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NUMERICAL SIMULATION OF HIGH-ENERGY-ELECTRON
GENERATED FIELD IN DIELECTRICS OF VARIOUS GEOMETRIES

FINAL REPORT FOR
SUBCONTRACT NO. 4803709

Kane S. Yee, Principal Investigator

Department of Mathematics
Kansas State University
Manhattan, Kansas 66502

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INTRODUCTION

From June, 1979 to May 15, 1980 the following problems were addressed relating to the High-Energy-Election Generated Field in Dielectrics.

- A. The electric field in a finite cylindrical dielectric due to a high-energy-electron beam when the beam axis is the same as the cylindrical axis.
- B. Numerical scheme devised for calculating the electric field when the electron beam axis is not the same as the cylindrical axis.
- C. Further development of the electron-generated electric field in a concentric spherical geometry.

The documentation of the majority of the effort on these problems have been collected in two appendices, Appendix A and Appendix B, found at the end of this report.

High-Energy-Electron Generated Field in Dielectrics

It has been observed that the exposure of dielectrics to electron beams can produce electric field of sufficient magnitude to cause dielectric break-down. The present investigations will be directed to calculate the electric field intensity in dielectric under spherical and cylindrical geometries. In the spherical geometry the method of multiple images renders the full numerical calculation unnecessary whereas in a finite length cylindrical geometry the full numerical calculation seems to be inevitable. A description and results of the spherical geometry is presented in Appendix A and a more detail presentation of the finite cylinder geometry is given in Appendix B.

APPENDIX A

QUASI-STATIC ELECTRIC FIELD BUILD-UP BETWEEN
TWO SPHERICAL CONDUCTORS

(UCID 18236 By K. S. Yee and J. Kasher)

The results of this appendix has been documented in UCID 18236, June, 1979. Here we shall only quote the introduction of the report. Interested readers may obtain the lengthy document quoted above.

Prior to dielectric breakdown the illuminated region of the medium is rendered conducting by the electron beam. When the time interval of interest is large compared to the time needed for the electromagnetic signal to travel in the spatial dimension of interest, it is plausible that a quasi-static model, in which one neglects the magnetic field, will supply some useful information. We shall describe our problem in terms of the electric field and charge density. The most important contribution of this report is that in solving Poisson's equation for the electric field we employ the method of multiple image, thus avoiding the brute force full numerical solution of the partial differential equations.

APPENDIX B

NUMERICAL INTEGRATION OF THE QUASI-STATIC
APPROXIMATION TO MAXWELL'S EQUATIONS FOR
AN ELECTRON BEAM IN A FINITE CYLINDER

(K. S. Yee and J. Kasher)

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K. S. Yee,* J. Kasher**

1. Introduction and Summary

In some dielectric breakdown problems where the magnetic field is neglected one obtains a system of two partial differential equations. In this report we solve this system of equations in cylindrical geometry by using the finite difference method. A sample calculation will be presented.

2. Equations Describing the Model and the Resulting Finite Difference Equations

If we neglect the magnetic field the electric field due to an external charge deposition can be described by the following two differential equations:

$$\nabla^2 \phi = -\rho/\epsilon \quad (1)$$

$$\frac{\partial \rho}{\partial t} + \frac{\sigma}{\epsilon} \rho = \frac{\partial \rho_s}{\partial t} + \nabla \sigma \cdot \nabla \phi \quad (2)$$

where ρ_s, σ are known functions of position and time, and ϵ is a known constant.

The equations will be integrated inside a finite circular cylinder. We shall assume cylindrical symmetry with cylindrical coordinates r and z . The cylinder is described by the set

$$S = \{ (r, z) : 0 \leq r \leq R, 0 \leq z \leq L \} \quad (3)$$

The cylinder S is discretized by the partition (r_i, z_j) , where

*Department of Mathematics, Kansas State University, Manhattan, Kansas 66506

**Department of Physics, University of Nebraska at Omaha, Omaha, Nebraska 68182

$$r_1 = 0, \quad r_{i+1} = r_i + \Delta r_i; \quad i = 1, 2, 3, \dots, I-1 \quad (3a)$$

$$z_1 = 0, \quad z_{j+1} = z_j + \Delta z; \quad j = 1, 2, 3, \dots, J-1$$

The zoning in the r -direction may not be uniform, but the zoning in the z -direction will be. Written in cylindrical coordinates (1) becomes

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} = -\rho/\epsilon \quad (4)$$

The cylindrical axis is a mathematical singularity. A straightforward finite differencing may lead to difficulty. The following mathematical manipulation will avoid the mathematical singularity.

Figure 1. A volume element of integration

Shown in Figure 1 is a small cylinder whose center is located at $(0, z_0)$. The radius is a and the length is l . It occupies a volume V .

We integrate (1) over the volume V to get

$$\begin{aligned} - \int_V \frac{\rho}{\epsilon} dV &= \int_V \nabla \cdot (\nabla \phi) dV = \int_{\partial V} \frac{\partial \phi}{\partial n} dS \\ &= \int_{z_0 - l/2}^{z_0 + l/2} 2\pi a \left. \frac{\partial \phi}{\partial r} \right|_{r=a} dz + \int_{\partial V_T} \frac{\partial \phi}{\partial z} dS - \int_{\partial V_B} \frac{\partial \phi}{\partial z} dS \end{aligned} \quad (5)$$

where in (5) ∂V denotes the boundary of the volume, ∂V_T denotes the top of the cylinder and ∂V_B denotes the bottom of the cylinder. On the assumption that a and l are small (5) can be approximated by

$$-\frac{1}{\epsilon} 2\pi a^2 \rho \Big|_{r=0}^{r=a} = 2\pi a l \frac{\partial \phi}{\partial r} \Big|_{r=a} + \pi a^2 \left\{ \frac{\partial \phi}{\partial z} \Big|_{z=z_0} - \frac{\partial \phi}{\partial z} \Big|_{z=z_0 + l} \right\} \quad (6)$$

Equation (6) will be used later to derive an equation involving the values of ϕ on the axis of the cylinder.

2a. Finite Difference Equations Based on Constant Δr and constant Δz

In this section we shall write down the difference equations with constant Δr and constant Δz . With the usual notation $U(r_i, z_j) = U_{i,j}$; $r_i = (i-1)\Delta r$; and $z_j = (j-1)\Delta z$ we have:

$$\frac{1}{r_i \Delta r} \left\{ r_{i+\frac{1}{2}} \left(\frac{\partial \phi}{\partial r} \right)_{i+\frac{1}{2},j} - r_{i-\frac{1}{2}} \left(\frac{\partial \phi}{\partial r} \right)_{i-\frac{1}{2},j} \right\} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{(\Delta z)^2} = -\left(\frac{\rho}{\epsilon} \right)_{i,j}$$

Further approximation to the first derivatives on the above equations yields

$$\frac{1}{r_i \Delta r} \left\{ r_{i+\frac{1}{2}} \frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta r} - r_{i-\frac{1}{2}} \frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta r} \right\} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{(\Delta z)^2} = -\left(\frac{\rho}{\epsilon} \right)_{i,j}$$

The above equation is reduced to

$$\begin{aligned} & \frac{1}{(\Delta r)^2} \frac{r_{i-\frac{1}{2}}}{r_i} \phi_{i-1,j} - \frac{1}{(\Delta z)^2} \phi_{i,j-1} + 2 \left[\frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \right] \phi_{i,j} \\ & - \frac{1}{(\Delta r)^2} \frac{r_{i+\frac{1}{2}}}{r_i} \phi_{i+1,j} - \frac{1}{(\Delta z)^2} \phi_{i,j+1} = \frac{1}{\epsilon} \rho_{i,j}, \quad \begin{matrix} i = 2, \dots, I-1 \\ j = 2, \dots, J-1 \end{matrix} \end{aligned} \quad (7)$$

For another set of equations relating the values of ϕ on the cylindrical axis we use equation (6) with $a = r_{1,5}$, $l = \Delta z$, and $z_0 = z_j$ to get

$$-\frac{1}{2\epsilon} \rho_{1,j} = \frac{\phi_{2,j} - \phi_{1,j}}{r_{1,5} \Delta r} + \frac{\phi_{1,j+1} - 2\phi_{1,j} + \phi_{1,j-1}}{2(\Delta z)^2}$$

or

$$\begin{aligned} & -\frac{1}{2(\Delta z)^2} \phi_{1,j-1} + \left(\frac{1}{r_{1,5} \Delta r} + \frac{1}{(\Delta z)^2} \right) \phi_{1,j} \\ & - \frac{1}{2(\Delta z)^2} \phi_{1,j+1} - \frac{1}{r_{1,5} \Delta r} \phi_{2,j} = \frac{1}{2\epsilon} \rho_{1,j} \end{aligned} \quad (8)$$

$j = 2, 3, \dots, J-1$

Boundary conditions to be imposed for our problem are:

$$\begin{aligned}\phi_{I,j} &= 0 & j = 1, 2, \dots, J \\ \phi_{i,1} &= \phi_{i,J} = 0 & i = 1, 2, \dots, I\end{aligned}\quad (9)$$

Since the system of equations ((7), (8) together with (9)) constitutes a so-called diagonally-dominant, irreducible system, the sequential iteration method can be used to solve them.

We calculate ρ at the same grid points as ϕ . Specifically the charge density is advanced by the following equation:

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \frac{\sigma^n}{\epsilon} \rho^{n+1} = \left(\frac{\partial \rho_s}{\partial t} \right)^n + (\nabla \sigma \cdot \nabla \phi)^n$$

or

$$\rho^{n+1} = \frac{1}{1 + \frac{\sigma^n}{\epsilon} \Delta t} \left\{ \rho^n + \Delta t \left[\left(\frac{\partial \rho_s}{\partial t} \right)^n + (\nabla \sigma \cdot \nabla \phi)^n \right] \right\} \quad (10)$$

Along the cylindrical axis $\nabla \phi$ has only a z-component, as $\partial \phi / \partial r = 0$.

2b. Finite Difference Equations Based on a Nonconstant Δr but a constant Δz

Let $U(x)$ be a smooth function in the neighborhood of x . Let us define three constants A , B , and C as follows:

$$A = \frac{z}{\Delta x_1(\Delta x_1 + \Delta x_2)} \quad ; \quad B = \frac{-z}{\Delta x_1 \Delta x_2} \quad ; \quad C = \frac{z}{\Delta x_2(\Delta x_1 + \Delta x_2)}$$

It can be shown that

$$AU(-\Delta x_1) + BU(0) + CU(\Delta x_2) = U''(0) + O(\Delta x_1) + O(\Delta x_2) \quad (11)$$

Also if we define D , E , and F as follows

$$D = \frac{-\Delta x_2}{\Delta x_1(\Delta x_1 + \Delta x_2)} \quad ; \quad F = \frac{\Delta x_1}{\Delta x_2(\Delta x_1 + \Delta x_2)} \quad ; \quad E = -(F + D)$$

we will get

$$DU(-\Delta x_1) + EU(0) + FU(\Delta x_2) = U'(0) + O((\Delta x_1)^2) + O((\Delta x_2)^2) \quad (12)$$

To derive the difference equation at a grid point where Δr is not constant we first write (4) in the form

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = -\rho/\epsilon \quad (13)$$

Shown in Figure 2 is an r-z grid.

Figure 2. An r-z grid with nonuniform spacing

The grid points are defined as in (3a). Making use of the approximations in (11) and (12) we will difference (13) as follows:

$$A_i \phi_{i-1,j} + B_i \phi_{i,j} + C_i \phi_{i+1,j} + \frac{1}{r_i} (D_i \phi_{i-1,j} + E_i \phi_{i,j} + F_i \phi_{i+1,j}) + \left(\frac{1}{\Delta z}\right)^2 (\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}) = -\frac{1}{\epsilon} \rho_{i,j} \quad (14)$$

where

$$A_i = \frac{z}{\Delta r_{i-1} (\Delta r_{i-1} + \Delta r_i)} ; B_i = \frac{-z}{\Delta r_{i-1} \Delta r_i} ; C_i = \frac{z}{\Delta r_i (\Delta r_{i-1} + \Delta r_i)}$$

$$D_i = \frac{-\Delta r_i}{\Delta r_{i-1} (\Delta r_{i-1} + \Delta r_i)} ; E_i = \frac{1}{\Delta r_{i-1} + \Delta r_i} \left(\frac{\Delta r_i}{\Delta r_{i-1}} - \frac{\Delta r_{i-1}}{\Delta r_i} \right) ; F_i = \frac{\Delta r_{i-1}}{\Delta r_i (\Delta r_{i-1} + \Delta r_i)}$$

3. The Sequential Iterative Method for Solving the System of Linear Equations Derived in Section 2

The system of linear equations derived in section 2 can be cast in the following form:

$$\begin{aligned} AL(i)\phi_{i-1,j} + AD(i)\phi_{i,j-1} + \phi_{i,j} + AR(i)\phi_{i+1,j} \\ + AU(i)\phi_{i,j+1} = AS(i)q_{i,j} \end{aligned} \quad (15)$$

$$i = 1, 2, \dots, I-1; \quad j = 2, \dots, J-1$$

The sequential iterative scheme is

$$\begin{aligned} AL(i)\phi_{i-1,j}^{k+1} + AD(i)\phi_{i,j-1}^{k+1} + \phi_{i,j}^{k+1} + AR(i)\phi_{i+1,j}^k \\ + AU(i)\phi_{i,j+1}^k = AS(i)q_{i,j}^k \end{aligned} \quad (16)$$

$$i = 1, \dots, I-1; \quad j = 2, \dots, J-1$$

Experience has shown that convergence will be obtained if the number of iterations is approximately equal to twice the number of grid points, which is $I \times J$.

3a. The Coefficients of Equation (15) for Uniform Spacing

From (7) and (8) we get

$$AL(1) = 0, \quad AD(1) = AU(1) = \frac{-1}{2(\Delta z)^2} / \left(\frac{1}{r_{1,5}\Delta r} + \frac{1}{(\Delta z)^2} \right)$$

$$AR(1) = \frac{-1}{r_{1,5}\Delta r} / \left(\frac{1}{r_{1,5}\Delta r} + \frac{1}{(\Delta z)^2} \right)$$

$$AS(1) = \frac{1}{2\epsilon} / \left(\frac{1}{r_{1,5}\Delta r} + \frac{1}{(\Delta z)^2} \right)$$

$$AL(i) = \frac{-1}{2(\Delta r)^2} \frac{r_{i+\frac{1}{2}}}{r_i} / \left(\frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \right)$$

$$AD(i) = AU(i) = \frac{-1}{2(\Delta z)^2} / \left(\frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \right)$$

$$AR(i) = \frac{-1}{2(\Delta r)^2} \frac{r_{i+\frac{1}{2}}}{r_i} / \left(\frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \right)$$

$$AS(i) = \frac{1}{2\varepsilon} / \left(\frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \right) \quad i = 2, 3, \dots, I-1$$

3b. The Coefficients of Equation (15) for Nonuniform Spacing in the r-Direction

$AL(1)$, $AD(1)$, $AU(1)$, $AR(1)$, $AS(1)$ will be the same as in (3a) when we use Δr_1 for Δr . Define A_i , B_i , C_i , D_i , E_i , and F_i as in section 2. Then

$$AL(i) = \left(A_i + \frac{D_i}{r_i} \right) / \left(B_i + \frac{E_i}{r_i} - \frac{2}{(\Delta z)^2} \right)$$

$$AD(i) = AU(i) = \frac{1}{(\Delta z)^2} / \left(B_i + \frac{E_i}{r_i} - \frac{2}{(\Delta z)^2} \right)$$

$$AR(i) = \left(C_i + \frac{F_i}{r_i} \right) / \left(B_i + \frac{E_i}{r_i} - \frac{2}{(\Delta z)^2} \right)$$

$$AS(i) = -\frac{1}{\varepsilon} / \left(B_i + \frac{E_i}{r_i} - \frac{2}{(\Delta z)^2} \right)$$

$$i = 2, \dots, I-1$$

4. Explanation of the Code

Code CYL calculates r and z components of the electric field, as well as the absolute value of the electric field, caused by an electron beam passing through the z -axis of a dielectric cylinder grounded on its surface. Since there is symmetry in the azimuthal angle the problem is two-dimensional, depending only on r and z . The origin of the cylindrical coordinate system is at the center of the bottom of the cylinder, and the beam enters at the top and proceeds downward. If Sandy1 data is fed in, the beam is defined by these numbers. Otherwise provision is made for the beam to spread ($SIG0 > SIG1$) or remain constant in radius ($SIG0 = SIG1$); and it can be gaussian in the r -direction ($IGAUS = 1$) or of uniform charge density in the r -direction ($IGAUS = 0$).

If the non-Sandy1 beam spreads, charge is conserved by decreasing the charge density proportionally. The grid spacing in the r -direction (i.e., dr) can be constant ($IEQDR = 1$) or can be changed once ($IEQDR = 0$) at the radius of the electron beam (i.e., at $SIG1$), which is one standard deviation for a gaussian beam or simply the beam edge if the charge density is constant. If dr is to be changed once two approaches are possible. First, the number of r -zones within the beam can be set at $NR1 - 1$ ($I2NR1 = 0$, set $NR1$ to desired value); or the dr spacing within the beam can be set at half of dr outside the beam ($I2NR1 = 1$). This appears to be a reasonable ratio, judging from test calculations we have made.

At the start of the program the following data are initialized:

- IMX - number of r grid points
- JMX - number of z grid points ($(JMX-1)/4$ should be an integer)
- IGAUS - type of beam (gaussian or constant)
- RMX - radius of cylinder (in meters)
- ZMX - length of cylinder (in meters)
- SIG1 - beam radius at entry (one standard deviation)
- SIG0 - beam radius at exit (one standard deviation)

TT - life of beam (seconds)
 DOSMX - peak dose (calories/gram). Not used if Sandy1 data fed in.
 CONDMX - peak conductivity (mnos/meter - based on 40 nanosecond pulse. Adjusted automatically in the code if beam lasts longer or shorter. Not used if Sandy1 data is fed in.
 RHOMX - peak source charge density (coulombs/cubic meter - based on beam of one centimeter radius. Adjusted automatically to smaller or larger value if beam is wider or narrower. Not used if Sandy1 data is fed in.
 NR1 - number of r grid points within beam (should be odd)
 IEQDR - if = 1, dr does not change at edge of beam (if = 1, neutralizes NR1)
 TACCNM - number of time loops (defined in terms of accuracy)
 I2NR1 - if = 1, makes dr inside beam half of dr outside (replaces NR1 if = 1)
 IMEV - if = 500, runs a gaussian or constant beam for Sandy1 calculations at 500 MeV
 AKA - current strength of beam, in kilamps. This replaces CONDMX and RHOMX if Sandy1 values are written in.
 ISAND - if = 1, Sandy1 data for dose and charge are to be fed in.

After several constants are defined, the r and z grid points are set up, as shown in Figure 3.

The electron beam functions are then defined. There are three options here:

(1) The beam is a functional form that is explicitly defined. Currently the code can set up either a gaussian beam or one of constant density in the r-direction (the latter ends abruptly at the edge of the beam). Either of these can spread or remain of constant standard deviation or radius. With this option CONDMX and RHOMX are used as given in the data. The beam functions defined are the time derivative of the

source charge density, the conductivity, partial derivatives of the conductivity with respect to r and z , and the charge density that would hold after one time loop (this latter is needed because the charge density is not calculated in the time loop until after the field is defined). Finally, if the beam spreads, its standard deviation as a function of z is defined.

(2) The beam consists of 500 MeV electrons. This option models the total charge in each z level (as given by Sandy1 for 500 MeV) into either a gaussian or a constant-radius beam, and uses a conductivity that remains constant in the z -direction and is equivalent to a dose of one calorie/gram. CONDMX and RHOMX as given in the data are replaced by the proper values for 500 MeV.

(3) Values from Sandy1 calculations for dose (MeV/gram/source electron) and charge (electrons/cell/source electron) are fed in as input data. The code then calculates the corresponding conductivity and time derivative of the source charge density and interpolates to the grid used in CYL for that particular run. The rest of the electron beam functions are then appropriately defined.

Next the coefficients used in the finite difference equation for the potential are defined, followed by the initialization (all equal zero) of the potential and r and z components of the electric field. The running time of the code thus far is negligible -- on the order of a thousandth of a minute.

Finally comes the time loop, during which in sequence the potential is advanced, the r and z components of the field, as well as the absolute value of the total field, are calculated, and the charge density is advanced. As noted above, the surface of the cylinder is kept grounded throughout the calculations.

The flow chart shown in Figure 4 may help to clarify the code.

Figure 3. The grid used.

Figure 4. Flow chart for the program.

5. An Example -- A 500 MeV Electron Beam

A Sandyl calculation was run for a 500 MeV gaussian beam passing through a dielectric cylinder with thin metal plates on either end. The length of the cylinder was 5 centimeters, its radius 4 centimeters, and the beam width one centimeter. It turns out that a net positive charge was left in the cylinder in a region one centimeter thick (z-direction) near the side where the beam entered, and negative charge was deposited in the last centimeter on the other side. The region in the middle had very little charge. The dose, however, was nearly the same for a given radius all through the cylinder. That is, the dose did not diminish in the z-direction.

We modeled the total charge deposited as a function of z into both a gaussian beam of standard deviation one centimeter, and a beam of constant radial charge density of radius one centimeter. (The charge density in the latter case is twice that of the central density of the gaussian beam -- see Appendix II for proof.) No charge was placed in the middle region. We also fed the data from Sandyl directly into our code.

The maximum fields for the three cases were all on the z-axis of the cylinder on the side where the beam entered. They are:

constant model	--	73.2×10^6	volts/meter
gaussian model	--	38.3×10^6	volts/meter
direct data	--	26.5×10^6	volts/meter

Figures 5 through 7 show contour plots for the constant and gaussian models and the direct Sandyl data, respectively. Since the Sandyl beam itself was gaussian, it makes sense that its peak field is closer to the gaussian model. The differences in the contour plots for the Sandyl data and gaussian model can be attributed to statistical fluctuations in Sandyl results, particularly for the source charge density. This would seem to suggest that the Sandyl data should be

graphed and modeled first, then fed into the computer. A functional form, such as a gaussian, would not be necessary -- direct numerical data could be gotten from the graphs and put in. But at least the statistical fluctuations could be smoothed out, and the general pattern more accurately described.

Figure 5. Contour plot from the constant-beam model from the Sandyl data for 500 MeV. The maximum field is 73.2×10^6 volts/meter.

Figure 6. Contour plot from the gaussian-beam model from the Sandyl data for 500 MeV. The maximum field is 38.3×10^6 volts/meter. The peak charge density is only half that of the constant beam, since the charge is more spread out. This leads to the lower maximum electric field.

Figure 7. Contour plot from the actual Sandyl data for 500 MeV. The maximum field is 26.5×10^6 volts/meter. Since the incoming beam is gaussian, the maximum field is closer to the gaussian model (Figure 6).

APPENDIX I

Three-Dimensional Solution of Poisson's Equation
in a Finite Cylinder by Finite Difference

Poisson's equation in cylindrical coordinates is

$$\nabla^2 \phi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} + \frac{\partial^2 \phi}{\partial z^2} = -\frac{\rho}{\epsilon} \quad (1)$$

where (r, θ, z) are the cylindrical coordinates, ϕ is the potential, and ρ is the charge density. We wish to solve (1) in the finite cylinder $\mathcal{B}$

$$\mathcal{B} = \{ (r, \theta, z) : 0 \leq r \leq R; 0 \leq \theta \leq 2\pi; 0 \leq z \leq L \}$$

subject to the boundary condition

$$\phi = 0 \quad \text{on} \quad \partial \mathcal{B} \quad (2)$$

The difficulty involving the coordinate singularity in (1) can be removed by integrating over a small cylindrical volume shown in Figure 1.

Figure 1. A small cylindrical volume

$$-\int_V \frac{e}{\epsilon} dV = \int_V \nabla \cdot (\nabla \phi) dV = \int_{\partial V} \frac{\partial \phi}{\partial n} dS \quad (3)$$

$$= \int_{z_0 - \frac{\Delta}{2}}^{z_0 + \frac{\Delta}{2}} \int_0^{2\pi} \left. \frac{\partial \phi}{\partial r} \right|_{r=a} a \hat{a} \delta \hat{a} dz + \int_{\partial V_T} \frac{\partial \phi}{\partial z} dS - \int_{\partial V_B} \frac{\partial \phi}{\partial z} dS$$

where ∂V_T is the top of the cylinder and ∂V_B is the bottom of the cylinder. Equation (2) will be used to derive an approximate relation for the values of ϕ .

A. "Uniform" Zoning

Δr , $\Delta \theta$, and Δz are constant. We define

$$r_0 = 0, \quad r_{i+1} = r_i + \Delta r, \quad i = 0, \dots, I-1; \quad r_I = R$$

$$\theta_0 = 0, \quad \theta_{j+1} = \theta_j + \Delta \theta, \quad j = 0, \dots, J-1; \quad \theta_J = 2\pi$$

$$z_0 = 0, \quad z_{k+1} = z_k + \Delta z, \quad k = 0, \dots, K-1; \quad z_K = L$$

We can center difference (1) to get

$$\begin{aligned} & \frac{1}{r_i \Delta r} \left\{ r_{i+\frac{1}{2}} \frac{\phi(i+1, j, k) - \phi(i, j, k)}{\Delta r} - r_{i-\frac{1}{2}} \frac{\phi(i, j, k) - \phi(i-1, j, k)}{\Delta r} \right\} \\ & + \frac{1}{r_i \Delta \theta} \left[\phi(i, j+1, k) - 2\phi(i, j, k) + \phi(i, j-1, k) \right] + \frac{1}{r_i \Delta z} \left[\phi(i, j, k+1) - 2\phi(i, j, k) + \phi(i, j, k-1) \right] \\ & = -\frac{1}{\epsilon} \rho(i, j, k) \quad i=1, 2, \dots, I-1; \quad j=0, 1, \dots, J-1; \quad K=0, 1, \dots, K \end{aligned}$$

The above equation can be written as

$$\begin{aligned} & AE(i, j, k) \phi(i-1, j, k) + AW(i, j, k) \phi(i+1, j, k) + AS(i, j, k) \phi(i, j-1, k) \\ & + AN(i, j, k) \phi(i, j+1, k) + AD(i, j, k) \phi(i, j, k-1) \\ & + AU(i, j, k) \phi(i, j, k+1) + \phi(i, j, k) = AC(i, j, k) \rho(i, j, k) \end{aligned}$$

and we can derive the sequential scheme

$$\begin{aligned}
 & AE(i,j,k)\phi^{m+1}(i-1,j,k) + AW(i,j,k)\phi^m(i+1,j,k) \\
 & + AS(i,j,k)\phi^{m+1}(i,j-1,k) + AN(i,j,k)\phi^m(i,j,k+1) \\
 & + AD(i,j,k)\phi^{m+1}(i,j,k-1) + AU(i,j,k)\phi^m(i,j,k+1) \\
 & + \phi^{m+1}(i,j,k) = AC(i,j,k)\phi(i,j,k)
 \end{aligned} \tag{4}$$

where the coefficients in (4) are given as follows

$$DEN = - \left\{ \frac{1}{(\Delta r)^2} \left(\frac{r_{i+\frac{1}{2}}}{r_i} + \frac{r_{i-\frac{1}{2}}}{r_i} \right) + \frac{2}{r_i^2 (\Delta \theta)^2} + \frac{2}{(\Delta z)^2} \right\}^{-1}$$

$$AF(i,j,k) = DEN \left[\frac{1}{(\Delta r)^2} \frac{r_{i-\frac{1}{2}}}{r_i} \right]$$

$$AW(i,j,k) = DEN \left[\frac{1}{(\Delta r)^2} \frac{r_{i+\frac{1}{2}}}{r_i} \right]$$

$$AS(i,j,k) = DEN \left[\frac{1}{r_i^2 (\Delta \theta)^2} \right] = AN(i,j,k)$$

$$AD(i,j,k) = DEN \left[\frac{1}{(\Delta z)^2} \right] = AU(i,j,k)$$

$$AC(i,j,k) = -DEN/\epsilon$$

In actual iteration we write (4) as

$$\begin{aligned}
 \phi_{(i,j,k)}^{m+1} &= AC(i,j,k)\phi(i,j,k) - AE(i,j,k)\phi^{m+1}(i-1,j,k) \\
 &- AW(i,j,k)\phi^m(i+1,j,k) - AS(i,j,k)\phi^{m+1}(i,j-1,k) \\
 &- AN(i,j,k)\phi^m(i,j+1,k) - AD(i,j,k)\phi^{m+1}(i,j,k-1) \\
 &- AU(i,j,k)\phi^m(i,j,k+1)
 \end{aligned} \tag{5}$$

with

$$i = 1, 2, \dots, I-1; \quad j = 0, 1, \dots, J-1; \quad k = 1, 2, \dots, K-1$$

At the cylindrical axis (corresponding to indices $(0, j, k)$) we use

(3) with $a = r_{0,5} = 0.5\Delta r$ to get

$$-\frac{1}{\varepsilon} \rho(0, j, k) \pi \left(\frac{1}{2}\Delta r\right)^2 \Delta z = \frac{1}{2} \Delta r \Delta z \Delta \theta \frac{1}{\Delta r} \left[\sum_{j=0}^{J-1} \phi(1, j, k) - J \phi(0, j, k) \right] \\ + \pi \left(\frac{1}{2}\Delta r\right)^2 \frac{1}{\Delta z} \left[\phi(0, j, k+1) - 2 \phi(0, j, k) + \phi(0, j, k-1) \right]$$

The above equation will yield iterative equations

$$\phi^{m+1}(0, 0, k) = AC(0, 0, k) \phi(0, 0, k) - AW(0, 0, k) \sum_{j=0}^{J-1} \phi^m(1, j, k) \\ - AD(0, 0, k) \phi^{m+1}(0, 0, k-1) - AU(0, 0, k) \phi^m(0, 0, k+1) \quad (6)$$

$$\phi^{m+1}(0, j, k) = \phi^{m+1}(0, 0, k) \quad j = 1, 2, \dots, J-1$$

where the coefficients in (6) are calculated as follows:

$$D = - \left\{ \frac{1}{2} \Delta z (J \Delta \theta) + 2 \pi \left(\frac{1}{2}\Delta r\right)^2 \frac{1}{\Delta z} \right\}^{-1} = - \left\{ \pi \Delta z + \frac{1}{2} \pi (\Delta r)^2 \frac{1}{\Delta z} \right\}^{-1}$$

$$AC(0, 0, k) = -\frac{1}{\varepsilon} \frac{\pi}{4} (\Delta r)^2 \Delta z D$$

$$AW(0, 0, k) = \frac{1}{2} \Delta z \Delta \theta D$$

$$AD(0, 0, k) = \frac{\pi}{4} (\Delta r)^2 \frac{1}{\Delta z} D = AU(0, 0, k)$$

The iterative scheme defined by (5) and (6) ought to converge as the original system is diagonally dominant and irreducible.

B. Nonuniform Δr , $\Delta \theta$, but uniform Δz

The procedures will be entirely similar to that discussed in detail in section 2b. We are assuming here that the first two Δr will be the same.

APPENDIX II

Comparison of Charge Densities for Constant and Gaussian Beams
Containing the Same Total Charge

It is of interest to study both gaussian and constant beams, and often the same total charge is desired for each. In this section we compare a constant beam to a gaussian beam with standard deviation equal to the radius of the former. It turns out that the central charge density for the gaussian is only half that of the constant beam.

Since the charge is the same in both cases,

$$Q = \int_{z_1}^{z_2} \int_0^{2\pi} \int_0^R \rho_c r dr d\theta dz = \int_{z_1}^{z_2} \int_0^{2\pi} \int_0^\infty \rho_g \exp(-r^2/2R^2) r dr d\theta dz$$

$$(z_2 - z_1) 2\pi \rho_c R^2/2 = (z_2 - z_1) 2\pi \rho_g (-R^2) \left[\exp(-r^2/2R^2) \right]_0^\infty$$

$$(z_2 - z_1) 2\pi \rho_c R^2/2 = (z_2 - z_1) 2\pi \rho_g R^2$$

or $\rho_c = 2\rho_g$.

APPENDIX III

Derivation of the Expressions for Conductivity and Time Derivative
of the Source Charge Density, As Used When Reading Sandyl Data
Directly into the Code

A. Time Derivative of the Source Charge Density

Sandyl calculates electron/cell/course electron. In the code (subroutine BEAM) this is converted to electrons/cubic meter/source electron by dividing by the appropriate ΔV_i . Multiplying both numerator and denominator units by the number of electrons in a coulomb, then dividing both numerator and denominator by the length of the pulse, leads to the same number in amps/cubic meter/source current. Thus, multiplying the data from Sandyl (after converting to electrons/cubic meter/source electron) by the beam current gives the rate of charge deposition/cubic meter in the cylinder:

$$\dot{\rho}_{s_i} = IN_q/\Delta V_i$$

where I is the beam current and N_q is the direct data from Sandyl.

B. Conductivity

The conductivity can be expressed as follows:

$$\sigma = KD$$

where σ is the conductivity, K the conductivity constant (we used $K = 2 \times 10^{-17} \text{ mho/meter//rad/sec}^1$), and D the dose rate in rad/second, or some equivalent energy unit. In Sandyl the dose is given in Mev/gram/source electron, so we change K to units of mho/meter//Mev/g-sec). If N_e is the number of source electrons, N_d is the dose from Sandyl,

¹Richard C. Weingart, internal progress report, Lawrence Livermore Laboratory

and T is the duration of the beam, the equation becomes

$$\sigma = KN_e N_d / T$$

It is more convenient in the code to express N_e in terms of a fraction of the number of electrons in a one kilamp beam of duration 40 nano-seconds. This number is

$$\begin{aligned} N_1 &= IT = 10^3(\text{coul/sec})(4 \times 10^{-8} \text{sec})(1e/1.6 \times 10^{-19} \text{coul}) \\ &= 2.5 \times 10^{14} e \end{aligned}$$

Thus multiplying N_1 by the number of kilamps in the beam, I , gives N_e . Putting all the numbers together,

$$\begin{aligned} \sigma &= 2 \times 10^{-17} \omega\text{-s/m-rad}(1.6 \times 10^{-8} \text{rad/MeV/g})(2.5 \times 10^{14}) I N_d / T \\ \sigma &= (8 \times 10^{-11} I N_d / T) \text{mho/meter} \end{aligned}$$

APPENDIX IV

Accuracy Checks for the Code

A. The Time Integration

We tested the accuracy of the time integration by integrating for the case of constant conductivity the differential equation used to advance the charge density, and then comparing our results with the known analytical solution. The equation is

$$\frac{\partial \rho}{\partial t} + \frac{\sigma}{\epsilon} \rho = \frac{\partial \rho_s}{\partial t} + \nabla \sigma \cdot \nabla \phi \quad (1)$$

where ρ is the charge density, σ and ϵ are the conductivity and permittivity, respectively, $\partial \rho_s / \partial t (= \dot{\rho}_s)$ is the rate of charge deposition by the beam, and ϕ is the potential. If the conductivity is constant the gradient term drops; and for constant $\dot{\rho}_s$ the charge density integrates to

$$\rho = \frac{\epsilon}{\sigma} \dot{\rho}_s (1 - e^{-\frac{\sigma t}{\epsilon}}) \quad (2)$$

The charge is advanced in the time loop according to the equation

$$\frac{\rho_{n+1} - \rho_n}{\Delta t} + \frac{\sigma}{\epsilon} \rho_{n+1} = \dot{\rho}_s + (\nabla \sigma \cdot \nabla \phi)_n$$

or

$$\rho_{n+1} = [\rho_n + \Delta t (\dot{\rho}_s + (\nabla \sigma \cdot \nabla \phi)_n)] / (1 + \sigma \Delta t / \epsilon)$$

which becomes, for constant conductivity,

$$\rho_{n+1} = (\rho_n + \dot{\rho}_s \Delta t) / (1 + \sigma \Delta t / \epsilon) \quad (3)$$

For $\sigma \Delta t / \epsilon \ll 1$ (= TACCM in the code) ρ should be fairly

accurate. We ran off quite a number of different values for TACCNM, bypassing the loops that calculate the potential in order to save computing time (each run required less than 0.001 minutes). Table I lists the TACCNM, and the resulting accuracy (equation 3 compared with equation 2), and the number of time loops required (NTMX).

One thing to bear in mind is that in a true run of the code the conductivity will probably not be constant, and thus that the gradient term will not drop out of equation 3. This means that some of the error in calculating the potential would be propagated through the charge density calculation, and would lead to a larger error than we have found in our example. However, we think this possibility is minimized for two reasons. First, $\bar{\rho}_s$ will probably be considerably larger than $\nabla \sigma \cdot \nabla \phi$, and so will dominate the advance of the charge density. Second, in test calculations using different grid sizes we have found that potential calculations are uniformly either too high or too low, and not a combination of the two. Since the difference of successive potential values appears in the gradient, the error would tend to be subtracted out.

B. Comparison with a Known Function of r

Poisson's equation in cylindrical coordinates is

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \phi}{\partial r} \right) + \frac{\partial^2 \phi}{\partial z^2} = -\rho/\epsilon$$

For an infinitely long cylinder of constant charge density ρ_0 this reduces to

$$\frac{1}{r} \frac{d}{dr} \left(r \frac{d\phi}{dr} \right) = -\rho_0/\epsilon$$

If the cylinder is grounded on its surface, which is at radius R, the equation has the solution

$$\phi = \frac{\rho_0}{4\epsilon} (R^2 - r^2) \quad (4)$$

If we use the constant charge density ρ_0 throughout our finite cylinder, ground the outer surface, and define the above value for the potential on the top and bottom surfaces, our code should give us the corresponding value from equation 4 for each grid point in the interior of the cylinder. For a ten by ten grid our computed values were accurate past the fifth significant figure.

C. Variation of Grid Spacing for a One-Centimeter Gaussian Beam

We ran three different checks on the accuracy of the integration of Poisson's equation using a one-centimeter gaussian beam with peak source charge density and conductivity of 0.02 coulombs/cubic meter and 2×10^{-4} mho/meter, respectively.

(1) We used a cylinder 20 centimeters high of radius 10 centimeters, and tested various grid sizes from three z-zones by ten r-zones up to 60 x 60. Assuming the 60 x 60 grid to be the most accurate, a satisfactory compromise between running time and accuracy would seem to indicate a 40 x 20 grid. For these values the maximum field is off by less than one percent and the maximum potential varies by about three percent. Running time would be about thirteen minutes. See Table II.

(2) The code can use smaller r-zoning within the beam, and we found through various runs that twice as many r-zones per unit length within the beam gives stable results that appear to be sufficiently accurate.

(3) We tested various grid spacings for a cylinder that is five centimeters high with a four centimeter radius (see Table III). Clearly these cylinder parameters give extremely stable results. The maximum and minimum values for all those tested differ by only 1.5%. A 20 x 20 grid seems sufficient, and takes about 3.5 minutes to run with 150 time loops.

D. Variation of Grid Spacing for the 500 MeV Beam from Sandy1

We checked several grid spacings for the 500 MeV beam given by Sandy1. This beam is peculiar, in that there is a cluster of positive charge within the first centimeter on the side where the beam enters,

negative charge in the last centimeter on the other side, and very little charge in between. We found that for some reason the results were quite insensitive to the number of time loops used for this beam -- the difference in the maximum field between using an apparently quite coarse time integration of 4 loops and a very accurate one of 152 loops was only about 4%. Thus we were able to test a number of grid spacings by using 4 time loops (otherwise the running time would have been far too large). The results are shown in Table IV. Changing from 20 to 40 z-zones lowers the peak field by about 9% for both the 152 and 4 time loop runs. Changing from 20 to 40 r-zones at 40 z-zones makes no difference at all, and going from 40 x 40 to 60 x 40 reduce the peak field by only 3% more. Clearly, a 40 x 20 grid should be sufficient for 152 time loops (about 13 minutes running time), while a 20 x 20 grid would probably be accurate enough, and takes only about 3.5 minutes.

E. Recommendation for Grid Spacing and Number of Time Loops

Considering all the accuracy checks we made for different kinds of situations, we would recommend a 40z by 20r grid with 152 time loops to ensure sufficient accuracy (about 13 minutes running time), although in some cases a 20 x 20 grid would give a sufficiently close answer. The 40 x 20 x 152 run would require the following parameters:

IMX = 21

JMX = 41

TACCNM = 2.01E-03

<u>TACCNM</u>	<u>NTMX</u>	<u>% ERROR</u>
3.00×10^{-1}	1	57.4
1.00×10^{-1}	3	22.3
6.02×10^{-2}	5	13.8
3.01	10	7.1
1.00	30	2.4
6.02×10^{-3}	50	1.4
4.02	75	1.0
3.01	100	0.73
2.01	150	0.49
1.51	200	0.36
1.00	300	0.24
7.53×10^{-4}	400	0.19
5.02	600	0.12
3.76	800	0.09
3.01	1000	0.08

Table I. $\sigma \Delta t / \epsilon$ (= TACCNM), the number of time loops this leads to (NTMX), and the accuracy of the resulting charge density for the case of constant conductivity.

60	2.212 (0.045)	2.060 (0.15)	2.032 (0.34)	2.023 (0.59)	2.018 (0.91)	2.016
40	2.157 (0.022)	2.002 (0.074)	1.974 (0.16)	1.965 (0.27)	1.960 (0.41)	1.957 (0.59)
28	2.078 (0.013)	1.920 (0.038)	1.892 (0.078)	1.882	1.876 (0.21)	1.870 (0.29)
20	1.969 (0.0074)	1.809 (0.022)	1.780 (0.043)	1.767 (0.071)	1.757 (0.11)	1.744 (0.15)
12	1.733 (0.0043)	1.574 (0.0094)	1.541 (0.017)	1.514 (0.028)	1.484 (0.042)	1.450 (0.06)
$\uparrow$ z-zones r-zones $\rightarrow$	10	20	30	40	50	60

Table II. Peak field for various grid spacings for a one-centimeter gaussian beam in a cylinder of radius 10 centimeters and length 20 centimeters. (Peak source charge density = 0.02 coul/m^3 , peak conductivity = $2 \times 10^{-4} \text{ mho/meter}$) All values in 10^6 volts/meter. Running time (minutes) for one time loop is in parentheses.

60		1.4944	1.4926	1.4920		
40	1.5016	1.4923	1.4905	1.4899	1.4896	1.4894
20	1.4916	1.4818	1.4799	1.4793	1.4790	1.4788
↑ z-zones r-zones →	10	20	30	40	50	60

Table III. Peak field for various grid spacings for a one-centimeter gaussian beam in a cylinder of radius 4 centimeters and length 5 centimeters. (peak source charge density = 0.02 coul/m^3 , peak conductivity = $2 \times 10^{-4} \text{ mho/meter}$) All values in 10^6 volts/meter .

60			35.9×10^6 (g4) 68.9 (c4)
40		37.0×10^6 (g4) 71.0 (c4) 38.2 (g152) 33.2 (c152)	37.0 (g4) 70.9 (c4)
20		40.4 (g4) 77.0 (c4) 41.6 (g152) 79.3 (c152)	
12	40.6×10^6 (g4) 77.2 (c4) 41.8 (g152) 79.6 (c152)		
↑ z-zones r-zones →	12	20	40

Table IV. Values for the 500 MeV beam for gaussian (g) and constant (c) models. 4 and 152 refer to the number of time loops in the run.