of co-ordinates is necessary to obtain the self-adjoint forms for problems of the form (1.1).

Applying the shift transformation $R = r - a$, and converting to polar co-ordinates $R = \rho \cos \theta$, $z = \rho \sin \theta$, (5.3) - (5.5) become

$$\frac{\partial^2 u}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial u}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2 u}{\partial \theta^2} + g(\rho,\theta)\, u = 0 \quad . \tag{5.8}$$

$$\frac{\partial u}{\partial \theta} = 0 \quad \text{on} \quad \theta = 0 \; ; \quad u = 0 \quad \text{on} \quad \theta = \pi \quad , \tag{5.9}$$

where

$$g(\rho,\theta) = \frac{1}{4(\rho \cos \theta + a)^2} \quad . \tag{5.10}$$

Equation (5.10) can be written as

$$g(\rho,\theta) = \sum_{n=0}^{\infty} \rho^n g_n(\theta) \quad \text{where } g_n(\theta) = \frac{(-1)^n (n+1)}{4a^{n+2}} \cos^n \theta \ . \tag{5.11}$$

Following Fox and Sankar (1969), the separable-variable form

$$u(\rho,\theta) = \sum_{j=0}^{\infty} \rho^{\alpha+j} A_{\alpha,j}(\theta) \tag{5.12}$$

is sought such that the simple homogeneous conditions (5.9) are satisfied. Substitution of (5.12) into (5.8) gives the following set of differential equations for the $A_{\alpha,j}(\theta)$.

$$A''_{\alpha,0}(\theta) + \alpha^2 A_{\alpha,0}(\theta) = 0 \tag{5.13}$$

$$A''_{\alpha,1}(\theta) + (\alpha+1)^2 A_{\alpha,1}(\theta) = 0 \tag{5.14}$$

$$A'_{\alpha,m+2}(\theta) + (\alpha+m+2)^2 A_{\alpha,m+2}(\theta) + \sum_{j=0}^{\infty} g_{m-j} A_{\alpha,j}(\theta) = 0 \tag{5.15}$$

$$m = 0, \ 1, \ 2, \ ...$$

The simplest way for (5.12) to satisfy (5.9) is for

$$A'_{\alpha,j}(0) = 0 \qquad\qquad j = 0, 1, \quad 2, \ ... \quad , \tag{5.16}$$

$$A_{\alpha,j}(\pi) = 0 \qquad\qquad j = 0, 1, \ 2 .... \tag{5.17}$$

Using these conditions to solve for the $A_{\alpha,j}(\theta)$ in (5.13)—(5.15) it is easily shown that non-trivial solutions only exist if

$$\alpha = p + \frac{1}{2} \qquad , \qquad P = 0, \ 1, \ 2, \ ... \quad , \tag{5.18}$$

and that these solutions are:

$$A_{\alpha,0}(\theta) = a_{0,p} \cos (p+\tfrac{1}{2}) \,(\theta) \quad , \tag{5.19}$$

$$A_{\alpha,1}(\theta) = a_{1,p} \cos (p+\tfrac{3}{2}) \,(\theta) \quad , \tag{5.20}$$

$$A_{\alpha,2}(\theta) = a_{2,p} \cos(p+\tfrac{5}{2}) - \frac{a_{0,p}}{8(2p+3)\,a^2} \cos(p+\tfrac{1}{2})\theta \quad , \tag{5.21}$$

:

etc.

In the above the $a_{j,p}$, $j = 0,1,2,\ \ldots\ $, are arbitrary constants. The three terms (5.19)-(5.21) are all that is needed to give a

truncated series expression for $u(\rho,\theta)$ up to terms involving $\rho^{\frac{5}{2}}$, for

$$u(\rho,\theta) = \sum_{j=0}^{\infty} \sum_{p=0}^{\infty} \rho^{p+\frac{1}{2}+j} A_{p+\frac{1}{2},j}(\theta)$$

$$= \rho^{\frac{1}{2}} A_{\frac{1}{2},0} + \rho^{\frac{3}{2}} A_{\frac{3}{2},0} + \rho^{\frac{5}{2}} A_{\frac{5}{2},0} + \rho^{\frac{3}{2}} A_{\frac{1}{2},1}$$

$$+ \rho^{\frac{5}{2}} A_{\frac{3}{2},1} + \rho^{\frac{5}{2}} A_{\frac{1}{2},2} + 0(\rho^{\frac{7}{2}})$$

$$= c_1 \rho^{\frac{1}{2}} \left[1 - \frac{\rho^2}{24a^2} \right] \cos \frac{\theta}{2} + c_2 \rho^{\frac{3}{2}} \cos \frac{3\theta}{2} + c_3 \rho^{\frac{5}{2}} \cos \frac{5\theta}{2} + 0(\rho^{\frac{7}{2}}) \quad , \tag{5.22}$$

where $c_1 \equiv a_{0,0}$, $c_2 \equiv a_{0,1} + a_{1,0}$, $c_3 \equiv a_{0,2} + a_{1,1} + a_{2,0}$ represent the new unknown constants. To transform back to the original unknown function ϕ, it is necessary to use (5.2) in the form

$$\phi(\rho,\theta) = a^{-\frac{1}{2}} \{1 + (\rho/a)\cos\theta\}^{-\frac{1}{2}} u(\rho,\theta) \quad . \tag{5.23}$$

On using the binomial expansion in (5.23), then (5.22) and (5.23) give the truncated series form

$$\phi(\rho,\theta) = c_1\left[\left(\frac{\rho}{a}\right)^{\frac{1}{2}}\cos\frac{\theta}{2} - \frac{1}{4}\left(\frac{\rho}{a}\right)^{\frac{3}{2}}\left(\cos\frac{\theta}{2} + \cos\frac{3\theta}{2}\right) + \frac{1}{96}\left(\frac{\rho}{a}\right)^{\frac{5}{2}}\left(14\cos\frac{\theta}{2} + 9\cos\frac{3\theta}{2} + 9\cos\frac{5\theta}{2}\right)\right]$$

$$+ c_2 a\left[\left(\frac{\rho}{a}\right)^{\frac{3}{2}}\cos\frac{3\theta}{2} - \frac{1}{4}\left(\frac{\rho}{a}\right)^{\frac{5}{2}}\left(\cos\frac{\theta}{2} + \cos\frac{5\theta}{2}\right)\right] + c_3 a^2\left(\frac{\rho}{a}\right)^{\frac{5}{2}}\cos\frac{5\theta}{2} + 0\left(\rho^{\frac{7}{2}}\right), \qquad (5.24)$$

for ø in the neighbourhood of the singularity at   (a,0) .

6.   Modified Five-point Approximations near   (a,0)

Modified five-point approximations for points in N[a]   are   formed
for each of the terms in (5.3) using the truncated series form of
the solution (5.22).   The constants c_i , i = 1, 2, 3,   are approximated
in terms of the (values at neighbouring points. Modified approximations
of (3.1) for points in N[a]   follow readily.

For the derivative terms in (5.3) five-point approximations are formed
by taking the following three-term truncated form of (5.22):

$$u*(\rho,\theta) = \sum_{i=1}^{3} c_i h_i(\rho,\theta) \text{ with truncation error } 0(\rho^{\frac{7}{2}}), \qquad (6.1)$$

where the $h_i(\rho,\theta)$ are obtained by comparison with (5.22).   Using the
standard differential relations

$$\frac{\partial^2 u}{\partial r^2} = \frac{\partial^2 u}{\partial R^2} = \cos^2\theta\,\frac{\partial^2 u}{\partial\rho^2} - \frac{\sin 2\theta}{\rho}\,\frac{\partial^2 u}{\partial\rho\partial\theta} + \frac{\sin^2\theta}{\rho^2}\,\frac{\partial^2 u}{\partial\theta^2} + \frac{\sin^2\theta}{\rho}\,\frac{\partial u}{\partial\rho} + \frac{\sin 2\theta}{\rho^2}\,\frac{\partial u}{\partial\theta}, \quad (6.2)$$

$$\frac{\partial^2 u}{\partial z^2} = \sin^2\theta\,\frac{\partial^2 u}{\partial\rho^2} + \frac{\sin 2\theta}{\rho}\,\frac{\partial^2 u}{\partial\rho\partial\theta} + \frac{\cos^2\theta}{\rho^2}\,\frac{\partial^2 u}{\partial\theta^2} + \frac{\cos^2\theta}{\rho}\,\frac{\partial u}{\partial\rho} - \frac{\sin 2\theta}{\rho^2}\,\frac{\partial u}{\partial\theta}, \quad 6.3)$$

where approximations for the ρ and θ derivatives are obtained by
differentiating (6.1), the following three-term series approximations

for $\frac{\partial^2 u}{\partial r^2}$ and $\frac{\partial^2 u}{\partial z^2}$ are found :

$$\frac{\partial^2 u*}{\partial r^2} = \sum_{i=1}^{3} c_i \omega_i (\rho,\theta)$$

$$\left.\right\} \text{ with truncation error } 0(\rho^{\frac{3}{2}}) , \qquad (6.4)$$

$$\frac{\partial^2 u*}{\partial z^2} = \sum_{i=1}^{3} c_i \omega'_i (\rho,\theta)$$

$$(6.5)$$

where $\quad \omega_1 = \omega_0 - \dfrac{\rho^{\frac{1}{2}}}{8a^2} \cos \dfrac{\theta}{2} \quad , \quad \omega_0 = -\dfrac{\rho^{\frac{1}{2}}}{4}\left(\dfrac{1}{8a^2} + \dfrac{1}{\rho^2}\right)\cos \dfrac{3\theta}{2} ,$

$$\left.\right\} \qquad (6.6)$$

$$\omega_2 = \frac{3 \cos \frac{\theta}{2}}{4\rho^{\frac{1}{2}}} \quad , \qquad\qquad \omega_3 = \frac{15\rho^{\frac{1}{2}}}{4} \cos \frac{\theta}{2} \qquad .$$

and , from the similariti es between (6.2) and (6.3) ,

$$\omega'_1 = \omega'_0 - \frac{\rho^{\frac{1}{2}}}{8a^2}\cos\frac{\theta}{2} \quad , \quad \omega'_i = -\omega_i \quad , \; i = 0, 2 \text{ and } 3. \qquad (6.7)$$

For the 'heat source' term $\dfrac{u}{4r^2} u \qquad$ in (5-3) the approximation (6.1) is used.

Approximations for the constants c_i ,   i = 1, 2, 3 are found in terms of neighbouring ø values by using the following three-term truncated form of (5.24):

$$\phi * (\rho,\theta) = \sum_{i=1}^{3} c_i f_i (\rho,\theta) \text{ with truncation   error }\; 0(\rho^{\frac{7}{2}}) , \qquad (6.8)$$

where the $f_i (\rho,\theta)$ are obtained "by comparison with (5.24).   Referring to Fig. 5 and denoting ϕ^*_j, ρ_j, θ_j to be the corresponding , ϕ^*, ρ , θ values at the points j = 1, 2, 3, 4, 5, then ϕ^* values at three neighbouring points in the horizontal direction are used to find the

c_i in (6.4) for $\dfrac{\partial^2 u*}{\partial r^2}\bigg|_{\text{po int } 1}$.   The most obvious choice, and that

which leads to a five-point formula, is to use points j = 1, 2 and 3 to give the   following three equations   for the c_i ,

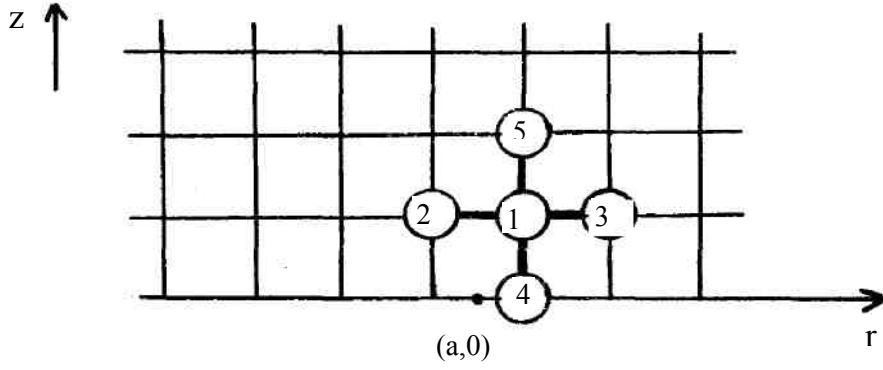$$\phi^*_j = \sum_{i=1}^{3} c_i f_i (\rho_j,\theta_j) , \qquad\qquad j = 1, 2, 3 \quad . \qquad (6.9)$$

FIG.5. Typical 'molecule' of neighbouring points.

The solution of (6.9) is denoted by

$$c_i \; = \; B_i \, \phi^*_2 \; + \; C_i \, \phi^*_1 \; + D_i \, \phi^*_3 \qquad , \quad i \; = \; 1, \; 2, \; 3 \; . \tag{6.10}$$

Similarly, to find the c. in (6.5) for $\left. \dfrac{\partial^2 u^*}{\partial z^2} \right|_{\text{point} \; 1}$, points 4, 1

and 5 are used in the vertical direction. The solution is denoted by

$$c_i \; = \; B'_1 \; \phi^*_4 \; + \; C'_1 \; \phi^*_1 \; + \; D'_1 \; \phi^*_5 \quad , \qquad i \; = \; 1, \; 2, \; 3 \qquad . \tag{6.11}$$

Substitution of (6.10) and (6.11) in (6.4) and (6.5) respectively, gives the five-point approximation

$$\frac{\partial^2 u^*}{\partial r^2} + \frac{\partial^2 u^*}{\partial z^2} \; = \; e_2\phi^*_2 + e_3\phi^*_3 + e_4\phi^*_4 + e_5\phi^*_5 + e_1\phi^*_1 \; = \; 0 \quad , \tag{6.12}$$

where

$$\left. \begin{array}{l} e_2 \; = \; \displaystyle\sum_{i=1}^{3} \omega_i B_i \; , \quad e_3 \; = \; \displaystyle\sum_{i=1}^{3} \omega_i D_i \; , \quad e_4 \; = \; \displaystyle\sum_{i=1}^{3} \omega'_i B'_i \; , \\[4mm] e_5 \; = \; \displaystyle\sum_{i=1}^{3} \omega'_i D'_i \; , \quad e_1 \; = \; \displaystyle\sum_{i=1}^{3} (\omega_i C_i \; + \; \omega'_i C'_i) \; , \end{array} \right\} \tag{6.13}$$

for a typical point 1 in N[a], the ω_i and ω'_i being evaluated at the point (ρ_1, θ_1)

The corresponding approximations for the original problem (3.1) are obtained by equivalencing (5.3) to (3.1), viz.

$$\frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial z^2} + \frac{u}{4r^2} = 0 = \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r}\frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} \qquad , \qquad (6.14)$$

where $\dfrac{\partial^2 u}{\partial r^2}$ and $\dfrac{\partial^2 u}{\partial z^2}$ are approximated by (6.12), and the 'heat source' term by (6.1) using the c_i given by (6.10). This gives the following modified five-point approximation to (3.1) for a typical point 1 in N[a]:

$$e_2' \phi_2^* + e_3' \phi_3^* + e_4' \phi_4^* + e_5' \phi_5^* + e_1' \phi_1^* = 0 \quad , \qquad (6.15)$$

where

$$\left. \begin{array}{l} e_2' = e_2 + g \sum\limits_{i=1}^{3} h_i B_i \quad , \quad e_3' = e_3' + g \sum\limits_{i=1}^{3} h_i D_i \quad , \\[4mm] e_1' = e_1 + g \sum\limits_{i=1}^{3} h_i C_i \quad , \quad g \text{ given by (5.10)} \qquad , \end{array} \right\} \qquad (6.16)$$

all functions being evaluated at the point (ρ_1, θ_1).

The method used above was first given by Crank and Furzeland (1976) and is a generalisation of the ideas of Bell and Crank (1975) in that

(i)   both derivatives are treated

(ii)   the approximations (6.4) and (6.5) are written in a general way so that the neighbouring points chosen need not lie on the same horizontal or vertical line.

The generalisation (ii) is useful in developing higher‑order, multi‑point modified approximations by varying the number of terms included in the truncated series expansion and the set of neighbouring points used for any one point in N[a]. The method can be extended to the time‑dependent case by following Bell and Crank.

The neighbourhood N[a] can include points away from the singularity, as long as the three-term approximations (6.1) and (6.8) remain valid. This may be checked as described in Motz (1946). The approximate size of N[a] can be determined by noting that the discretisation error in the standard finite-difference approximations (4.5) is $0(h^2)$ whereas the modified approximations (6.4) and (6.5) contain a truncation error of $0(\rho^{\frac{3}{2}})$. Thus application of the modified approximations is advantageous as long as the truncation error does not exceed the discretisation error. An approximate rule is then to choose N[a] such that the maximum ρ value m N[a], ρ_{max} say, is such that $\rho_{max}^{\frac{3}{2}}$. is of the same order of magnitude as h^2. However, practical experience suggests that the size of N[a] can he increased further, and with beneficial effect, as long as $\rho_{max}^{\frac{3}{2}}$ is of the same order of magnitude as h (rather than h^2).

Five-point 'molecules' differing from that given in Fig.5 are needed for points in N[a] which involve the boundary. Points to the right of (a,0) on $j = 0$ do not have a point at the j-1 level, necessitating a different molecule, e.g. Fig. 6. Points to the left of (a,0) on $j = 1$ involve points on $j = 0$ for which $\theta = \pi$. The fact that $\theta = \pi$ means that each of the $f_i(\rho,\theta)$ in (6.8) are zero, and thus solutions to (6.9) cannot be found. A suggested alternative is given in Fig. 7. The first point on the right of (a,0) on $j = 0$ involves both the above problems and a suggested molecule is given in Fig. 8. The general form of the modified approximations allows for any combination of five neighbouring points provided $\theta \neq \pi$.
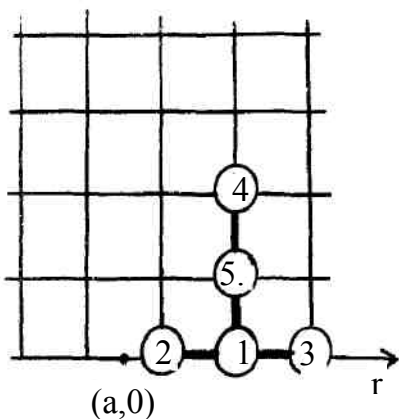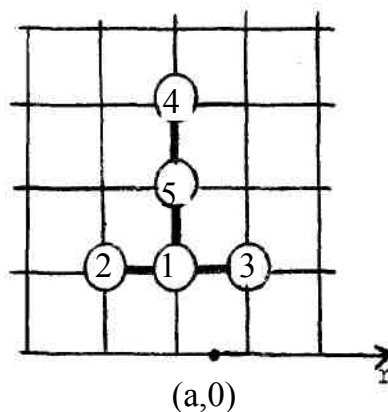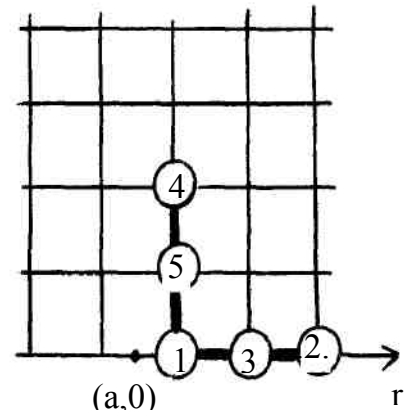

FIG. 6.   FIG. 7.   FIG. 8.

7. Calculation of Flux through Disc-Shaped Electrode

The flux Q given in (3.7) is calculated, using $\phi_{i+\frac{1}{2},i}$ values from (4.5) and (6.15), by a similar method to that of Evans and Gourlay (1976) who used a quadrature process of summing integrals of the form (3.7) over boxes in the narrow band $\{0 \leq r \leq a, 0 \leq z \leq \delta z\}$ in Fig. 9.
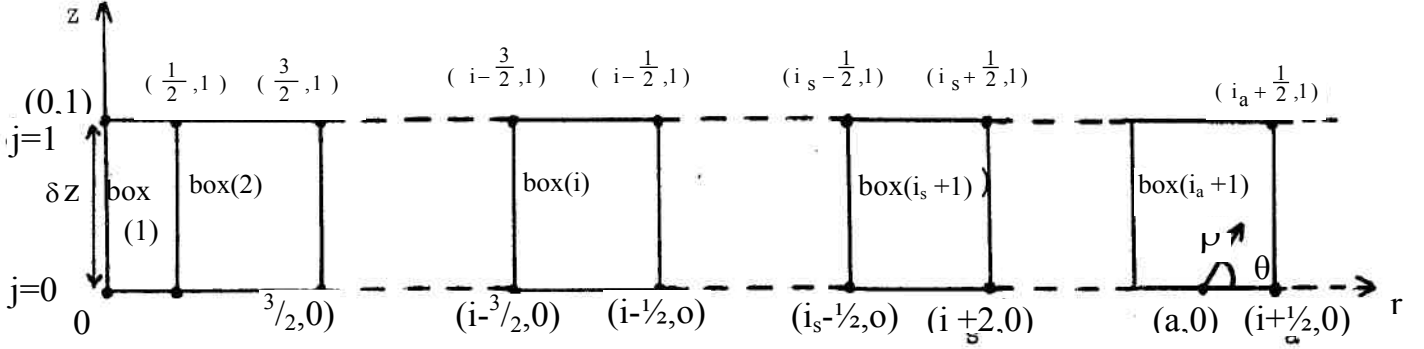

FIG. 9.   Region used for flux quadrature.

In Fig. 9, i_a denotes the value of i at r = a.   A standard quadrature process would give inaccurate results for boxes $(i_s+1, \ldots, i_a + 1)$ near the singularity and so special treatment is used for these boxes. Practical experience suggests that i_s should he chosen such that the line $i = i_s + \frac{1}{2}$ coincides with the boundary of N[a].

For boxes $(1, \ldots, i_s)$ away from the singularity a standard quadrature process is used.   Evans and Gourlay used the local interpolant

$$\phi^* = \alpha z + \beta rz + \gamma r + \delta \quad , \quad \alpha, \beta, \gamma, \delta \text{ constants}, \tag{7.1}$$

thus

$$\frac{\partial \phi^*}{\partial z} = \alpha + \beta r \quad , \tag{7.2}$$

and Q_i, the flux through box (i), is, from (3.7) with (7.2),

$$Q_i \approx 2\pi D \int_{box(i)} r(\alpha + \beta r)dr = 2\pi D \left[\frac{\alpha r^2}{2} + \frac{\beta r^3}{3} \right]_{box(i)} . \tag{7.3}$$

The constants in (7.1) are evaluated in terms of the four surrounding ø values for each box. This gives, remembering (3.2),

$$\alpha = \frac{1}{\delta z}\left[(i-\tfrac{1}{2})\phi^{*}_{i-\frac{3}{2},1} - (i-\tfrac{3}{2})\phi^{*}_{i-\frac{1}{2},1}\right] , \quad \beta = \frac{1}{\delta r \delta z}\left[\phi^{*}_{i-\frac{1}{2},1} - \phi^{*}_{i-\frac{3}{2},1}\right] ,$$

$$\gamma = 0 , \qquad \delta = 0 .$$

$$(7.4)$$

The ϕ^{*} values are obtained from the finite-difference approximations (4.5) and (6.15). For box (1), the limits of integration are $r = 0$ and $r = \frac{\delta r}{2}$, and

$$\alpha = \frac{1}{\delta z}\phi^{*}_{0,1} , \qquad \beta = \frac{2}{\delta r \delta z}\left[\phi^{*}_{\frac{1}{2},1} - \phi^{*}_{0,1}\right] ,$$

$$\gamma = 0 , \qquad \delta = 0 .$$

$$(7.5)$$

For boxes $(i_s +1, \ldots, i_a+1)$, the local interpolant must take into account the behaviour of the singularity. The most convenient interpolant to use is (6.1). From (5.2),

$$r\frac{\partial \phi}{\partial z} = r^{\frac{1}{2}}\frac{\partial u}{\partial z} , \qquad (7.6)$$

and so

$$r\frac{\partial \phi}{\partial z}\bigg|_{z=0} = (a-\rho)^{\frac{1}{2}}\left\{\frac{\partial u}{\partial \rho}\frac{\partial \rho}{\partial z} + \frac{\partial u}{\partial \theta}\frac{\partial \theta}{\partial z}\right\}\bigg|_{\theta = \pi} \qquad (7.7)$$

Approximations for $\frac{\partial u}{\partial \rho}$ and $\frac{\partial u}{\partial \theta}$ are obtained from the interpolant (6.1) to give, from (3.7) with (7.7),

$$Q_i \approx \pi D a^{\frac{1}{2}}\int_{\rho_{i-\frac{1}{2}}}^{\rho_{i-\frac{3}{2}}} (1-\rho/a)^{\frac{1}{2}}\left\{c_1\left[\rho^{-\frac{1}{2}} - \frac{\rho^{\frac{3}{2}}}{24a^2}\right] - 3c_2\rho^{\frac{1}{2}} + 5c_3\rho^{\frac{3}{2}}\right\}d\rho . \qquad (7.8)$$

Expanding (7.8), and integrating, gives

$$Q_i \approx 2\pi Da^{\frac{1}{2}}\left[c_1\rho^{\frac{1}{2}}\left(1 - \frac{\rho}{6a} - \frac{\rho^2}{30\,a^2}\right) + c_2\rho^{\frac{3}{2}}\left(\frac{3\rho}{10\,a} - 1\right) + c_3\rho^{\frac{5}{2}}\right]_{\rho_{i-\frac{1}{2}}}^{\rho_{i-\frac{3}{2}}}, \qquad (7.9)$$

for a typical box (i) for boxes (i_s +1, ..., i_a +1) near the singularity. Approximations for the c_i , i = 1, 2, 3, in (7.9) are found in terms of neighbouring ø values by using (6.8) and the ø values at the three points $(i-\frac{3}{2},1)$, $(i-\frac{1}{2},l)$, $(i+\frac{1}{2},l)$. For the last box, the three points $(i_a -\frac{1}{2},1)$, $(i_a+\frac{1}{2},l)$, $(i +\frac{1}{2},0)$ are used and the limits of integration in (1.9) are $\rho = 0$ and $\rho=\frac{\delta r}{2}$.

It should be noted that Evans and Gourlay chose the form of the singular interpolant to be

$$\phi^*(\rho,\theta) = c_1\rho^{\frac{1}{2}}\cos\frac{\theta}{2} + c_2\rho^{\frac{3}{2}}\cos\frac{3\theta}{2} + c_3\rho^{\frac{5}{2}}\cos\frac{5\theta}{2}, \qquad (7.10)$$

without any formal derivation. Comparison with (5.24) shows that this form is not strictly correct.

8. Numerical results

Referring to Table 1, the region ABCD was chosen for N[a] since this gave optimal improvement (here $\rho^{\frac{3}{2}}_{max.} \approx 0.1$ and h $= 0.1$).

The concentration (ø) values were calculated in the following three ways and are compared in Table 1:

   (I)   using the standard finite-difference scheme (4.5) throughout the region in Fig. 4,

   (II) using the standard finite-difference scheme (4.5) outside N[a] and the modified scheme (6.15) inside N[a] based on Figs. 6-8 where appropriate,

   (III)   using the exact forms (3.9) and (3.10).

The flux (Q) values were calculated in the following three ways and are compared in Table 2:

(IV)   using the ø values from (I) and the standard quadrature process
         (7.3) for all boxes in Fig. 9,

 (V)   using the ø values from (II) , the standard quadrature process
         (7.3) for boxes (1,   ..., i_s) arid the modified quadrature process
         (7.9) for boxes   (i_s +1,   ...,i_a+1),

(VI)   using the exact   form (3.12).

Both tables show that   a marked improvement   occurs   if modified treatments
(II)   and (V) are used rather than (I) and (IV).

9.   Time-Dependent Problems

The time-dependent   form of (1.1) is

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{k}{x} \frac{\partial \phi}{\partial x} + \frac{\partial^2 \phi}{\partial y^2} = \frac{\partial \phi}{\partial t} \ , \quad x \neq 0 \ , \quad t > 0 \ , \quad k > 0 \ \text{and known} . \tag{9.1}$$

Modified finite-difference approximations for problems of the   form (9.1) ,
with mixed boundary conditions such as (2.1), can be developed in a
similar way to the steady-state case.   Using the transformation (5.6)
on (9.1) gives the self-adjoint form

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{k}{2} (1 - \frac{k}{2}) \frac{u}{x^2} = \frac{\partial u}{\partial t} \ , \tag{9.2}$$

and, after converting (9.2) to polar co-ordinates centred on (a,0),
a truncated series solution can be   formed by seeking a solution of
th e   form

$$u(\rho,\theta, t) = T(t)R(\rho)\Theta(\theta) + \omega(\rho,\theta) \ , \tag{9.3}$$

where $\omega(\rho,\theta)$ represents the solution of the corresponding steady-state
problem.   Modified approximations can then be developed as before with
the unknown coefficients in the truncated series solution being found
in terms of neighbouring solution values at each time step, see Bell
and Crank (1973,1975).

TABLE 1

A comparison of solution (ø) values x 10³ :

$C_0 = 1.0$, $\delta r = \delta z = 0.1$, $r_L = 2.0$, $z_L = 1.1$, $a = 1.0$, $N[a] = ABCD$.

Each cell shows three values: Standard F.D. scheme (4.5) / Modified F.D. scheme (6.15) / Exact values from (3.9) and (3.10).

331 / 329 / 329	347 / 345 / 345	367 / 364 / 364	390 / 388 / —	418 / 415 / 415	444 / 445 / —	480 / 476 / —	512 / 507 / 508	541 / 538 / 538	569 / 566 / 566
278 / 275 / 275	294 / 291 / 291	315 / 312 / 312	342 / 338 / 338	374 / 369 / 370	412 / 406 / 407	451 / 445 / 445	488 / 483 / 483	523 / 518 / 519	554 / 550 / 551
217 / 215 / 215	233 / 230 / 230	254 / 251 / 251	283 / 279 / 280	322 / 316 / 317	370 / 362 / 363	419 / 411 / 412	465 / 458 / 458	506 / 500 / 500	541 / 537 / 537
150 / 148 / 148	163 / 161 / 160	182 / 179 / 179	211 / 207 / 207	256 / 250 / 251	322 / 310 / 312	387 / 375 / 377	443 / 434 / 435	490 / 483 / 484	530 / 525 / 526
77 / 76 / 76	84 / 83 / 83	97 / 95 / 94	119 / 115 / 115	163 / 159 / 159	269 / 248 / 250	357 / 342 / 344	426 / 415 / 417	480 / 472 / 473	523 / 517 / 518
				B	C	D	418 / 408 / 410	475 / 467 / 469	520 / 514 / 516
		A		224 / 196 / 197	341 / 327 / 329				
				(a,0)					

$$\frac{\partial \phi}{\partial z} = 0$$

$\phi = 0$

Standard F.D. scheme (4.5)	Modified F.D. scheme (6.15)
	Exact values from (3.9) and (3.10)

TABLE 2

Flux (Q) values for each-box in Fig. 9.

$C_0 = 1.0$, $\delta r = \delta z = 0\text{-}1$, $r_L = 2.0$, $z_L = 1.1$, $D = 1.0$, $a = 1.0$,

$N[a] = ABCD$ (see Table 1), $i_s = 8$.

Box	Standard F.D. (4.5) ϕ values and standard quadrature (7.3)	Modified F.D. (6.15) ϕ values and modified quadrature (7.9)	Exact values from (3.12)
1	0.005	0.005	0.005
2	0.040	0.040	0.040
3	0.082	0.082	0.082
4	0.127	0.126	0.126
5	0.176	0.175	0.175
6	0.234	0.231	0.231
7	0.305	0.301	0.301
8	0.399	0.392	0.394
9	0.543	0.541	0.539
10	0.798	0.856	0.858
11	1.361	1.243	1.249
Total	4.070	3.992	4.000
% Error	1-76	-0.20	

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