A THREE DIMENSIONAL SIMULATION OF THE ION-DRIFT PROBLEM IN ELECTROSTATIC PRECIPITATORS USING AN ANALYTICAL FINITE ELEMENT APPROACH APPROPRIATE TO A WIDE VARIETY OF GEOMETRIES

Thesis submitted for the degree of Doctor of Philosophy at the University of Leicester

by

Kay Bromley
Department of Engineering
University of Leicester

June 1996
1. IMPROVING THE DESIGN OF ELECTROSTATIC PRECIPITATORS

1.1 What is an Electrostatic Precipitator?

1.2 Physical Processes Within Electrostatic Precipitators

1.2.1 Corona discharge and charge injection

1.2.1.1 Active and passive regions in the inter-electrode space

1.2.2 Particulate charging

1.2.2.1 Charging by ion-bombardment

1.2.2.2 Charging by ion-diffusion

1.2.3 Particle migration

1.2.4 Effects of particulate properties on precipitation

1.2.5 Back-ionisation

1.2.6 Effects of discharge electrode radius of curvature

1.2.7 The Townsend criterion

1.2.8 Paschen's Law

1.2.9 Charge injection laws

1.3 Role of the electric field in a precipitator

1.3.1 Current - voltage characteristics

1.4 Estimation of the Efficiency of an Electrostatic Precipitator

1.4.1 The Deutsch equation of precipitator efficiency

1.4.2 The effect of turbulent diffusion

1.5 Research Objectives

1.5.1 Industrial motivation

1.5.2 Possible Improvements in Electrode Design

1.5.3 Key Considerations

1.6 Scope of the model

1.6.1 Assumptions
1.6.2 Limitations ............................................................................................ 1-25

2. ELECTROSTATIC THEORY

2.1 Electric Field ......................................................................................... 2-1
2.2 Electric potential .................................................................................... 2-1
2.3 Equations for conduction in free space .................................................. 2-2
2.4 Mobility and velocity of charged species ................................................. 2-3
2.5 Ionic mobility .......................................................................................... 2-5
   2.5.1 Relationship between ion mobility and electric field ...................... 2-6
      2.5.1.1 Dynamic equilibrium ................................................................. 2-6
      2.5.1.2 High fields .............................................................................. 2-7
2.6 Current continuity .................................................................................... 2-8
2.7 The Deutsch approximation .................................................................. 2-9
   2.7.1 Criticisms and developments of the Deutsch approximation ............ 2-9

3. REVIEW OF PRECIPITATOR MODELLING

3.1 Introduction ............................................................................................ 3-1
3.2 General requirements ............................................................................. 3-3
3.3 Finite Difference Techniques .................................................................. 3-3
   3.3.1 Alotto, Gallimberti, Molinari and Repetto 1995 .............................. 3-4
3.4 Finite Element ........................................................................................ 3-5
   3.4.1 Janischewskyj and Gela 1979 .......................................................... 3-6
   3.4.2 Takuma, Ikeda and Kawamoto 1981 .............................................. 3-7
   3.4.3 Davis and Hoburg 1983. Hoburg and Davis 1985 ......................... 3-9
   3.4.4 Davies, Goldman, Goldman and Jones 1987 ................................. 3-10
   3.4.5 Levin and Hoburg 1988 ................................................................. 3-11
   3.4.6 Cristina and Feliziani 1989 ............................................................ 3-11
   3.4.7 Abdel-Salam and Al-Hamouz 1992 ................................................ 3-14
3.5 Charge Simulation Techniques ............................................................... 3-16
   3.5.1 Elmoursi and Castle 1984 and 1987, Elmoursi and Speck 1989 ........ 3-18
3.6 Combination Methods ............................................................................ 3-20
   3.6.1 Kallio and Stock 1985 .................................................................... 3-20
3.7 Other Methods ....................................................................................... 3-21
   3.7.1 Zamany 1995 ................................................................................. 3-22
3.8 Comparison of Standard Techniques .................................................... 3-22
5.3.2 Hardware ................................................................................................. 5-8
5.4 Design - high level .................................................................................... 5-9
  5.4.1 Principles of program design ................................................................. 5-9
  5.4.2 Consideration of Object Oriented Programming .................................. 5-10
  5.4.3 Flow chart for the iterative solution ...................................................... 5-11
5.5 Design - low level ..................................................................................... 5-13
  5.5.1 Reusable functions ................................................................................ 5-17
  5.5.2 Use of Global Variables ................................................................. 5-17
5.6 Implementation .......................................................................................... 5-18
  5.6.1 Development of Structure Diagrams .................................................. 5-18
  5.6.2 Imposition of boundary conditions ................................................... 5-18
    5.6.2.1 Implementation of the fixed field injection law ............................ 5-19
  5.6.3 Use of commercial software packages .............................................. 5-20
    5.6.3.1 Convert FEMGEM output into MATLAB data file format .......... 5-23
    5.6.3.2 Convert optimised C code in MATLAB function format ............ 5-24
5.7 Testing ........................................................................................................ 5-24
  5.7.1 Testing during coding ........................................................................... 5-24
  5.7.2 Checking the Laplace solution ............................................................ 5-25
  5.7.3 Checking the Poisson solution ............................................................ 5-26
  5.7.4 Comparison to analytical solutions ..................................................... 5-27
  5.7.5 Problems that were difficult to solve ................................................ 5-27
    5.7.5.1 The missing volume factor ......................................................... 5-27
    5.7.5.2 Right handed tetrahedra ............................................................ 5-29
  5.7.6 Typical run-time errors ....................................................................... 5-32
    5.7.6.1 Duplicate node numbers in an element ....................................... 5-32
    5.7.6.2 No coronating nodes .................................................................. 5-32
    5.7.6.3 Inconsistencies in defining node types ....................................... 5-32
6. IMPLEMENTATION OF 1D MODEL WITH FIELD DEPENDENT MOBILITY
  6.1 Variation of ion mobility with high electric field .................................... 6-1
  6.2 Derivation of the Galerkin Residual ....................................................... 6-4
  6.3 The Galerkin Residual with cylindrical symmetry .................................. 6-5
  6.4 Implementation of 1D field dependent mobility ..................................... 6-7
6.5 Structure of 1D Model........................................................................................................ 6-7
6.6 Testing of the 1D FDM Model.......................................................................................... 6-10
   6.6.1 Comparison to constant mobility model..................................................................... 6-10
6.7 Results from 1D Model..................................................................................................... 6-13
   6.7.1 Mobility independent of field.................................................................................. 6-15
   6.7.2 Comparison of increasing to decreasing mobility..................................................... 6-16
   6.7.3 Comparison of different increases in mobility............................................................. 6-19
   6.7.4 The effect of different zero field mobility values....................................................... 6-22
   6.7.5 Summary.................................................................................................................. 6-22
6.8 Considering other mobility-field relationships................................................................. 6-22
6.9 Conclusions..................................................................................................................... 6-24

7. THE 3D CONSTANT MOBILITY MODEL

7.1 Overview of the 3D model............................................................................................... 7-1
7.2 Potential and space charge approximation within an element......................................... 7-2
7.3 Design of MATLAB program to incorporate complex discharge electrode geometries.................................................................................................................. 7-4
7.4 Structure diagrams of the 3D model............................................................................... 7-8
   7.4.1 Structure diagrams for construction of disconnected matrix.................................. 7-11
7.5 Convergence.................................................................................................................... 7-15
7.6 Boundary Conditions...................................................................................................... 7-15
   7.6.1 Field magnitude and direction at the discharge electrode......................................... 7-16
   7.6.2 Space charge at the discharge electrode..................................................................... 7-17
   7.6.3 Symmetry boundary conditions.................................................................................. 7-17
   7.6.4 Cyclical boundary conditions.................................................................................... 7-17
7.7 Grid Generation............................................................................................................... 7-18
   7.7.1 Element definition...................................................................................................... 7-18
   7.7.2 FEMGEN.................................................................................................................. 7-18
   7.7.3 Convert grid of prisms to Tetrahedra.......................................................................... 7-18
   7.7.4 Grids designed by hand............................................................................................. 7-19
7.8 Data files to define the grid and it's properties................................................................. 7-19
7.9 Grid data input files......................................................................................................... 7-21
7.10 Improvements to the model.......................................................................................... 7-25
   7.10.1 Pre-processor.......................................................................................................... 7-26
8. RESULTS AND IMPROVEMENTS TO THE 3D MODEL

8.1 Introduction ........................................................................................................... 8-1
  8.1.1 Cyclical boundary conditions ........................................................................ 8-1
  8.1.2 Symmetric grid .............................................................................................. 8-1

8.2 Visualisation of the results .................................................................................. 8-1
  8.2.1 Post processor .............................................................................................. 8-2
  8.2.2 Output data file format ................................................................................. 8-2

8.3 Results for plane-plane geometry ....................................................................... 8-3
  8.3.1 Grid for testing ............................................................................................ 8-3
  8.3.2 Plane-plane geometry using only bulk elements ......................................... 8-4
  8.3.3 Plane and curved electrode elements .......................................................... 8-6
  8.3.4 Introduction of cyclical boundary conditions .............................................. 8-8

8.4 Results for Cylindrical geometry ....................................................................... 8-12
  8.4.1 Checking for symmetry ............................................................................... 8-12
  8.4.2 Effect of angle of grid on Laplace solution ............................................... 8-16
    8.4.2.1 Grid with 4 radial nodes, angle of $24^\circ$ ........................................ 8-18
    8.4.2.2 Grid with 4 radial nodes, angle of $8^\circ$ ........................................ 8-19
    8.4.2.3 Grid with 6 radial nodes, angle of $8^\circ$ ........................................ 8-20
    8.4.2.4 Summary .......................................................................................... 8-21
    8.4.2.5 Effect on space charge calculations ................................................. 8-22
    8.4.2.6 Non-convergence of iterative solution ........................................... 8-23

8.5 Comparison of the model's predictions to experimental data ............................ 8-23

8.6 Summary ............................................................................................................ 8-25

9. CONCLUSIONS AND FURTHER WORK

9.1 A model that can be adapted to include new features ....................................... 9-1
  9.1.1 Background dust ....................................................................................... 9-1
  9.1.2 Time varying potential ............................................................................. 9-2
  9.1.3 Field dependent mobility ......................................................................... 9-2

9.2 Detailed modelling of discharge electrode geometry ......................................... 9-3
  9.2.1 User interface .......................................................................................... 9-3
  9.2.2 Practical discharge electrodes ................................................................... 9-4
  9.2.3 Corona fluctuations ................................................................................. 9-4

9.3 Improved design technique for discharge electrodes ........................................ 9-5
  9.3.1 Limitations of the model and further work ............................................. 9-5
ACKNOWLEDGEMENTS

This research was carried out with the financial support of EPSRC, DTI and National Power PLC.

I sincerely thank Dr John Fothergill for his help and encouragement throughout this project. Also, John Houlgreave for many helpful discussions and I acknowledge his work on the mathematical background to the model.

I also thank Dave and my Mum and Dad for their support and confidence in me. Especially I thank Chris, Andrew and Jonathan for their patience whilst I have been rather ‘distracted’ by the writing of this thesis.
A computer simulation of the ion drift problem in air has been developed to predict the potential, electric field and space charge density in various geometries applicable to wire-duct electrostatic precipitators.

The development of the design of the model is explained and its implementation in a fourth generation language is described. The generality of the overall design allows new features to be included.

The model uses existing analytical expressions derived using the variational functionals for Poisson's equation and the Galerkin residual for current continuity which are solved iteratively. The resulting system of simultaneous equations are represented in a matrix formulation. Routines in the program: construct the matrices; set the boundary conditions; identify 'known' and 'unknown' node parameters; iteratively solve the system of equations; test for convergence and output the solution.

The Galerkin residual using a field dependent mobility has been derived and a one dimensional simulation for cylindrical geometry has been developed. Predictions are compared for linear relationships between field magnitude and ion mobility. The feasibility of extending this to other relationships is considered.

The design and implementation of a three dimensional model with constant mobility is described. The grid can be fitted to a variety of geometries, with plane and curved electrodes, using a functional for equipotential surfaces. No further adaptations to the model are required to make predictions for these different geometries. Charge injection is modelled using a fixed field injection law. Predictions for plane-plane and cylindrical geometries are compared to analytical solutions.

The need to improve the efficiency of the program is identified. Possible options to achieve this are discussed so that the model may be developed as a design tool for novel discharge electrodes in electrostatic precipitators.
DECLARATION

This thesis is submitted in fulfillment of the requirements for the degree of Doctor of Philosophy in the Department of Engineering, University of Leicester, UK. All work recorded in this thesis is original unless otherwise acknowledged in the text or by references. No part of it has been submitted for any other degree either to the University of Leicester or to any other university.

Kaye Brealey
1. IMPROVING THE DESIGN OF ELECTROSTATIC PRECIPITATORS

1.1 What is an Electrostatic Precipitator?

Electrostatic precipitators are devices for removing dust particles from gas flow. Their commercial operation is described in [46] and [48]. In particular, precipitators are used by power stations, cement works and other industrial units where a by-product of the process is dusty gas. A precipitator consists of high-voltage corona discharge electrodes suspended in ducts which act as earthed particulate collecting electrodes. The corona floods the inter-electrode gap with electrons which soon attach themselves to molecules which are thereby ionised. Gas-borne particles flowing past the discharge electrodes become charged through collision with the gas ions and "migrate" through electrostatic attraction towards the collecting electrodes where they adhere and lose their charge. The earthed electrodes are periodically mechanically rapped to detach the collected particles which fall mainly into hoppers below, although some become re-entrained into the gas flow.

![Figure 1-1 Schematic representation of a section of a wire-plate precipitator](image-url)
1.2 Physical Processes Within Electrostatic Precipitators
In this section the factors that are of particular importance in relation to the design of the discharge electrodes are described.

1.2.1 Corona discharge and charge injection
A unipolar corona discharge is produced when a sufficiently high DC voltage is applied to two electrodes, one of which has a small radius of curvature. A non-uniform electric field results. This causes an electrical discharge in a limited region near the sharp electrode that is known as the active region. If the voltage is further increased a threshold is reached above which sparkover between the electrodes occurs.

Electrical discharges in gases are complex, involving elastic and non-elastic collisions and resulting in excitation, ionisation, recombination, charge transfer and dissociation. [50] details these processes. An overview of the major processes within a precipitator is given here.

Just below sparkover voltage the electric field close to the sharp electrode is very high and exceeds the breakdown field of the gas. Any electron entering this region will be accelerated. The result is an electron avalanche initiated close to the point of the electrode. During this process light is also emitted and this can be seen as a glow around the sharp electrode, hence the name of corona. Accelerated electrons then inelastically collide with neutral gas molecules. These have sufficient energy to detach electrons from the molecules leaving positive ions and additional electrons. The additional electrons are accelerated in turn producing more ion-electron pairs. The heavier positive ions have a much shorter mean free path and do not contribute to the avalanche process. Some electrons attach themselves to molecules of the electro-negative gases that are present, producing negative ions. The process is self-sustaining as the electron-atom interactions also produce photons which excite further electrons to be emitted from the discharge electrode.
The conditions in which coronas arise and develop in ESPs vary according to:

- the pollutant contents of the gas
- the build up of deposits on the electrodes
- the continuing charging separation and collection of the particles.

These changes are spatially and time dependent. Theoretical investigations of current-voltage characteristics are based typically on two simplifying assumptions:

1. the part of the electric field induced by the surface charges on the electrodes can be found by solving Laplace's equation with appropriate boundary conditions
2. in any transversal cross section of the precipitator the space charge of the pollutant particles is uniform throughout this section.

When the high voltage is applied the ionisation is limited to a region very close to the electrode with small radius of curvature where the field is high. Only carriers which are expelled from this region are found in the inter-electrode space.

The ions are of similar size to the neutral molecules. When collisions occur momentum is transferred to the molecule and there is bulk movement of the neutral gas in the same direction as the ions. This movement is often referred to as ion wind. The field strength necessary to initiate a corona discharge is dependent on the field required to accelerate the electrons sufficiently to produce ionising collisions in the gas present.

Historically, theories have been developed to quantify the processes of corona discharge in uniform fields. In particular:

- Townsend's criteria for the avalanche of electrons, described in section 1.2.7,
- Pashen's law relating breakdown voltage to gas pressure and electrode spacing, described in section 1.2.8.
1.2.1.1 Active and passive regions in the inter-electrode space

Figure 1-2 shows the active region close to the discharge electrode. This region contains the electrons emitted by the electrode and accelerated by the applied field to produce an electron avalanche. In the passive region the field is not sufficiently high to sustain the avalanche and the main charge carriers are now the electronegative gas ions that have captured electrons escaping from the active region. The motion of the negatively charged particles towards the collection plate is superimposed on the turbulent motion of the gas. See section 1.4 which details the Deutsch efficiency equation and section 1.4.2 which describes the effects of turbulent diffusion.

\[
\begin{align*}
\text{e}^- &= \text{electron} \\
\text{i}^- &= \text{gas ion} \\
\text{d}^- &= \text{charged dust} \\
\text{d} &= \text{dust on the collecting plate}
\end{align*}
\]

**Figure 1-2  Schematic representation of active and passive regions in the inter-electrode space (not to scale)**

In electrostatic precipitators a unipolar negative corona discharge is used. This is obtained by applying a high negative DC voltage to a set of highly-curved electrodes, the discharge electrodes. The other electrodes have much lower curvature and are earthed, these are the collecting electrodes. For negative corona the emerging carriers are electrons.

The behaviour of the space charge close to the discharge electrode can be approximated by a charge injection law. In principle this charge injection law
can be calculated from the characteristics of the device. See section 1.2.9 for a review of charge injection laws and the use of the fixed field injection law in the model being constructed.

The curvature of the electrodes is also important in determining the emission characteristics. This is discussed in section 1.2.6.

1.2.2 Particulate charging

The gas-borne particulate in a precipitator is predominantly charged by collision with the negative ions in the passive region. When a collision occurs between an ion and a dust particle the charge on the ion causes a polarisation of the charge within the dust particle so that the ion is then attracted to and sticks onto one side of the particle. As the number of ions attached to the particle increases it becomes more difficult for further ions to become attached. Charging occurs by the combination of two processes:

1. ion-bombardment - a deterministic process whereby ions drift along field lines and impinge on any particles in their path
2. ion-diffusion - a stochastic process in which ions have a random thermal velocity component which can be high enough to overcome any repulsive potential that a particle may have.

Ion bombardment charging increases with current density and electric field, whereas ion diffusion charging increases with space charge density. Hence, increased current for the same field will give higher rates of particle charging. However, additional benefits with increased charging fall as currents get higher, and there also comes a point at which power dissipation becomes prohibitively high.

For smaller particles, diameter less than 0.2μm, ion diffusion charging dominates. For larger particles, diameter greater than 2μm ion bombardment dominates. For particle diameters between these both charging methods are significant. Very small particles, diameter less than 0.1μm, are difficult to collect as the average charge is less than that of one electron.
1.2.2.1 Charging by ion-bombardment

In the mono-ionised field due to a DC unipolar corona discharge, a saturation charge is reached when the attractive field due to the field distortion is equal to the repulsive field due to the charge on the particle. For the general case of conducting or insulating particles of radius \( a \), in an electric field \( E \), the saturation charge \( q_{\text{sat}} \) is given by, see [45]

\[
q_{\text{sat}} = a^2 p E
\]
\[
p = \frac{3\varepsilon_r}{(\varepsilon_r + 2)}
\]

where \( \varepsilon_r \) is the relative permittivity; \( p \) varies between 3 for a conducting particle and 1 for insulating particle.

This is the equation for ion bombardment charging in a unipolar field. It can be seen from this equation that the maximum charge on the particle is:

1. proportional to the electric field
2. proportional to the square of the particle radius
3. dependent on particle conductivity.

It is weakly dependent on the relative permittivity, but is independent of the density of the charging ions. The density of ions affects only the time taken to reach the maximum charge. Particle charging by ion bombardment is also referred to as field or Pauthenier charging.

1.2.2.2 Charging by ion-diffusion

Charging also takes place by ion diffusion. Diffusion charging arises from the collisions due to the random thermal motion of the ions in the gas. Using the kinetic theory of gases the charge acquired by a particle can be calculated, see [45] and [35].
By considering:

1. the density of ions
2. the repulsive energy between an ion and a dust particle
3. the number density \( N \) of ions that have sufficient energy to reach the particle
4. the mean ion speed
5. the cross-sectional area of the particle

the number of charges, \( n \), on the particle after time, \( t \), is shown to be:

\[
E_{q-2} \quad n = \frac{a k T}{e^2} \ln \left( \frac{\pi a N_0 e^2 u t}{k T} + 1 \right)
\]

where \( u \) is the kinetic theory mean ion speed, \( a \) is the radius of the particle, \( N_0 \) is the ion concentration, \( k \) is Boltzmann's constant, \( T \) is the temperature of the gas and \( e \) is the charge on an electron.

The accumulation of charge on the particle tends to repel ions and progressively reduces the charging rate.

1.2.3 Particle migration

Once charged, the particulate experiences a force due to the electric field. It therefore moves in such a way that this electrostatic force is balanced by a drag force, due to motion relative to the surrounding gas, and a diffusive force. The particulate will experience both turbulent and molecular diffusion, although the latter will only be significant for very small particles. On average, the charged particulate will move towards the earthed collecting plate, to which it adheres on impact.

The efficiency of particulate collection is highly dependent on the electric field in the vicinity of the earthed collecting plate. Good collection efficiency requires that this field be as high as possible.
1.2.4 Effects of particulate properties on precipitation
The Deutsch theory of precipitator efficiency, see section 1.4.1, coupled with simple (bombardment) charging theory under fixed field conditions predicts that only the particle radius and dielectric constant will affect particulate collectability, but practice shows that other properties have significant effects. This is to be expected since the theory is based on assumptions that are, at best, first order approximations. For example: non-ideal mixing and variable gas flow have significant effects on migration velocity, particle re-entrainment and 'sneakage' efficiency by changing the field and current distributions.

1.2.5 Back-ionisation
Deposits of a resistive dust on the electrodes reduces the collection efficiency at a given voltage by a mechanism known as back ionisation. It reduces the maximum voltage achievable before arcing.

Back-ionisation is the result of the electrical breakdown that can occur when a layer of high-resistivity dust is deposited on the earthed collecting electrode and this can cause a significant reduction in dust collection efficiency. The electric field, $E$, that builds up in the deposited layer of dust due to corona current flow can be estimated using Ohm's Law:

$$E = \frac{1}{\sigma} j$$

where $\sigma$ is the electrical conductivity of the dust layer and $j$ is the current density.

If this field gets large enough, the dust layer will suffer electrical breakdown. Positive ions and electrons will be created within the layer when an electrical discharge occurs through it and will be expelled back into the inter-electrode space. The electrons will move through the layer towards the collector and the positive ions will move through the inter-electrode space towards the discharge electrode. The travelling positive ions will discharge some of the charged dust particles, thereby reducing the efficiency of the precipitator. The increased
number of charge carriers result in a higher power dissipation and a greater likelihood of arcing between electrodes.

1.2.6 Effects of discharge electrode radius of curvature

It was shown semi-empirically by Peek in [51] that the field required for corona onset is given by

\[
E_{cor} = \delta \left( \frac{A}{r} + \frac{B}{(r \delta)^{1/2}} \right)
\]

where \(A\) and \(B\) are constant functions of the gas, \(r\) is the radius of the wire and \(\delta\) is the relative air density. The experiments were limited to densities of \(\delta \leq 1\).

\(A\) and \(B\) were determined for several geometries and are shown in Table 1-1.

<table>
<thead>
<tr>
<th>Geometry</th>
<th>A</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>concentric cylinders</td>
<td>31.0</td>
<td>0.308</td>
</tr>
<tr>
<td>adjacent cylinders</td>
<td>30.0</td>
<td>0.301</td>
</tr>
<tr>
<td>adjacent spheres</td>
<td>27.2</td>
<td>0.540</td>
</tr>
</tbody>
</table>

Table 1-1 Constants for Peek semi-empirical corona onset field

These constants were confirmed in [65] by reference to other experimental data, although the constants determined there for concentric cylinders were \(A=30.5\) and \(B=0.305\).

Equ. 1-4 has been generalised in [37] to obtain an expression for the corona onset field dependent on the local radius of curvature in two perpendicular directions and is given here:

\[
E_{cor} = A \left( 1 + \frac{B}{r} \right)
\]

where \(A = 3.0 \times 10^6\) V/m, the breakdown strength of a plane-plane electrode air gap, \(r\) is the mean radius of curvature, and \(B\) is characteristic mean radius of curvature.

When applied to parallel wires, concentric cylinders or adjacent spheres the expression approximates closely to the Peek expressions.
1.2.7 The Townsend criterion

This criterion for a self-sustaining discharge was formulated by Townsend in 1914, [64]. If $N_{e0}$ electrons with mobility $\mu_e$ are released in a gas in an electric field $E$ they will drift with a velocity $u = \mu_e E$. This drift will be along the electric field line. The electrons will collide with gas atoms and each electron will produce $\alpha$ new electron-ion pairs and suffer $\eta$ attachments per unit path length. $\alpha$ is the primary ionisation coefficient and $\eta$ is the attachment coefficient, both are functions of local field. Therefore, for uniform field the change in number of electrons in a path length $dl$ is

$$dN_e = N_e \left( \alpha - \eta \right) dl$$

which is integrated to give

$$N_e(l) = N_{e0} \exp \left( (\alpha - \eta)l \right)$$

$N_{e0}$ is the number of electrons initially released, therefore the number of new electron-ion pairs is:

$$N_{new} = N_e - N_{e0} = N_{e0} \left\{ \exp \left( (\alpha - \eta)l \right) - 1 \right\}$$

If the discharge is to be self-sustaining there must be a secondary process such as photoionisation which replaces the initial electrons. The secondary processes are combined in the secondary ionisation coefficient, $\gamma$, defined as the number of replacement electrons produced per ionising collision in the ionisation region.

The number of secondary electrons for $\eta \ll \alpha$ is given by

$$N_{\gamma e} = \gamma N_{e0} \left\{ \exp \left( (\alpha - \eta)l \right) - 1 \right\}$$
The Townsend criterion for the discharge to be self-sustaining is that there should be at least one secondary electron for every initial electron released, i.e.

\[ \gamma \left\{ \exp[(\alpha - \eta)\gamma] - 1 \right\} = 1 \]

The coefficients \( \alpha, \eta \) and \( \gamma \) as functions of the local field are reasonably well known for many gases. However the local field is non-uniform and is a function of space charge density therefore the conditions required for a self-sustaining discharge must be determined by analysis which for most situations will involve numerical techniques. Corrections also need to be made if the gas molecules are electron-attaching.

1.2.6 Paschen's Law

The breakdown voltage across a uniformly-stressed gap with metal electrodes was investigated experimentally by Paschen and is explained in [19]. Experiments were made using air, carbon dioxide and hydrogen. The breakdown voltage \( V_b \), in a uniform field gap was found to be governed by:

\[ V_b = f(pd) \]

where \( p \) is the gas pressure, \( d \) is the electrode spacing.

Provided that field enhancement effects are taken into account then this law can be verified by theory and by experiment, see [19]. To get ionisation by an electron the kinetic energy of the electron must be greater than the ionisation energy required by the molecule.

In an electrostatic precipitator the electrode spacing is too wide to be a limiting factor at normal pressures.

1.2.9 Charge injection laws

Budd and Hare 1992 [11] review the theories of charge injection. The bulk distribution of the field and the charge is governed by a single third order differential equation, known as the space charge equation. Microscopic behaviour of steadily glowing gas discharge has been studied to gain
information about the boundary conditions that apply. The behaviour is complex with charge carriers of opposite polarity to the coronating electrode having a significant effect near the electrode but not moving into the gas as a whole.

In sections 2.3 and 2.6 the equations that describe the physical processes for the bulk of the inter-electrode space are considered. These equations are not a good representation of charge motion close to the electrode because of the other physical effects.

In the coronating gas there is a thin region close to the electrode in which electrons, negative ions and positive ions act as charge carriers. These charge carriers result from both ionising collisions and photoelectric effects. The width of the corona is determined by the curvature of the electrode, the rate of ionisation in the gas, the thermal diffusion speed and the efficiency of the photoionisation process. Macroscopically the corona acts as a charge source, since the ions of the same polarity as the electrode leave the corona and drift into the gas.

It has been shown experimentally in [51] and theoretically in [64] that if the potential applied to the electrode is increased from zero then a corona first occurs close to the electrode when the field reaches a critical value $E_c$. $E_c$ is above the value $E_i$ where ionisation first occurs and is the lowest value of the field at which photo-ionisation is sufficient to maintain steady corona, i.e. at which Equ. 1-10 is satisfied. $E_c$ depends on the type of gas and the electrode geometry and is given by:

$$E_c = E_i \left( 1 + \left( \frac{0.7}{a} \right)^{1/2} \right)$$

where $\delta$ is the corona thickness and $a$ is the local radius of curvature of the electrode (m), (see [10] although this paper is primarily concerned with positive corona).

If the potential is increased further then, although the corona acts as the source of more charge, the field on the surface of the electrode remains close to $E_c$. 

$$E^*$$
This occurs because, if the field on the surface is greater than \( E_s \) then the ionisation processes in the corona are enhanced and a substantial amount of charge is created. This charge then drifts into the gas and the resulting field due to the space charge suppresses the surface field on the electrode below \( E_c \). This then reduces the ionisation so that less charge is produced and the surface field rises. Generally, in a gas, either an equilibrium field close in value to \( E_s \) is reached or the whole system oscillates, possibly in a chaotic manner, and Trichel pulses are generated. At higher voltages sparkover occurs.

A realistic injection law describing a steadily coronating gas is therefore a fixed field law:

\[
E|_{\Omega_a} = E_s
\]

In the Mott-Gurney approximation \( E_s \) is set to zero. Budd and Hare [11] state that this is only a reasonable approximation provided that the true \( E_s \) is much less than the harmonic field \( E_{hi} \), i.e. the solution of Laplace's equation, which would occur on the electrode surface in the absence of any space charge.

Alternative injection laws are respectively the constant charge and current specified laws:

\[
P|_{\Omega_a} = 0
\]

and

\[
\frac{d}{d\Omega_a} = B(E|_{\Omega_a})
\]

In their review [11] Budd and Hare use the concept of a current-surface-field characteristic. For a symmetric geometry, so that solutions may be exact, they deduce and plot the voltage-current characteristics resulting from each of the three charge injection laws.
The following conclusions are drawn.

1. For the field-limited injection law there is no current for small voltages. For voltages close to a critical value there is a small current and for large voltages the current varies as a quadratic function of the amount by which the voltage exceeds the critical value.

2. For the fixed charge injection law, at low voltage, the current is saturated and varies quadratically. For larger voltages it varies linearly.

3. For the approximate current injection law the current is saturated for both small and larger voltages, although behaviour at very small voltages is unclear.

These conclusions were drawn from calculations made for simple geometries. In extending to more general geometries, approximations must be made and the calculations become numerical. Principally the Deutsch approximation is used with the needle plane geometry to determine the characteristic curve and saturation current. The results closely resemble those obtained for the simple case.

Finally Budd and Hare consider the stability of the solutions of the space charge equations with different charge injection laws. The stability is investigated by considering a small perturbation to the steady state solution. It is shown that for either the constant field charge injection law or the constant charge model the space charge solution is stable to small perturbations. The stability of systems governed by the current specified injection law is less clear and may depend on the coefficients of the injection process.
1.3 Role of the electric field in a precipitator

The electric field consists of three components:

- $E_c$ - the field from the surface charges of the electrode (that is due to the high voltage),
- $E_j$ - the field induced by the ionic space charge,
- $E_p$ - the field set up by the charged gas-borne particulate.

$E_j$ and $E_p$ arise as a consequence of the impact ionisation of the gas molecules and the charging of the gas-borne particles respectively. Space charge due to electrons is typically negligible in a precipitator apart from in the active region close to discharge electrodes.

As the gas-borne particulate is gradually collected along the precipitator duct conditions change, and hence the field contributed by the ions and charged particulate also varies. The formation of layers of deposit on both the collecting and discharge electrodes and corrosion/erosion of the discharge electrodes also cause variations along the duct and over time.
Factors giving rise to variation along the duct include:

- monotonically diminishing concentration of dust particles
- alteration of particle size distribution along the duct
- gradual additional charging of the particles
- build up of deposit layers on the electrodes causing an extra voltage drop over the layer.

There are also variations with time for example:

- increasing layer thickness of deposit on collecting electrodes between rapping
- corrosion of the discharge electrodes
- variations in input burden, gas flow rate, pressure and temperature.

In cylindrical geometry the gas flow is along the discharge electrode whereas in wire-plate type precipitators the flow is across the wires. For modelling purposes, the latter electrode system can therefore be broken up into what may be considered as a system of repetitive modules. It can be seen that, in a parallel-plate precipitator, the electric field is subject to a periodic variation along the direction of the gas flow corresponding to the discharge electrode spacing.

The electric field is integral to three important mechanisms in electrostatic precipitation:

1. the charge injection process
2. the charging of gas-borne particulate
3. the migration of charged particulate towards the collecting plate.

Mechanism 1. requires a high non-uniform field; 2. is maximised by a current density distribution that prevents particulate from following a low-field path; whereas 3. is maximised by a uniform field.
1.3.1 Current - voltage characteristics

The mechanism by which the electrostatic precipitator removes the dust from the gas flow is the charging of this dust, known as the particulate, which is then attracted to the collecting electrode.

For efficient charging of the particulate the design of precipitator electrodes must ensure that corona discharge is well-distributed over the discharge electrodes. Figure 1-3 shows that in reality corona occurs as tufts, irregularly spaced over the electrode. The current density in a corona discharge is typically relatively low and can be described for a given electrode arrangement by its current-voltage characteristic. The characteristic begins at a critical initial voltage below which there is negligible current and terminates at the current and voltage just below sparkover. The shape of the characteristic depends on the
configuration of the electrode system, the gas, the type of voltage waveform and the charged particulate in the gas flow.

The VI curve represents the average current flow over the whole electrode, i.e. it is the sum of all the individual corona points as they change over time and over the surface of the electrode.

1.4 Estimation of the Efficiency of an Electrostatic Precipitator

The overall objective of the research project is to improve the efficiency of the collection process within the electrostatic precipitator especially by consideration of the discharge electrodes. It is therefore necessary to estimate the efficiency to test whether suggested alterations in design are likely to lead to improved collection rates.

1.4.1 The Deutsch equation of precipitator efficiency

A theory for the efficiency of precipitators with turbulent flow was developed by Deutsch in 1922.
An explanation of the Deutsch Equation is given in [26]. The Deutsch equation can be written to give efficiency, $\zeta$, in the form

$$\zeta = 1 - \exp\left(\frac{-AW}{Q}\right)$$

where $A$ is the collecting surface area, $W$ is the migration velocity and $Q$ is the volumetric flow rate.

Assumptions made in the derivation of Equ. 1-16 are given below:

- The particulate concentration across the precipitator cross section is assumed to be uniform. This implies infinite mixing by turbulent diffusion. In practice there is a relatively dust-free zone near the discharge electrode which broadens as the dusty gas moves through the precipitator.
- There is a uniform gas velocity in the precipitator, except near the boundary layer.
- $W$ is constant and small compared to the gas velocity.
- There is no particle reentrainment.

The Deutsch equation generally overstates the efficiency of full-scale precipitators. Despite the gas-borne particles in a precipitator having a distribution of sizes, the general form of Equ. 1-16 is obeyed; but the effective migration velocity $W$ is lower than expected and is dependent on the gas turbulence and the average gas velocity.

In practice, significant reentrainment does occur, commencing after only a few seconds of deposition onto a clean electrode. The reentrainment is mainly due to the friction of the particulates, rather than the friction of the gas molecules. The effects of turbulent diffusion are considered in section 1.4.2.
1.4.2 The effect of turbulent diffusion

The assumptions used in deriving the Deutsch efficiency equation are listed in the section 1.4.1. There is, however, experimental evidence, Rose & Wood [54], to suggest that in practice there is a concentration gradient in the cross section.

Feldman, Kumar and Cooper [26], give a table summarising the value of the coefficient of diffusion in several precipitation theories:

- for laminar boundary layer:
  1. infinite (or constant) coefficient of diffusion in the core, zero in the boundary layer
  2. diffusion not explicitly described in the core but falls to zero at the boundary

- for turbulent boundary layer:
  3. diffusion falls continuously to zero as the wall is approached
  4. diffusion is constant over the duct cross section.

In considering turbulent diffusion the uncollected dust inside the precipitator is mixed in two ways:

1. turbulent eddies in the gas system
2. turbulence caused by the electric wind.

Feldman, Kumar and Cooper [26] used a finite difference method to study diffusion theory using the particle flux factor, introduced by Cooperman [15]. They concluded that the particle flux factor characterises re-entrainment at the collecting plates. The particle flux factor is the ratio of particle flux due to diffusive forces to that due to electrical migration forces.

The Deutsch efficiency equation, based on diffusivity $D = \infty$, and the laminar flow model, $D = 0$, do not accurately represent the physical conditions present in the precipitator. For modelling purposes however, use of the Deutsch efficiency equation can be used for comparison purposes.
1.5 Research Objectives

The specific objectives of the project are to facilitate the improved design of electrostatic precipitator discharge electrodes by developing a technique whereby the effect on the potential, electric field and charge density in the interelectrode region can be modelled with a variety of discharge electrode geometries. A computer modelling capability for discharge electrodes is seen as a long term necessity. This may be incorporated into a more complete precipitator model later. The predictions from the model will be compared to analytical solutions and will predict a V-I curve for near-cylindrical geometry.

Construction of the model will result in greater understanding of the interaction of the electrical processes within the precipitator and new insight into the detailed effects of the discharge electrode geometry. This is particularly interesting for the design of novel electrodes to increase the collection of small particles - such particles are thought to pose a high risk of increased respiratory diseases such as asthma, and may therefore become the subject of stricter legislative control in the future.

1.5.1 Industrial motivation

Many plants in the UK need to reduce particulate emissions to meet new environmental legislation which requires that the amount of particulate exhausted to the atmosphere be strictly controlled. As concerns over health and the environment increase then the legislated requirements are becoming more stringent for example as stated in 1988 EC directive [1], which also specifies requirements for emission of SO$_2$ and NO$_x$.

Improving, in a cost-efficient way, the removal of suspended particles from gases is therefore of major scientific and technological interest. Typically an electrostatic precipitator will use up to 0.1% of the power station output. Any electrostatic research must take into account the requirements of the different mechanisms that are integral to the overall process, see section 1.2. In addition engineering constraints such as size, complexity, reliability and running costs must be allowed for. Historically, an optimisation approach was felt to be
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promising because of the conflicting requirements of the charging and collecting mechanisms underlying electrostatic precipitation, see [31] and [46].

To reach the very high efficiency required for existing plants, at a reasonable cost, it is preferable to modify by fitting improved components rather than full replacement. This is known as retrofitting.

This research programme originated with the premise that a way to improve electrostatic precipitator efficiency would be to find a systematic way of optimising electrode design such that the large-scale geometry enables a high collection field, whilst interaction between large and small scale geometry results in a well-distributed discharge that is not strong except at the highest applied voltages. The general aim is that electrodes should produce a reasonably uniform large scale field and low emission up to fairly high voltages. A comparatively rapid increase in emissions is required above the high critical voltage.

1.5.2 Possible Improvements in Electrode Design

The main techniques by which electrode designs could be improved are listed below.

- Ideas suggested by previous experience which can then be trialed on in-service precipitators. Whilst it is possible to be fairly sure that these ideas will work on the real system it is not practicable to try radically new solutions. It is also difficult to pass on the experience built up over many years and therefore this approach can be unsystematic.

- Development of a simple well instrumented laboratory analogue of a precipitator. This enables radical new solutions to be tried and accurate measurements taken. However it is generally not possible to accurately scale up to full size and without very large resources it is not possible to include conditions such as high gas temperature and rapping.
Use of full-scale test facilities. This is likely to give representative results provided it is well instrumented. Novel solutions can be trialed without risks although it may be time consuming to manufacture and fit the trial electrodes. Such a facility can be very costly to manage.

Development of a computer mathematical model describing the physical processes. In this case novel electrodes can be tried quickly and at low cost and insights may be gained as to why a particular solution is good or bad, although it may be beyond the scope of the simulation to model all possible electrode designs. As yet no sufficiently realistic computer simulation has been developed.

1.5.3 Key Considerations
The key considerations in the design of the discharge electrodes are:

- Sharp emission points produce strong corona which are useful for boosting particle charging near the gas inlet. Re-entrainment downstream of the inlet, particularly through rapping, makes it necessary to produce corona downstream, (re-entrainment also occurs continuously due to the gas flow, particularly if it contains a high concentration of particulates).

- A high collection field is of paramount importance. Flat plate high-voltage electrodes enable higher fields to be achieved within the duct thereby boosting migration velocities.

1.6 Scope of the model
A major part of the research project is the design, construction and use of a computer simulation of the electric potential, field and space charge between the discharge electrode and the collection electrode. Inclusion of the detail of the curvature of the discharge electrode will enable the effects of variations in the curvature to be studied, see section 1.2.6. Such a model would enable the effects of novel discharge electrode designs on the current density at the collection plate.
to be predicted. This will provide a new and significantly more useful and informative tool than previously published models.

A comprehensive literature review, see chapter 3, shows that existing 3D models do not model the detail of the discharge electrode geometry. Many use an ‘equivalent wire radius’ to represent a barbed or spiked electrode. This model will enable accurate modelling of such electrodes as cylindrical or square wires, twisted square wires and spiked electrodes. Many previous models use numerical techniques to solve the differential equations that govern the electrical processes within the precipitator. If these techniques are to be applied to a variety of discharge geometries the reworking of the model can be complicated and time consuming, eg [5]. An analytical formulation of an iterative procedure to solve the differential equations has been reported by Houlgreave, Bromley and Fothergill in [36], see Appendix C. This model makes use of the analytical formulation in such a way that data for different electrodes can be provided to the program and the potential, field and space charge can be predicted without any modifications to the underlying analytical expressions.

This is achieved by using the symbolic formulation of the Finite element Poisson variational functionals and Galerkin residuals described in [36]. See chapter 4 for a resume of the Finite Element method. For these functionals and residuals it is required to develop a technique whereby the construction of the matrices, the handling of the electrode geometries, the imposition of the boundary conditions can all be undertaken without the need for any further analytical derivations. This has been achieved by the building of a computer model, described in chapter 5, that requires the user to create only input data files relating to the geometry and properties of the electrodes and the finite element grid. The model is based on a series of functions that will handle the construction and manipulation of all the matrices required for Finite element analysis of the region. This is explained in detail in chapter 7.

The time taken to produce the prediction is dependent on the accuracy required and the hardware limitations of the chosen computer platform.
1.6.1 Assumptions

In the symbolic formulation [36] it has been assumed that the electron mobility at any point is independent of the electric field at that point. For the implementation of the 3D model, described in chapter 7, this assumption has been maintained. For the 1D model described in chapter 6, a linear representation of the relationship between field magnitude and mobility has been incorporated and the current continuity Galerkin residual has been rederived. This illustrates that new functionals or residuals could be used in conjunction with the matrix handling method described here without material alterations.

1.6.2 Limitations

Although the model uses the underlying symbolic formulation described in [36] this formulation was itself in the development stage whilst the model was being constructed. It was therefore a requirement that the model design be such that new symbolic forms of the functionals and residuals could be incorporated at any stage, see section 5.2. The has led to the model design being 'inelegant' in some aspects and some of the computation could be arranged to be more efficient.

As more complex discharge electrode geometries are modelled the run-time becomes prohibitive. This is mainly due to the memory limitations of running under Windows 3.1. Whilst the memory management is handled transparently within MATLAB it requires the setting of a large, 80 Mbyte, swap file and computing time is used in transferring variables in RAM into virtual memory. This memory limitation would not be so severe on a workstation running under UNIX and the run-time would be reduced, even without a faster processor.

The input of grid data and node properties is via 12 input data files, described in section 7.8. This is not a ‘user-friendly’ method of data input and has arisen because the model has been developed as a prototype, rather than a piece of user software, and the input requirements have evolved throughout the construction of the model.
The output data is recorded in a text file and simple plots are given using MATLAB. For visual representation of the predictions further processing would be required to import the data to a graphics package.

A pre and post processing package could be developed that would not require alteration to the main functions of the model. This is considered in sections 7.10.1 and 8.2.1.
2. ELECTROSTATIC THEORY

The charged particles (electrons, ions and dust) within the electrostatic precipitator are moving under the influence of the electric field. The velocities are low enough for the magnetic effects to be ignored however, 'quasi-electrostatic' is a more appropriate description than electrostatic, although it is the electrostatic equations that govern the electrical properties within the duct.

2.1 Electric Field

The electric field between the discharge electrode and the collection electrode of the precipitator arises from the superposition of two electric fields:

■ The field due to the charge on the surface of the electrodes
■ The field due to the space charge moving between the plates.

The Electric field strength, $E$, measured in volts per metre, at a given point, is the force per unit charge at that point [53].

An electric field, $E$, must satisfy:

$$\int E \cdot ds = 0$$

Equ. 2-1

this shows that an electric field cannot do any resultant work on a charge moving around a complete circuit, i.e. an electric field cannot sustain a steady current. To achieve a steady current an electromotiveforce is needed.

2.2 Electric potential

The electrical potential is the work required to bring unit positive electric charge from infinity to the point, [53]. It is measured in volts.

The electric potential at a point $A$ is given by:

$$\varphi_A = -\int_A E \cdot d\tau$$

Equ. 2-2

for any path from infinity to $A$. 

2-1
The electric field at $A$ can be found using the gradient of the potential at $A$:

$$\text{Equ. 2-3} \quad E_{A} = \left(-\frac{d\Phi}{dn}\right)_{A} = -\vec{\nabla}\Phi|_{A}$$

where $n$ is normal to the equipotential surface at $A$.

### 2.3 Equations for conduction in free space.

The conditions in the inter-electrode space can be investigated by considering the quasi-electrostatic equations for negligible magnetic effects. For a general case, the electric field must satisfy the following equations together with appropriate boundary conditions:

**Equ. 2-4**

$$\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_{0}}$$

**Equ. 2-5**

$$\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t}$$

where the right-hand side of Equ. 2-5 equals zero in steady-state conditions,

**Equ. 2-6**

$$\vec{E} = -\nabla \Phi$$

**Equ. 2-7**

and $\vec{J} = \sigma \vec{E} + \rho \vec{v} - \kappa \nabla \rho$

where $\kappa$ is the diffusivity coefficient and $\vec{v}$ is the gas flow velocity.

In general the current density, $\vec{J}$, is the sum of the current densities of electrons, positive ions, negative ions and the charged particulate. In addition the current density includes, not only the transport of these charged species under the action of the electric field, but also their movement due to the turbulent gas flow. Similarly, the space charge density, $\rho$, and the conductivity, $\sigma$, are due to the combined effect of the charged species listed above.
Therefore:

Equ. 2-8 \[ \sigma = \sum_s \mu_s \rho_s \]

Equ. 2-9 \[ \rho = \sum_s \rho_s \]

where the sums are taken over all the charged species, s, present. \( \mu_s \) is the mobility.

Equ. 2-5 may be written as

Equ. 2-10 \[ \nabla \left( j + \frac{\partial D}{\partial t} \right) = 0 \]

where the electric displacement \( D = \varepsilon_0 E \); \( j \) is the conduction current density; \( \frac{\partial D}{\partial t} \) is the displacement current density; their sum is the total current density.

Combining Equations Equ. 2-4 and Equ. 2-6 we obtain Poisson’s equation:

Equ. 2-11 \[ \nabla^2 \varphi = \frac{-\rho}{\varepsilon} \]

This equation is often considered as the first fundamental equation in the modelling of the inter-electrode conditions.

If there were no space charge, i.e. \( \rho = 0 \), then

Equ. 2-12 \[ \nabla^2 \varphi = 0 \]

which is Laplace’s equation.

2.4 Mobility and velocity of charged species

The mobility of a charged species is a direct measure of its ability to move in an electric field. In general, the mobility of the gas-borne charged particulate is influenced by individual particle charge, size and shape. Gas-borne charged sub-micron particulate travels relatively slowly in an electric field due to viscous
effects, and will often be influenced more by gas flow than by electrostatic forces.

To consider the mobility Ohm's Law in vector form may be written as:

Equ. 2-13  \[ i = \sigma E \]

where \( \sigma \) is the conductivity at a point.

Equ. 2-14  \[ i = \sum_s n_s q_s \nu_s \]

gives current density in terms of its constituent parts; where there are \( n_s \) members of charged species \( s \) per unit volume, each with charge \( q_s \) and velocity \( \nu_s \). Assuming all current flow is due to the electric field, if the carriers of current in a conductor all possess a single electronic charge \( e \) and the same velocity, this is the average velocity (the drift velocity), and if it is in the direction of the electric field, then

Equ. 2-15  \[ \sigma = \frac{i}{E} = \frac{nev}{E} \]

The drift velocity per unit electric field, \( \frac{\nu}{E} \) is known as the mobility, \( \mu \). Using the definition

Equ. 2-16  \[ \mu(E) = \frac{\nu}{E} \]

Therefore \( \sigma = ne\mu \) or, if more than one carrier exists

Equ. 2-17  \[ \sigma = \sum_s n_s e_s \mu_s \]

Within the precipitator the mobilities, \( \mu_s \), include the mobilities of all the charged particles: the electrons, the ions, and the charged gas-borne particulate.
2.5 Ionic mobility

The theory of ionic mobility is explained in various books on electrical discharge in gases, e.g. Samaras, [56]. The ion moves through the gas under the influence of the electric field. It will collide with uncharged particles and lose some of its kinetic energy, but can be considered as having a mean velocity. If the following assumptions are made:

1. the ions have the same thermal velocities as the uncharged particles
2. the drift velocity is much smaller than the thermal speed
3. after a collision the ion has zero velocity
4. the ion concentration is small and the pressure is low
5. the presence of electrons has no effect on the motion of the ions,

then ionic mobility is the constant of proportionality between the mean drift velocity and the electric field:

\[ \mu = \frac{v_d}{E} \]

To find \( \tau \) the time between collisions, \( \lambda \), the thermal velocity of the ions, \( u \), the mean free path, \( \lambda \), and \( \eta \), the charge over mass ratio of the ion, must be considered. The force acting on the ion between two collisions is due only to the electric field, if the electric field is uniform then the mean velocity of the ion is given by:

\[ v_d = \frac{1}{2} \left( \frac{\eta \lambda}{u} \right) E \]

which leads to:

\[ \mu = \frac{\eta \lambda}{u} = \eta \tau \]
Making similar assumptions, and calculating the ‘distance distribution’ of $\lambda$, Cobine, [14], obtains the expression:

\[ \mu = \frac{e\lambda}{mc} \]

Equ. 2-21

where $c$ is the average thermal velocity of the gas particles. It is assumed that the charge on the ion is $e$.

These expressions depend on the assumptions outlined above. Experimental measurements of mobility can show variations of up to 5 times the calculated value, [56]. Chapter 3 shows that many previous models do not consider the relationship between mobility and field strength. The feasibility of incorporating field dependent mobility of ions into the present model is considered in chapter 6.

2.5.1 Relationship between ion mobility and electric field

Experimental data for $\mu$ is usually given in terms of $\frac{E}{p}$, where $p$ is the gas pressure. At a constant temperature $\frac{E}{p}$ is the essential parameter in controlling the energy acquired by an ion between collisions. Loeb, [44], states that $\mu$ is independent of field strength for $E$ up to 1600 kV/m or $\frac{E}{p}$ up to 2 MV/m².

2.5.1.1 Dynamic equilibrium

Dynamic equilibrium occurs when the thermal speed is much greater than the drift velocity, so that the mean time between collisions, $\tau$, does not change with field. The motion of the ion is analogous with the motion of electrons in a crystal lattice. This is known as ohmic conduction, see [19]. It is assumed that the electrons are moving randomly due to thermal energy. The probability of a collision in time $dt$ is $\frac{dt}{\tau}$.
The total momentum of \( n \) electrons, of mass \( m \), is the sum of the momentum of each individual electron. Therefore the average drift velocity is:

\[
\text{Equ. 2-22} \quad V = \frac{P_{\text{tot}}}{nm} = \frac{v_1 + v_2 + \ldots + v_n}{n}
\]

The electric field accelerates the electrons, and if it were not for the collision, the momentum would increase in time \( dt \), as:

\[
\text{Equ. 2-23} \quad dP_{\text{tot}} = -neEdt
\]

The decrease in momentum, due to the collisions, in \( dt \), is given by:

\[
\text{Equ. 2-24} \quad dP_{\text{tot}} = -P_{\text{tot}} \frac{dt}{\tau}
\]

Equating Equ. 2-23 and Equ. 2-24 gives

\[
\text{Equ. 2-25} \quad P_{\text{tot}} = -neE\tau
\]

i.e.

\[
\text{Equ. 2-26} \quad v_{\text{drift}} = -\frac{e}{m}E\tau
\]

therefore

\[
\text{Equ. 2-27} \quad \mu = \text{constant} = \frac{e\tau}{m}
\]

which is the same as Equ. 2-20. For ions in air, since \( \tau \propto \frac{1}{p} \), where \( p \) is the gas pressure, then \( \mu \) is constant for constant pressure.

### 2.5.1.2 High fields

At high fields the drift velocity is much greater than the thermal speed. In this case the motion of the ion is analogous to the motion of a charged oil drop moving under gravity and an applied electric field; Millikan's oil drop experiment, see [21]. When the oil drop reaches its terminal velocity,
electric force equals the force due to the weight of the drop. Therefore the equivalent Stokes equation for an ion is:

\[ eE = \rho v^2 C \]

where \( \rho \) is the density of the gas and \( C \) is a constant. By definition \( \mu = \frac{v_d}{E} \), so that:

\[ \mu = \frac{2e}{\sqrt{pEC}} \]

Therefore at high fields ion mobility and field strength are related by

\[ \mu \propto \frac{1}{\sqrt{E}} \]

**2.6 Current continuity**

The general property of current continuity follows from the principle of conservation of charge. The outward current over a closed surface \( S \) for steady conditions and zero charge source enclosed by the surface can be written as:

\[ \oint j \cdot dS = 0 \]

However if the currents vary then:

\[ \oint j \cdot dS = -\frac{dQ}{dt} \]

where \( Q \) is the charge enclosed by \( S \) at time \( t \).

This can be converted to apply at a point and becomes the charge continuity equation:

\[ \nabla \cdot j = -\frac{\partial Q}{\partial t} \]

This is the second fundamental equation in modelling inter-electrode conditions with corona discharge.
2.7 The Deutsch approximation

Deutsch 1933 made the assumption that for unipolar ion fluxes, the space charge affects the magnitude of the electric field, but not its direction, this is considered in [34]. A number of researchers have shown that the Deutsch approximation is inaccurate apart from cases of spherical or cylindrical symmetry, or where space charge density is very low.

2.7.1 Criticisms and developments of the Deutsch approximation

Hoburg and Davies, [34], have tested the validity of the Deutsch approximation by use of a modelling technique based on finite elements and the method of characteristics. Their model does not use the Deutsch approximation. The shape of field lines for a HVDC transmission line are plotted and compared with the field using the Deutsch approximation. This and other calculations show that the Deutsch equation is a very rough approximation. It will only give reasonable results in fortuitous cases such as with cylindrical electrode symmetry. This indicates that precipitator models that have used this approximation are seriously limited in their accuracy. This is supported by Elmoursi and Castle, [22] and [24].

The use of the approximations and assumptions in models of the electrical processes within an electrostatic precipitator are considered in further detail in chapter 3.
3. REVIEW OF PRECIPITATOR MODELLING

3.1 Introduction

One of the uses of models of electrostatic precipitators is the prediction of the efficiency. Models may attempt to consider the many physical processes involved in the full precipitation operation to help in the development of understanding of the processes involved and their interaction with each other. Performance, however, depends on many factors, for example the precipitator design and the properties of the particulate. Many models concentrate on a particular aspect of the whole. A major factor in the efficiency is the charging and collection of dust particulate, which is governed by the electric field. This review focuses on the prediction of the electric field between the emitting discharge electrode and collection plate. The advantages of computer modelling over trial and error, use of laboratory rig and test rigs have been discussed in section 1.5.2.

Baker and Smith, [6], review the development of physical models. In the area of electric field modelling the first publications were primarily concerned with the point-plane geometry of a needle-point discharge electrode and a plane earthed, collection plate. In some cases back ionisation has been included.

In 1987 Gricco, [31], published a review of the types of design procedures that may be considered. The three main types are as follows.

1. Theoretical - equations are derived to represent fundamental physical and electrical mechanisms such as particulate charging rates, particulate space charge and electric field strength. Theoretical models may also include semi-empirical relationships. A common approach is to consider the precipitator as a series of sections and consider the performance in each section. Conditions can change from one section to the next, such as the average particulate diameter, gas flow velocity so that it is not a simple case of repeating the exact process several times.
2. Empirical - use large amount of existing data and regression techniques to make predictions, this means that the underlying physical processes do not have to be understood. Empirical models require a large accurate data base that has been derived from a broad range of electrostatic precipitator applications.

3. Design by analogy - uses the replication of previous applications, tried out on either a test rig or to full scale operation.

A major review of previous simulation techniques and computer models was undertaken to establish the best method to use in building the prediction program required by the research project. This review is fully reported in [8].

⇒ The remainder of this chapter summarises the main methods reviewed and aspects of the published models that were influential in the decision process are highlighted in this style.

The model proposed by the present project is a theoretical model. The possible mathematical modelling techniques that may be used are considered in this chapter. In planning the development of the computer model the techniques considered were:

- finite difference
- finite element
- charge simulation.

Additionally, adaptive meshing techniques could have been considered but the time required to develop these techniques is greater than was available for this research project.

The strengths and weaknesses of the possible techniques are considered further in section 3.8 and reasons for the choice of the method of finite elements are given in section 3.9.
3.2 General requirements
The general requirements listed below were considered when selecting which method to employ.

- The model should run on a PC so that it can easily be used, if required, by National Power PLC as sponsors of the research project.
- The software development should, where practicable, make use of existing software packages to speed up the development process. Where possible the packages should already be available or be purchased at a price to ensure that the project runs within budget.
- The model should be easily adaptable to include a variety of discharge electrode geometries.
- The run-times required to make specific predictions must be 'reasonable'.
- The model should avoid, as far as possible, the need for empirical data relating to the precipitator or the electrodes.
- The model should not rely on prior knowledge of any of the parameters to be modelled, for example the electric field pattern in the precipitator duct is not known.
- The model should be developed within the time frame of the 3 year research contract.

3.3 Finite Difference Techniques
The finite difference technique is a numerical method for the solution of partial differential equations, which is used when the problem to be solved is too complex for classical methods to be applied. It was originally developed by Thom in 1920 under the name of 'Method of Squares'. The finite difference technique is based on the solution of the governing differential equations over the required region by considering specific points, or nodes within the region and establishing how the value of a parameter at any node is influenced by the value of the same parameter at other nodes within the region. It requires the differential equation to be rewritten in an algebraic form as a finite difference
approximation between neighbouring nodes. The nodes may be produced by any net or grid laid down over the region. An irregular grid, however, would lead to a very complicated difference equation replacing the original partial differential equation, and to prohibitive numerical computations. The finite difference method is in general applied to a grid of regular polygons/polyhedrons although not necessarily in linear spatial co-ordinates. To fill a plane these regular polygons may be squares, triangles or hexagons. Squares and equilateral triangles are in common use. The technique is explained in [55]. Finite Difference methods can be applied to both linear and non-linear problems, although for non-linear cases the solution does not necessarily converge.

To summarise, the finite difference technique involves 3 steps.

1. Divide the solution region into a grid of nodes.
2. Approximate the given differential equation by the finite difference equivalent that relates the dependent variable at a point in the solution region to its value at the neighbouring points.
3. Solve the resulting system of simultaneous equations.

The method of finite differences can be applied in a variety of ways to the consideration of the potential distribution, electric field and space charge distribution within the precipitator inter-electrode space. Two examples are the solution of Poisson’s equation and the current continuity equation by McDonald, Smith, Spencer and Sparks 1977, [47], using a numerical solution to the governing equations, and the solution of Maxwell’s equations and the current continuity equation by Lawless and Sparks 1980, [42].

3.3.1 Alotto, Gallimberti, Molinari and Repetto 1995
This review paper, [5], considers the possible numerical methods that are now in use and summarises their advantages and disadvantages. Integral methods are particularly suited to unbounded problems but are not suitable for the solution of Poisson’s equation which is usually solved using differential methods. The paper considers several applications of these techniques and for electrostatic
precipitators the authors finite difference model is explained. This model considers the ionised region around the discharge electrode and the ionic drift region in the remaining space between the electrodes. The two regions are coupled together. The equations to be solved are:

\[ \nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \]  
Equation 3-1  

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mu \mathbf{E} - D \nabla \rho) = 0 \]  
Equation 3-2  

\[ \rho \mu \mathbf{E} = f(E) \]  
Equation 3-3  

Drift equation  
Glow equation on wire  

A steady state model and a time dependent model have been produced and initial results are shown. The paper states that the model is currently being adapted to practical geometries. Details of the adaptation are not given.

One of the reasons for the development of the present model is to avoid changing the program to make predictions for different geometries.

### 3.4 Finite Element

The finite element method was originally devised to analyse structural problems. It is primarily concerned with applying the minimum energy principle in the region of interest. The method has been extended to apply to electric and magnetic fields, which may be Laplacian or Poissonian. Typical areas of implementation are waveguide problems, semiconductor devices and transmission lines.

The finite element method may be generally described in four basic steps:

1. discretize the solution region into a finite number of elements
2. derive governing equations for a typical element and minimise the functional
3. assemble the elements of the solution region
4. solve the resulting system of equations.
Like finite difference methods, finite element analysis is also based on the identification of the differential equation governing the physical problem to be solved over a specified region. The solution region is divided into a grid of elements and the equations solved for all the individual elements simultaneously. The mathematical principles of finite elements are outlined in chapter 4. Many variations of finite element have been used to consider electrostatic problems but few directly address the effects of the detailed geometry of the discharge electrode.

### 3.4.1 Janischewskij and Gela 1979

In 1979 Janischewskij and Gela, [38], published a paper explaining their finite element approach to this area. Their paper considers the determination of the ionised electric field as a Boundary Value Problem and concentrates on the case of a DC field in air when a unipolar space charge is present. Knowledge of the space charge concentration and the distribution of electric field intensity will yield the current flow (if ion mobility is known).

Rigorous analytical solution of the ionised field is only possible for spherical or cylindrical geometry. Geometries with less symmetry involve simplifying assumptions and can therefore introduce errors. Janischewskij and Gela apply their model to one dimension assuming cylindrical geometry. This allows them to compare their results with the analytical solution of Townsend [64]. Their results show that the FEM is accurate in this application. The major assumptions made by Janischewskij and Gela are:

1. after initiation of the corona the electric field intensity remains fixed in magnitude at the onset value
2. that the region of corona activity consists of a sheath of negligible thickness.
The boundary values used by the authors are:

1. the known potential on the coronating electrode;
2. the potential on the other electrode is taken as ground;
3. the magnitude of the electric field at the coronating electrode is considered to be the constant onset value in air.

i.e. the potential, \( \phi \), and its derivative are constrained only on the boundaries of the region of interest.

⇒ An interesting aspect of this model is the use of two forms of approximation, linear and Hermite cubic, over a finite element. The Hermite cubic element method has the advantage of smaller errors in the results.

⇒ The quality of the solution also depends significantly on the discretization of the region. Boundaries with high curvature must be represented by a fine grid and similar regions where the solution is expected to vary significantly with position the grid must be fine. Regions where there are smaller variations, and away from the boundaries, can be represented by large elements.

In order to determine the optimum spacing a good understanding of the physical problem is required.

3.4.2 Takuma, Ikeda and Kawamoto 1981

The approach of Janischewskij and Gela, [38], for HVDC transmission lines was further considered by Takuma, Ikeda and Kawamoto 1981, [61]. Again the Finite Element Method is used and extended to include the effects of a wind (the effects of which are analogous to gas flow in a precipitator). Whilst recognising the value of using Hermite cubic elements, here the authors use upstream FEM and semi-automatic grid generation.
The assumptions used by Takuma, Ikeda and Kawamoto are as follows:

1. all values are steady in time and are two dimensional. Non-uniform corona occurrences are neglected
2. the diffusion of the ions is small compared to the drift by the electric field and can therefore be ignored
3. ion mobilities are taken as constants, independent of the electric field strength
4. the thickness of the ionisation region near the conductor can be neglected
5. the positive or negative charge density is constant on the surface of each source conductor of the corresponding polarity. (Assumption of constant ion density source).

Again the basic equations used are Poisson’s equation, current density and current continuity. The charge simulation method for a Laplacian field is used to determine the value of the potential without space charge at the artificial boundary. A significant proposal in this paper is the use of iterations between the solutions for charge density and potential, using the previously calculated values for the other parameter.

The calculated results were compared to an analytical solution and the agreement was satisfactory, the relative error in $j$ and $E$ being generally approximately 0.2% but larger near the boundaries with the electrode since the linear approximation of potential results in a constant electric field within each element. These errors, which occur only in the elements closest to the electrode boundary are not considered to invalidate the calculations.

⇒ It does however demonstrate the value of higher order approximations for potential, so that the electric field can be calculated more realistically. In an electrostatic precipitator the field is a very significant parameter in determining the efficiency of charging of the dust and its migration to the collection plate.
A significant proposal in this paper is the use of iterations between solutions for charge density and potential, using previously calculated values for the other parameter.

3.4.3 Davis and Hoburg 1983. Hoburg and Davis 1985

The earliest paper that deals with solving the electrostatic field within a precipitator, including a review of the finite element method applied to this problem, is Davis and Hoburg 1983, [18]. The procedure is developed further in their subsequent paper Hoburg and Davis 1985, [34], and includes the use of the method of characteristics to compute the charge density distribution for an assumed electric field. The method of characteristics is based on a technique whereby the partial differential equation governing the evolution of the charge density becomes an ordinary differential equation along specific "characteristic" space-time trajectories. The surface of the corona sheath is approximated by the corona wire surface.

The standard approach of minimising the functional is used to solve Poisson’s equation. The electric field magnitude is constrained according to Peek’s formula by considering the charge density as an unknown, and including an additional boundary condition at the surface of the corona sheath. Knowledge of the charge density at the corona sheath is required to determine the charge density values along the characteristic lines. The voltage drop through the corona sheath is neglected in approximating the radius of the sheath as the radius of the wire. The authors summarise that the model produces predictions that agree well with the experimental measurements of Penney and Matick, [52], and suggest the model could be extended to include further charge species.

The assumption that the radius of the corona sheath is the same as the radius of the electrode is a common approximation made in many of the published models. For simple geometries the potential at the outer edge of the corona sheath is the same as the potential applied to the wire, and as the corona sheath is very thin the approximation is valid. For more complex geometries, particularly those involving spikes or barbs, the equipotential, at the value of the
applied potential, around the electrode is determined by the local radii of curvature.

The later paper by the same authors, Hoburg and Davis 1985, [34], follows a similar approach to the 1983 paper, but the method is applied to steady-state situations with a superimposed wind velocity and applied to the geometry of HV transmission lines. The HVDC transmission line geometry calculations are compared to the experimental results of Hara, Hayashi, Shiotoku and Akazaki 1982, [32]. The model shows some discrepancies to the experimental data.

⇒ One of the possible causes of these errors are numerical differentiation errors. It would therefore be preferable to retain the analytical form of the differential equations for as long as possible, both to eliminate numerical errors and to make it easier to adapt the details of the method to different geometries. The need to re-evaluate differentials and integrals for each new geometry to be considered would be very time consuming.

3.4.4 Davies, Goldman, Goldman and Jones 1987

This paper, [17], reports analysis of negative point plane corona in air using field-theory and FEM in the needle-plane geometry. Whilst the geometry, and ease of making empirical measurements, is different from an electrostatic precipitator the paper is interesting because of its consideration of the corona region. The ionic current distribution on the earth-plate below the pencil shaped electrode has been measured experimentally. This is used as one of the boundary conditions in the simultaneous solution of Poisson's equation and the equation of current continuity. It would not be realistic to follow this approach for the electrostatic precipitator geometry, and possible alternative methods of implementing this boundary condition are discussed in section 1.2.9.

The paper also considers the corona region. This contains complex ionisation processes. It is desirable that only verifiable solutions are obtained for this region. If an approximated solution for this region is used, since it is a very small region compared to the other two, it will still lead to an acceptable solution overall. The researchers have used an existing FEM package available
through the Rutherford Appleton Laboratory. Error assessments of the results were made by comparing the numerical results with the exact solution for hyperbolic plane geometry.

⇒ Comparisons to analytical solutions are a valuable method of checking the accuracy of predictions to test the running of a complex computer model.

3.4.5 Levin and Hoburg 1988

The method of characteristics, whilst being an accurate and efficient tool for computing the field-to-source portion of the electric field (space charge coupling), is limited to models involving unipolar conduction based on only migration and convection. The method would not be easy to use if more than one charged species was included and cannot be used for modelling diffusion and charge transport. This paper proposes the use of the donor cell method. The donor cell method generalises to include multiple charge species and diffusive charge transport. Incorporation of multiple charge species enables back ionisation to be represented in the space charge density distribution. Inclusion of diffusive transport enables the time averaged effect of turbulence to be represented.

The authors give five examples in which they have used their method and found good agreement with previous analytical or numerical solutions. They suggest that their method, whilst giving good results, is less efficient than the combined method of characteristics and finite element approach and that their method may be impractical for a large number of nodes.

⇒ To model the effects of the detailed geometry of the discharge electrode effectively, it has already been established, [38], that the finite element grid needs to be finer near the discharge electrode, although it can be coarser in the regions of more slowly varying parameters. If the donor cell method requires the number of nodes in a grid to be limited this would prohibit the use of this method.
3.4.6 Cristina and Felliziani 1989

This paper, [16], is of particular interest as it shows the development of a model, applied to duct precipitator geometry, which was reported to have been of direct use to the Italian Electricity Board in the development of new precipitators. The authors put forward a method in this paper, [16], for calculation of space charge density due to corona phenomena and due to charged particulate. They calculate current density, potential and electric field distributions both with and without dust. The principle assumptions made are:

1. the ion space charge at the surface of the emitter is constant
2. secondary phenomena such as corona quenching and back corona are ignored
3. the ion mobility is constant
4. the dust comprises spherical particles of uniform size, distributed uniformly throughout the inter electrode space
5. charging of the dust particles by ionic attachment is ignored.

FEM is used together with two additional sub-procedures, both based on FEM, to determine respectively the ion density distribution due to corona discharge and the particle space charge density.

In the first stage of the iteration procedure both Poisson's equation and the equation of continuity, expressed as a function of potential, are solved using an arbitrary ion charge distribution. This arbitrary distribution is restricted only in that the corona onset electric field is determined by Peek's formulas, [51]. The distribution is assumed to be constant over the emitter. Solution of the two equations gives rise to two suggested potential distributions, and therefore two electric field distributions. A new ion charge distribution is calculated from these two and hence the convergence algorithm is defined. Iteration continues until the change in solution between steps is less than a specified value. The ion distribution at this last step is taken as the charge distribution in the inter-electrode space created by the electrodes.
Neutral particles in the precipitator duct are charged by a process of ion bombardment and ionic attachment by ion diffusion. For particles of diameter greater than 1\(\mu\)m then the dominant process is ion bombardment. The particle charge distribution is a function of the charging electric field and, because of fume turbulence, is considered constant over the inter-electrode space.

The first stage of the iteration process is to take the ion charge distribution already determined and add to it the particle charge distribution calculated from the previously determined electric field. It is assumed that the particle charge distribution is independent of the ion charge distribution. Poisson's equation is then integrated using this combined charge distribution. Iteration continues until convergence is achieved.

The boundary conditions employed in applying this method to the geometry of a duct type precipitator were: zero potential on the collecting plate; \(V\) on the discharge electrode; zero field perpendicular to the boundaries. The computed ion charge density was found to be in good agreement with measured values.

The electric field was calculated on the collecting plate and between the emitter and collecting plate. This calculation was made for both with and without charged dust particles and qualitative comparisons made. The authors feel that the proposed iterative method is simpler to apply than previous methods and is easy to use with complex geometries.

⇒ Assumptions 1 and 2 made in this model will also be made in the development of the new model. Dust in the new model is ignored and assumptions 4 and 5 therefore do not apply. The new model will be developed further to include the detailed geometry of the discharge electrodes and the model will be constructed so that different geometries can be tried without reworking the equations for the solution method. Ion mobility, assumption 3, is considered in ID, see chapter 6.
This paper, [4], is a further example of the use of an iterative procedure using FEA to solve for potential and space charge density. In this case, once the potential has been calculated the electric field can be calculated at each node. It is assumed that the boundary of the field flux tubes lie along the lines of the grid that has been devised to represent the solution region. In this case the geometry is that of a coaxial cylinder and it is reasonable to assume that the field lines are radial. For more complicated geometries this would require prior knowledge of the electric field pattern in the solution region.

Abdel-Salam and Al-Hamouz consider a unipolar ionised field in air. The potential is represented by a linear function of the node co-ordinates. The simplifying assumptions used in the solution of Gauss’s law and charge density continuity are:

1. The inter-electrode space is entirely filled with unipolar ions of the same polarity as the emitter. The thickness of the ionisation layer around the emitter is so thin that it can be considered as zero with respect to the distance between the emitter and the electrode.
2. The Deutsch assumption, see section 2.7.
3. The ions are of constant mobility.
4. The surface field of the coronating emitter remains constant at the corona onset value.

The limitations of the Deutsch assumption have been discussed in see section 2.1.7.

The applied boundary conditions, which are typical for these problems, are:

1. The potential on the stressed electrode is equal to the applied voltage.
2. The potential on the ground electrode is zero.
3. The magnitude of the electric field at the surface of the stressed conductor is constant at the corona onset value.
Since the mobility of the ions is assumed constant then

\[ \rho_n E_n A_n = \rho_0 E_0 A_0 \]

where \( n \) is the order of the node along the edge of the flux tube. \( A_n \) is the cross-sectional area of the flux tube which is proportional to \( r_n \) where \( r_n \) is the radial distance of the \( n \)th node. Therefore, since \( \rho_0 \) and \( E_0 \) are the charge density and electric field respectively at the outer cylinder,

\[ \rho_n = \rho_0 \frac{r_n}{r_0} \frac{E_0}{E_n} \]

The charge density \( \rho \) at the coronating electrode i.e. at radius \( r_i \) can be determined by extrapolation.

The paper explains the authors procedure:

1. assume an initial space charge distribution over the region, based on the radius of the wire and the radial distance of the point from the axis of symmetry
2. solve Poisson's equation for the first iteration of the finite element technique
3. calculate the electric field along the flux tube at all nodes
4. find the new charge distribution that satisfies Eqn. 3-5
5. repeat the calculation of the nodal values of potential as the second iteration
6. compare the potential error found at successive iterations relative to the potential value. If the potential error exceeds a specified value correct the charge distribution and continue the iteration.

The computed value of the space charge density and the electric field are compared to analytical solutions. The maximum errors are respectively 1.7%
and 2.0%. The authors emphasise the improved accuracy of their iterative method over previously reported methods.

⇒ This model has the advantage that both the potentials at each electrode and the electric field at the coronating electrode are implemented as boundary conditions rather than only the potentials being used and the subsequently calculated field at the electrode surface being checked.

3.5 Charge Simulation Techniques

The charge simulation method makes use of the method of images in that the total potential is obtained by summing the potentials due to individual charges. The description here is based on that given in [55].

⇒ The method of images can only be used for geometries that are enclosed by simple boundaries, for example plane or cylindrical.

If a line charge of density $q$ is at a distance $y'$ from the earthed plane at $y=0$ and a second earthed plane at $y=h$, then the resulting boundary condition on the potential distribution may be satisfied by constructing an infinite system of image line charges by replacing the plane with an image charge.
Figure 3-1 Line charge $+q$ at $(x',y')$ and images charges in the planes $y=0$ and $y=h$. All
charges are lines going into the page.

The potential due to such a sequence of charges, including the original is the
superposition of an infinite series of image charges.

The principle of the charge simulation technique is to find the potential
distribution of the field due to a distribution of charges by summing the
potential due to the individual charges.

In applying the charge simulation technique two aspects are of particular
significance:

1. correct choice of the type of simulation charges - e.g. point charges,
   line charges, ring charges

2. suitable arrangement of the charges and contour points.

It is important that the potential coefficients for the selected simulation charges
are known from analytical solutions. In general if more complex simulation
charges are chosen then the computations become more complicated.
There are many papers showing the application of the charge simulation method to a variety of geometries, for example: Abdel-Salam, Zeitoun and El-Ragheb, 1976 considers the space charge region that forms around a discharging HV conductor. Graf 1980, [30], takes the alternative approach of replacing the space charge in a point-plane gap with symmetrically arranged charged spheres which can penetrate each other.

A criticism of the charge simulation method to date is that considerable time can be taken in setting up the system of simulation charges. This process also requires insight into the physics of the situation together with guesswork, particularly in cases of no axial symmetry. This presents considerable difficulty for complex 3D geometries. The choice of position of the simulation charges will vary between individuals and therefore the accuracy of the results will also vary.

3.5.1 Elmorsi and Castle 1984 and 1987, Elmorsi and Speck 1989

The Elmorsi and Castle papers, [22] and [24], relate to charge simulation techniques specifically to duct-type electrostatic precipitators. The authors show that the Deutsch assumption is invalid for large corona current. The charge simulation technique is based on the method described Singer, Steinbigler and Weiss, [59].

Two models are developed:

1. Laplacian field within the duct

2. Poissonian field within the duct.

Due to the double symmetry the problem is two dimensional. The discharge electrode surface is represented by discrete infinite line charges, and the potential coefficient matrix can be constructed. The magnitude of the charges is found using the Gaussian elimination technique so that the known boundary conditions are satisfied.

The example explained by the authors suggests that eight charges be placed inside the corona wire with 31 image charges placed behind the collecting plate.
and 31 image charges along the line of symmetry between the discharge electrodes to represent the remainder of the precipitator. The boundary conditions are:

1. the component of the electric field perpendicular to the line of symmetry between the discharge electrode is zero along that line
2. the potential is zero on the collecting plate
3. the potential equals the applied potential at the discharge electrode.

⇒ If such a model were to be extended to 3 dimensions to model a complex discharge electrode geometry accurately the process of placing the image charges would become much more complex.

The model was checked by calculating the potential along the line of the collecting plate and compared to the expected value of zero. Agreement within 0.01% was found. The model was applied to the wire plate geometry of the experiments by Penney and Matick, [52]. Plots are given of the measured value and the computed value of potential across the duct. The accuracy of the computed values depend significantly on the chosen mobility factor for the ions. This is as expected since it is known that the V-I characteristic is also dependent on the mobility.

The Elmoursi and Speck paper, [25], follows the pattern of previous papers. The generation of the grid is again the network of field lines and lines of equipotential as explained in [23], applied to unbounded regions such as the rod-gap geometry. The method of characteristics is used to determine the charge density distribution along a characteristic line.

⇒ The application of the charge simulation techniques to 3D geometries would be complicated and time consuming. It would be especially difficult to deal with small scale variations in the local radius of curvature of the discharge electrode.
3.6 Combination Methods

Some of the papers discussed above use a combination of methods, particularly the method of characteristics with charge simulation e.g. Elmoursi and Speck 1990, [25], and method of characteristics with finite element e.g. Davis and Hoburg 1983, [18], Okubo Ikeda Honda and Yanari 1982, [49], describe a combination of the charge simulation technique and finite element method. The aim is to improve the overall solution by using each technique to overcome weaknesses in the other. It can be applied to various media with space charge and in open space. The authors suggest that their method gives a more accurate solution than any single method and could be precisely applied to three dimensional fields. Also they suggest that their method could be adapted to include other techniques such as finite difference.

3.6.1 Kallio and Stock 1985

Kallio and Stock, [41], put forward a combination method that utilises the finite element technique to determine the potential distribution from Poisson's equation with a triangular grid of variable spacing throughout the gap and the finite difference technique to determine the space charge distribution from the continuity equation. Since gradients are small a relatively coarse grid may be used. The wire-plate geometry is adopted, based on the co-ordinate system of McDonald et al, [47].

The authors base their method on the solution of Poisson's equation and the continuity equation using an iterative procedure. The space charge is assumed to consist solely of corona-generated unipolar ions of constant mobility. The technique has been used to compute the potential, electric field and charge density distribution. They have also predicted V-I characteristics. Their results are compared to conventional finite difference techniques to assess improvements in accuracy and computation time.

Plots of potential and electric field profiles are given to compare with the previous finite difference results and with analytical techniques. The present method is shown to be more accurate close to the wire due to the steep potential gradient. To improve the purely finite difference method the grid size would
have to be reduced making a significant increase in computation time as convergence is reached more slowly.

The results are also compared to Penney and Matick's experimental results, [52] with which good agreement is obtained.

⇒ This combination does not allow the calculation of the current density at all points in the region, only at the nodes. It would be of particular interest to be able to plot the predicted current density along the collecting plate so that the predictions can be compared to recent experimental measurements, [28].

3.7 Other Methods

There are other numerical techniques that have been applied to the study of electrical conditions within a precipitator. For example: numerical integration methods and the finite volume method. The finite volume method is commonly used in fluid flow studies. It algebraically equates flux into and out of small elements to a normally zero source term for that element. An example of the use of this method is given by Lawless and Sparks 1980, [42], in which the finite volume technique is based on a numerical solution of the integral form of Maxwell's equations rather than Poisson's equations and current continuity. This approach is considered by the authors as they encountered difficulties in extending the methods of McDonald et al, [47], to include back corona effects. The result is that the governing equations are based on the electric field rather than the potential distribution. The geometry considered is similar to that of McDonald et al but the co-ordinates correspond to the centres of the cells rather than the nodes.

In considering the accuracy of their method the authors relate their discussion to a square grid of cells of side length $h$. This present method is accurate to order $h^2$ except for the line integral equation where the cells are adjacent to the grid where the error is of order $h$. The authors discuss methods of improving the accuracy in this case. They note that the finite dimensions of the corona wire
have been ignored by McDonald et al, [47], which adds inaccuracies to those methods.

3.7.1 Zamany 1995

Two papers published recently by Zamany, [66] and [67], show the use of a 3D numerical model to solve the coupled quasi-static electro-dynamic Maxwell's equations for the electric field and the current density field. Time averaged diffusion of charges into regions where mathematically the space charge is zero is included. A variety of discharge electrodes, e.g. wires, helical wires and rigid with spikes together with corrugated plates are modelled and the results compared to experimental measurements - particularly the current density along the collecting plate - and good agreement is obtained. Data for the corona onset potential from VI characteristics for ESPs, under similar operating conditions, have been used in the model.

⇒ VI curves are general characteristics that do not take account of the small scale local differences in corona onset, which depends on the local radius of curvature of the discharge electrode.

3.8 Comparison of Standard Techniques

The techniques of finite difference, finite element and charge simulation have been described. All can be employed in the study of electric fields within electrostatic precipitators. Each technique, however, has strengths and weaknesses.

Finite difference and finite element both normally use numerical approximation techniques to solve the differential equations. Charge simulation uses numerical techniques to optimise the positioning of simulation charges. The field is calculated analytically once the position and location of the simulation charges has been established. If a space charge distribution is included the determination of the field becomes the addition of the components due to the simulation charges and the space charge. The finite difference method is mathematically easier than finite element and also software implementation is less involved. Numerical approximation techniques can introduce errors in the integration.
Analytical techniques are preferable, where it is possible to use them, as the method then remains general until a later stage, as it is easier to apply to different geometries and grids.

The finite element method is a more powerful and versatile numerical technique, and it is better able to cope with complex geometries and inhomogeneous media. The functional form of the solution allows inter-nodal values to be calculated. The functionals and residuals can be formulated symbolically so that the same expressions can be used for different geometries. This also reduces numerical errors.

Finite element has another advantage over finite difference that the inter-electrode region can be divided easily as required. The mesh size can be continuously varied across the inter-electrode gap. It is easy to use a finer mesh near to the wire where potential, field and charge distribution change rapidly. It is also easier to implement the boundary conditions especially fitting to a curved boundary. The disadvantages of FEM are possible numerical instability during iteration and the time consuming nature of grid generation.

The utilisation of the finite difference technique for wire plate geometry, the most applicable for electrostatic precipitator modelling, presents difficulties in that, because of the steep gradient in potential near the wire the grid size in that region must be small. If a uniform grid size is used the resulting matrices may be too large for the computer to manipulate. A possible solution is to divide the gap into regions, each of which has a constant grid size, with the grid size being larger in regions away from the wire. The finite element method can use a graded grid spacing so that nodes are set closer together in regions of greatest change of variable.

A further advantage of the finite element technique is that it can easily be implemented for elliptical partial differential equations such as Poisson's equation. The continuity equation is a hyperbolic partial differential equation, for which it is less easy to implement the finite element technique. An alternative is to use the method of characteristics in conjunction with the finite element technique.
The finite element technique can achieve considerable saving in computation time compared to finite difference, since finite difference usually employs a simple relaxation technique to reach convergence. Finite element requires fewer iterations since evaluation of all nodal values occurs simultaneously by solution of the linear matrix equation.

The accuracy of finite element techniques can be difficult to evaluate and compare due to the variable node spacing. To compare to finite difference the relative accuracy may be considered in terms of the ratio of nodal spacing for each method. Smaller errors for the same grid spacing can also be obtained by the use of higher order elements and the matching of gradients at nodes.

The main advantage of the charge simulation method is that it is normally the fastest method for electrostatic problems with no free space. Charge simulation can be used with curved boundaries, e.g. curved electrodes. The charge simulation method can be programmed with high precision however it is not suitable for considerably complicated fields. It can be applied to geometries containing partial fields or unbounded regions. However, it is not suitable for fields with many dielectric or complex electrode configurations. Although the ends of the discharge electrodes are an unbounded region, as is the end of each zone, these effects are small in a precipitator in comparison with the large central region. Okubo, Ikeda, Honda and Yanari 1982, [49], suggest that charge simulation is not suitable for Poissonian fields. However later work by others, e.g. Elmoursi and Speck, [25], suggest that space charge may be included.
3.9 Choice of Finite Element Method

Having reviewed the mathematical methods that may be employed to simulate the electrical conditions within electrostatic precipitators, the advantages of finite element analysis, compared to finite difference and charge simulation, can be summarised.

- The grid size may be varied to allow more detailed calculation over regions of rapidly varying physical properties and a wider grid over regions of more slowly varying solution. This increases the computation speed of the program and reduces the storage space required.

- The grid may be arranged to closely follow the curvature of the boundaries. This is particularly important in the modelling of the discharge electrode.

- The inclusion of space charge can be modelled more easily than for the charge simulation method.

- The solution is for all points in the solution region rather than for the nodes only as in the finite difference method. The calculated potential, field and charge density can therefore be compared to analytical solutions for all points in a region of simple geometry.

- There are good text books available explaining the application of finite element techniques to electromagnetic problems. Silvester and Ferrari, [58], and Sadiku, [55], give sample code that can be used as the starting point to develop programs specific to electrostatic precipitation.

- Although mathematically more complicated than finite difference, finite element is more adaptable. It is relatively easy to adapt it to cases of multiple carriers and variable mobility.
• It is easier to implement the boundary conditions in the finite element method as some are implied by the functional rather than being specified separately.

• Since the approximation for the potential is fitted over the whole of the solution region, the electric field may be legitimately evaluated by differentiating the solution for the potential.

• The coupled equations for Poisson and current continuity can be solved iteratively. To reach convergence finite element usually requires fewer iterations than finite difference.

• By matching the field components at nodes, as well as potential, a fixed field charge injection law may be simply implemented. This then allows the boundary conditions, at the discharge electrode, for current continuity to be fixed by reference to the Poisson boundary conditions.

3.10 Houlgreave, Bromley and Fothergill, 1996 - A quasi-electrostatic FEM with application to electrostatic precipitators

An iterative FEM for the solution of Poisson's equation, using the variational approach, and current continuity, using the Galerkin residual method, was presented initially in [9] and in more detail in [36], see also Appendix C. This model has been chosen as the basis for the prediction program and is explained in detail in section 5.2.3. The advantage of this particular model is the symbolic formulation that can be used with different electrode geometries.

The authors give the 8 steps for the solution of the non-linear system by means of the iterative solution of Poisson's equation and current continuity. The model includes geometry dependent charge injection at the discharge electrode surface. It uses a Hermite cubic representation of potential and a linear approximation for space charge over tetrahedral elements. The tetrahedral elements have been chosen for their ease of matching to complex electrode shapes. Hermite elements allow the field components to be matched at each node and this simplifies the imposition of the fixed field charge injection law.
The 1D results presented include an arbitrary static background space charge density due to the charged airborne particulate, which is assumed not to contribute to the current. This background dust is not included in the model presented in the thesis and therefore initially it is required to solve Laplace's equation rather than Poisson's equation.

In the paper the 1D results have been obtained using the iterative procedure derived and implemented in MAPLEV. The disadvantage is that the code would have to be revised to obtain predictions for other geometries, especially for the more complex case of 3D. This will be overcome by the development of the prediction program to handle the construction of matrices and vectors, imposition of boundary conditions and obtaining of the solutions, for a general geometry, within the outline of the symbolic computation described by the authors.
4. FINITE ELEMENT TECHNIQUES

4.1 Introduction

Finite element methods are ideally suited to solving bounded problems. To apply the method to unbounded situations the approach must be adapted. In the case of electric fields in the electrostatic precipitator, the geometric symmetry is used to formulate boundary conditions, usually of the first derivative of the potential to the boundary.

The standard way of numerically solving a Boundary Value Problem is to superimpose a suitable grid over the region of interest and to fit locally the known basis functions. This results in a transformation of differential equations into algebraic equations. Matrix methods are then used to calculate nodal values, i.e. values at the nodal points, which closely approximate the functions sought. The solution away from grid points is found using the approximation function defined on each element.

As mentioned in section 3.4 the finite element method may be generally described in four basic steps:

1. divide the solution region into a finite number of elements
2. derive governing equations for a typical region
3. assemble the elements of the solution region
4. solve the resulting system of equations.

The approach shown in this chapter follows that given in [55].

The parameter of interest in each element, e.g. \( \phi \) is approximated within each element by \( \varphi \). Such a \( \varphi \) for adjacent elements is identical at the common boundary. \( \phi \) can be calculated over the whole of the solution region, unlike the finite difference method where it can only be calculated at the nodes.
The approximate solution for the whole region is:

\[ \phi(x, y) = \sum_{e=1}^{N} \phi_e(x, y) \]

where \( N \) is the number of elements and \( \phi_e(x, y) = 0 \) outside element \( e \).

The approximation to be employed within each element must be selected, e.g. linear, quadratic, cubic etc. The higher the order of the approximation the better the fit that can be achieved. The increase in accuracy with higher order elements can reduce the number of elements required over the solution region i.e. the same level of accuracy can be achieved on a coarser grid.

Most commonly a linear form of approximation is used within an element \( e \), so that for a triangular element

\[ \phi_e(x, y) = a + bx + cy \]

where the constants \( a, b, c \) are unknowns.

The paper [36], see Appendix C, illustrates the use of a cubic expression for potential over a tetrahedral element. The derivation of such a cubic and the choice of the element shape is explained in section 7.2.

In 2 dimensions triangular elements are often chosen in preference to quadrilateral ones as they are easier to fit to a curved boundary in such a way that the resulting solution is a good approximation. Similarly in 3 dimensions tetrahedral elements are easier to fit to a curved boundary than cuboid ones.

4.2 Example: Solving Laplace's Equation in 2D

The procedure outlined in the following chapter is explained in 2D for clarity. In 3D the number of unknowns is larger, the matrices bigger and the expression to represent the parameter of interest, in this case \( \phi \), is much more complex, but the procedure is the same. It follows the four steps listed above in section 4.1.

4.2.1 Generation of the finite element grid

To find the potential distribution over a 2D region the first stage is to divide the area up into a number of non-overlapping triangular elements.
4.2.2 Derivation of the governing equations for an element

Consider a typical triangular element, for which by convention the local node numbering must be anticlockwise so that the area of the element is positive.

The equations for each element can be written in matrix form:

\[
\begin{bmatrix}
\phi_{e_1} \\
\phi_{e_2} \\
\phi_{e_3}
\end{bmatrix} =
\begin{bmatrix}
1 & x_1 & y_1 \\
1 & x_2 & y_2 \\
1 & x_3 & y_3
\end{bmatrix}
\begin{bmatrix}
a \\
b \\
c
\end{bmatrix}
\]

Equ. 4-3

To determine a, b, c, this can be rearranged as:
Equ. 4-4
\[
\begin{bmatrix}
a \\
b \\
c
\end{bmatrix} = \begin{bmatrix}
1 & x_1 & y_1 \\
1 & x_2 & y_2 \\
1 & x_3 & y_3
\end{bmatrix}^{-1}
\begin{bmatrix}
\varphi_n \\
\varphi_n \\
\varphi_n
\end{bmatrix}
\]

Equ. 4-3 may also be written

\[\varphi_s = \sum_{i=1}^{n} \alpha_i(x,y) \varphi_i\]

where

\[\alpha_1 = \frac{1}{2A} [(x_2y_3 - x_3y_2) + (y_2 - y_3)x + (x_3 - x_2)y]\]

\[\alpha_2 = \frac{1}{2A} [(x_3y_1 - x_1y_3) + (y_3 - y_1)x + (x_1 - x_3)y]\]

\[\alpha_3 = \frac{1}{2A} [(x_1y_2 - x_2y_1) + (y_1 - y_2)x + (x_2 - x_1)y]\]

\(\alpha\), are the linear interpolation functions, also known as the shape functions.

The required functional relating to the governing differential equation must be selected. Standard functionals are readily available in the literature e.g. [55]. For Laplace's equation

\[\nabla^2 \varphi = 0\]

the associated functional \(W(\varphi)\) is given by:

\[W(\varphi) = \frac{1}{2} \int dE \int dS = \frac{1}{2} \int d\nabla \varphi^2 dS\]

In two or three dimensions this functional may be expressed in matrix form, as

\[W(\varphi) = \frac{1}{2} d[\varphi^T][C^{(\sigma)}][\varphi] \]
where \([\phi^T]\) is the transpose matrix of \([\phi]\) and \([C^\alpha]\) is the element coefficient matrix or the stiffness matrix. This represents the coupling between the nodes or may be considered as giving the sensitivity of the functional in a particular element to the potential, in any given element.

4.2.3 Assembling the elements

All the elements must then be assembled by considering

\[ W(\phi) = \sum_{e=1}^{N} W(\phi_e) = \frac{1}{2} \epsilon [\phi]^T [C] [\phi] \]

where \(N\) = number of elements, \([\phi]\) = \([\phi_1, \phi_2, \ldots, \phi_n]\), \(n\) = number of nodes and \([C]\) is the global coefficient matrix. \(C_{ij}\) is the coupling between node \(i\) and \(j\). If there is no coupling \(C_{ij} = 0\). For large numbers of nodes \([C]\) is a sparse matrix.

For a homogenous region \(\epsilon\) is constant. If this is not the case, the grid must be generated so that each individual element is homogenous, i.e. \(\epsilon\) is constant for each element.

4.2.4 Solving the system of simultaneous equations

Laplace's or Poisson's equations are only satisfied when the total energy in the solution region is a minimum subject to boundary constraints. This same principle of minimum energy can be applied to all physical situations provided that the correct functional is chosen.
For total energy in the solution region to be zero the partial derivatives of $W$, with respect to each node value must be zero i.e.

$$\frac{\partial W}{\partial \varphi_1} = \frac{\partial W}{\partial \varphi_2} = \ldots = \frac{\partial W}{\partial \varphi_n} = 0$$

i.e. $\varphi_n$ is the total nodal value of the potential and $n$ is the total number of nodes in the mesh. Or equivalently,

$$\frac{\partial W}{\partial \varphi_k} = 0, \quad k = 1 \ldots n$$

in general terms

$$0 = \sum_{i=1}^{n} \varphi_i c_i, \quad k = 1, \ldots, n$$

By writing Equ. 4-13 for each of the nodes $k=1\ldots n$, and writing the boundary vector of known node potentials, a set of simultaneous equations is obtained the solution of which gives $[\varphi]$ i.e. $[\varphi_1, \varphi_2, \ldots, \varphi_n]$. This system can be solved by the band matrix method. The system of simultaneous equations is of the form

$$[A][X] = [B]$$

where $[A]$ is a matrix, $[X]$ is the vector of unknown $\varphi$ and $[B]$ is the vector of known $\varphi$. This may be rearranged to give

$$[X] = [A]^{-1}[B]$$

which can be solved to obtain $[X]$.

In practice in 3D it may be complicated to keep track of which node parameters are known and unknown values. This must be kept in mind for the construction of the matrix of coefficients of unknown node parameters; the rows and columns that would relate to known values must be excluded.
4.3 Solving Poisson’s Equation

Poisson’s Equation, see section 2.3 is given by:

\[ \nabla^2 \varphi = \frac{-\rho_s}{\epsilon} \]  

Equation 4-16

In considering this equation both the potential \( \varphi_s(x,y) \) and the source term \( \rho_s(x,y) \) over each triangular element can be approximated by say, linear combinations of the local interpolation polynomial, \( \alpha_i \), described in section 4.2.2.

\[ \varphi_s = \sum_{i=1}^{3} \varphi_{n_i} \alpha_i(x,y) \]  

Equation 4-17

\[ \rho_s = \sum_{i=1}^{3} \rho_{n_i} \alpha_i(x,y) \]  

Equation 4-18

Where \( \varphi_{n_i} \) and \( \rho_{n_i} \) are the values of \( \varphi \) and \( \rho \) at node \( i \) of element \( e \).

The variational functionals associated with Poisson’s equation are:

\[ F_u(\varphi) = \int \left[ \frac{\epsilon}{2} (\nabla \varphi)^2 - \rho \varphi \right] dV \]  

Equation 4-19

\[ F_u(\rho) = \int \left[ \frac{1}{2} \rho^2 + \epsilon \rho \nabla^2 \varphi \right] dV \]  

Equation 4-20

Equation 4-19 is the functional for the variation of \( \varphi \) with \( \rho \) constant and Equ. 4-20, see [40], is for the variation of \( \rho \) with \( \varphi \) constant.

Minimising the functionals is equivalent to solving Poisson’s equation and the same procedure is followed as described for the solution of Laplace’s equation, choosing the correct functional to construct the system of simultaneous equations.
4.4 Solving Current Continuity

The equation for current continuity, see section 2.6 is given by

\[ \nabla \cdot j = -\frac{\partial \rho}{\partial t} \]

For current continuity it is necessary to use the Galerkin weighted residual method, rather than a variational functional. In other respects the procedure is the same as for solving Laplace’s and Poisson’s equations. The Residual for constant mobility is given in [36], and Appendix C, and shown here:

\[ \text{Residual} = \int \left( \rho \nabla^2 \varphi + \nabla \cdot \rho \nabla \cdot \varphi \right) \omega^e_i \, dV \]

where \( \omega^e_i \) is the weighting function: \( \xi \) is the vertex of element \( e \).

The derivation of the field dependent mobility residual is shown in section 6.2.

4.5 Elements in 3 dimensions

In three spatial dimensions the elements are now also three dimensional. Typical elements for piecewise linear approximation of potential are four-node tetrahedral or eight-node hexahedral see Figure 4-3.
For a four-node tetrahedral element, a linear approximation is given by

\[ \varphi = a + bx + cy + dz \]

And similarly for the source function, giving rise to four ‘knowns’ and four ‘unknowns’.

The procedure for 3 dimensions is the same as described for 2 dimensional solution regions. The approximation equations are more complex and the expressions that result from the substitution of these approximations into the functionals and residuals are consequently more complex than in 2D. This complexity can be handled by modern computers. The aspect of 3D FEM that can be difficult to implement is the construction of a suitable grid. This can be done by hand but there are dedicated packages available, many such as FEMGEN, [27], are pre-processors to commercially available FEM solvers.

The use of linear elements restricts the accuracy that can be achieved. To overcome this a fine grid must be used. An alternative is the use of higher order elements.

4.6 Higher order elements

Higher order elements use a higher order polynomial to represent the parameter of interest within an element, e.g. parabolic, cubic, quartic, quintic etc. The choice of, for example, a parabolic expression of potential results in a linear field within an element which can result in a better fit than the constant field that goes with a linear expression for potential.

Higher order finite element schemes generally use co-ordinates local to each element rather than global co-ordinates. Such co-ordinates have a number of advantages in terms of simplifying implementation. In particular general software routines may be written in terms of local co-ordinates which enable most of the mathematical formulation of element equations to be achieved by simple co-ordinate transformations from prototype equations. Local coordinates are standard area coordinates for 2 dimensional shapes or volume coordinates for 3 dimensional elements. Figure 4-4 shows the cartesian \((x,y)\) and local coordinates \((l,m,n)\) for a triangular element.
In 2 dimensions the cartesian coordinates; \( x, y \), in terms of \( l, m, n \) are given by

Equ. 4-24

\[
x = l x_1 + m x_2 + n x_3,
\]

\[
y = l y_1 + m y_2 + n y_3,
\]

Total area, \( A = A_1 + A_2 + A_3 \) so that in terms of the area made from the point \( P \) to each side:

Equ. 4-25

\[
l = \frac{A_1}{A}, \quad m = \frac{A_2}{A}, \quad n = \frac{A_3}{A}
\]

In 3 dimensions the definition is similar, but using ratios in volume, see [55]

4.7 Computer modelling using Finite Element analysis

4.7.1 General aspects of constructing a computer model

To enable a complex, physical situation to be modelled on a computer the problem typically has to be translated from a system of differential or integral equations to a set of discrete algebraic equations in which continuous variables are approximated by discrete variables.

In constructing the system of discrete equations consideration must be given to the interdependence between variables. Efficient solution of the equations
normally requires an iteration process that produces a series of approximate solutions, each iteration using the results of the previous iteration to produce an improved approximation. In undertaking an iteration process the interim solutions must be checked for convergence to a final solution. An iterative procedure for the solution of Poisson’s equation and current continuity is reported in [36], see Appendix C.

4.7.2 Model structure

Ideally, before deciding on the solution algorithms to use or beginning to write computer code, the overall structure of the model must be specified. There are several recognised procedures for achieving this. The following is a typical approach, [20].

The design of the structure of a model is considered in four steps.

1. The physical quantities that will play a role in the model and their interconnectedness must be identified. This is done by first identifying the target quantities that are of primary interest. A causal network is then constructed. This shows the network of dependence between the quantities identified. The causal network should then be systematically checked to ensure that all factors affecting each of the quantities already identified is included, and any interdependencies are shown.

2. Physical quantities are identified or specified as:
   - the values of which can change during the process
   - values which do not change.

3. The dependencies between the quantities must be determined as either static or dynamic. In general, static relationships can be written in an algebraic form, whereas dynamic relationships cannot. These two types of dependence are denoted differently in the causal network. Starting point variables must also be identified. These are variables that may change with time but are not dependent on other variables in the system. They may be considered as input variables to the model (including boundary conditions if these are not fixed).
4. The causal network can then be simplified by condensing some or all of the static relationships. The output variables should be exempt from this process.

4.7.3 Modelling of Electrical Processes in an Electrostatic Precipitator

The charge density and potential distribution in an electrostatic precipitator are generally modelled as interdependent variables of a self-consistent set of equations. Computation of these quantities therefore requires the simultaneous computation of both physical quantities. This is because the fields and their sources are coupled: while charge density serves as a local source of electric field, the resultant field determines the charge density distribution by driving the ion motions. When the applied voltage is above corona onset there is, in effect, an injection of charged particles which flow away from the coronating electrode. The polarity of these ions is the same as that of the electrode. The flow of ions is determined by the magnitude and direction of the local electric field intensity, which is in turn governed by the potential and geometry of the electrodes as well as the presence and distribution of space charge. Therefore there is an inherent coupling between the inter electrode electric field, or potential, and the space charge and the problem to be solved is non-linear.

![Causal Network between electrode potentials, electric field and space charge.](image)

Even for two dimensional problems, highly divergent fields require a large number of elements to achieve sufficient accuracy. Since with linear approximation of potential the field is assumed constant within each element, an
error is introduced which increases if the size of elements is increased. The required increase in the number of finite elements means that the stiffness matrix $[C]$ becomes very large although many elements in it are zero. Sparse matrix techniques may be used to reduce the computer storage required.

In 3 dimensions the processing time is much longer, the memory requirements larger and more sophisticated techniques are required to number the nodes and elements of the grid, construct the disconnected matrix of coefficients and the connection matrix, impose the boundary conditions and keep track of the known and unknown node parameters. The vectors and matrices are much larger and therefore memory and storage requirements are much larger. The computation time is considerably increased especially if higher order elements are used, although in this case a coarser mesh may be satisfactory.

The design of a technique to build a computer model to carry out the iterative solution of Poisson’s equation and current continuity, as described in [36], also Appendix C, is explained in section 5.4.3.
5. SOFTWARE DESIGN AND DEVELOPMENT

5.1 The software life cycle

5.1.1 What is a 'good' program

There are many text books about the methods required to design good programs. Jones and Headon, [39], define a good program as one which:

1. gives correct results
2. is easy to understand
3. is easy to correct
4. is easy to alter
5. deals sensibly with unusual data.

This definition is a general one and the Finite Element model has been developed with the aim that each of these requirements is fulfilled.

5.1.2 Stages in the software life cycle

Somerville,[60], defines the software life cycle as:

1. requirements definition
2. specification and design
3. implementation
4. testing.

Figure 5-1 The software life cycle
There is forward flow and backward flow of information between each of the stages. In most software projects each of the four stages will be sub-divided, the divisions usually being specific to the project. For the current project each stage was 'revisited' as a new feature of the final program was identified.

5.2 Requirements definition - software

5.2.1 Rapid prototype development

The model was developed as part of a larger research project. The final specification had not been devised when the construction of the model was started, although the broad specification was available and the iterative procedure, described in section 5.2.3.1 had been formulated. The model was therefore developed as a prototype and an additional requirement was that the program should be capable of being rapidly adapted and developed; it should be able to:

- use new functionals as devised
- incorporate new ideas during development
- compare the effects of imposition of boundary conditions
- have reasonable run-times for testing
- use a variety of grids.

5.2.2 Principles of software specification.

Whichever methodology is chosen for a software project it is important that the requirements of the end product are clearly defined. In commercial software production the specification stage of the contract is critical as this defines how the software producer will meet the customer's requirements. All subsequent work will follow this specification. The high-level specification document can be written into the software contract.

In this research project it was not possible to initially define clearly the exact specification required of the final software program. By the nature of research the ideas to be incorporated into the program may be new and therefore need
investigation before deciding whether to include them or find alternatives. This research project, to build the FE model to be used for a variety of discharge electrode geometries was based on other research work; the development of the iterative procedure, which was continuing. The iterative procedure was being refined and the possible use of different functionals was concurrently being investigated. However the requirements of the model and some of the techniques and algorithms were known.

5.2.3 Specification of the model to solve the non-linear system

The modelled physical quantities which are important in determining precipitator performance are electric field, current density and space charge density as they control how the dust will be charged and collected. The ability to predict accurately how these quantities are affected by electrode geometry, and to optimise them for given operating conditions and power dissipation, would facilitate the development of more efficient electrodes.

To solve the electroquasistatic precipitator problem one must simultaneously solve Poisson's equation and the current continuity equation subject to the appropriate potential, charge injection and space charge boundary conditions. If the applied voltage is constant in time and stochastic time variations due to corona are ignored, the appropriate equations are:

\[ \nabla^2 \phi = -\frac{\rho}{\varepsilon} \]

which is Poisson's equation and

\[ \nabla \cdot \mathbf{J} = \nabla \cdot (\mu \rho \mathbf{E}) = -\nabla \cdot (\mu \rho \nabla \phi) = 0 \]

i.e.

\[ \rho \nabla^2 \phi + \nabla \cdot \nabla \phi = 0 \]

which is the equation of current continuity. Mobility \( \mu \) is taken as constant. Field dependent mobility is considered in chapter 6. This coupled set of equations is non-linear since the current continuity equation involves products of terms involving potential \( \phi \) with ones involving space charge \( \rho \).
In the model described here the general iterative procedure had already been devised and reported in [36], see Appendix C. This was used as the basis of the specification for the computer program. However new requirements or enhancements of this iterative procedure needed to be introduced during the development of the model.

5.2.3.1 Solution of the non-linear system

The finite element functionals and residuals are given here as background to the development of the iterative procedure, they are reported in [36]. They are not used directly by the model, but the expressions for the coefficients of the node parameters are derived from the functionals and residuals. The coefficients are used to form the matrices which represent the system of simultaneous equations to be solved, see section 5.2.4. The model initially used Equ. 5-3, Equ. 5-4 and Equ. 5-6, the functional for equipotential surfaces, Equ. 5-7 was incorporated at a later stage.

The iterative solution technique has the advantage over many previous techniques that only the field needs to be fixed at the coronating regions of the electrodes as the solution algorithm homes in on the space charge level at the injecting boundary; it does not require empirical data such as the current for a given applied voltage when dealing with complex electrodes. The initial guess at the space charge distribution is chosen to be uniform since for a general geometry there will be no prior knowledge from measurements or analytical solutions. In the solution to Poisson’s equation, ionic space charge density is assumed to have the form \( k \rho(x) \) where \( k \) is the scaling factor and \( \rho(x) \) is the previous estimate for the ionic space charge density.

The variational approach is used in solving Poisson’s equation. The appropriate functionals are, see [40]:

\[
\text{Equ. 5-3} \quad F_1(\phi) = \int \frac{1}{2} \rho \phi^2 - \rho \phi \, dV
\]

\[
\text{Equ. 5-4} \quad F_2(\phi) = \int \frac{1}{2} \rho^2 + \varepsilon_0 \varepsilon^2 \phi^2 \, dV
\]
for solution of Poisson's equation with variation of potential $\phi$ and space charge $\rho$ respectively. These functionals must be minimised by equating their partial derivatives with respect to appropriate parameters to zero. $E(\rho)$ is required for finding the ionic space charge scaling factor, and is in fact equivalent to the functional obtained by the least squares weighted residual method.

The current continuity equation is solved using the Galerkin weighted residual method. The space charge at any point within an element, $e$, may be found using a linear approximation in terms of the space charge at each vertex and the coefficients $b^e_i$ determined by:

$$\rho^e(x,y,z) = \sum_{i=1}^{4} b^e_i P^e_i,$$

where $P^e_i$ is the space charge at vertex $i$, to define the coefficients $b^e_i$ for an element $e$. The expressions, four per element, used in applying Galerkin method, that are equivalent to the partial derivatives of the functional over an element in the variational method, are:

$$\int_{e} \left( \rho \nabla^2 \phi - \nabla \cdot \mathbf{J} \right) b^e_i \, dV$$

The boundary conditions at the discharge electrode are determined as follows. Initially Laplace's equation is solved. The field at each node on the discharge electrode is compared with that obtained from a Peek-type empirical formula based on local curvature (or with the breakdown strength of air for flat or concave sections of surface). If the Poisson solution field exceeds this then the field is constrained to the appropriate magnitude in the direction of the Poisson solution and said to be coronating. Non-coronating nodes do not have their fields fixed but the ionic space charge density is fixed to zero.
The electrode surface boundary condition of being an equipotential surface is imposed during the initial Poisson FEM solution by forcing surface potential parameters to minimise the variational functional

\[ F_3(\phi) = \int_S \phi^2 - 2\phi V_\epsilon \, dS \]

over the electrode surface, where \( V_\epsilon \) is the applied electrode potential. (This functional is equivalent to using the least squares weighted residual method).

The problem is typically solved over a region bounded by a high-voltage discharge electrode, a planar earthed duct wall and several symmetry planes. The solution region is divided into a grid of tetrahedral elements each having 4 corner nodes and 4 mid-face nodes.

Table 5-1 summarises the iterative procedure described in [36]
step 1  Input grid data, electrode potentials, electrode radius of curvature at surface nodes and dust space charge distribution. Set ionic space charge distribution to be uniform and non-zero except at coronating nodes, where it is zero.

step 2  Find the variational FEM solution to Poisson's equation for potential using only dust space charge. Fix: electrode potentials, dust space charge distribution.

step 3  Identify the nodes on the coronating regions of electrode surface.

step 4  Find the variational FEM solution to Poisson's equation for potential and ionic space charge scaling factor. Fix: electrode potentials, field at coronating nodes, dust space charge distribution, shape of ionic space charge distributions.

step 5  Set potential and ionic space charge scaling factor to the Poisson solution values and change the ionic space charge at coronating surfaces in accordance with the scaling factor.

step 6  Find the Galerkin FEM solution to current continuity for ionic space charge. Fix: ionic space charge at coronating nodes, potential.

step 7  Set the ionic space charge to the current continuity solution.

step 8  If not converged go to step 2.

Table 5-1 Summary of iterative procedure

5.2.3.2 Assumptions, exclusions and limitations

The injection of charge at the discharge electrode is assumed to be governed by the fixed field charge injection law, see [11] for a discussion of this and other injection laws. For the 3D model it has been assumed that the electron mobility at any point is independent of the electric field at that point. Mobility therefore occurs as a constant in each term of the functionals and residuals and can be cancelled. This is considered further in chapter 6.

The model will not include temperature, humidity effects, turbulent gas flow or the dynamics of particle charging and collection. The applied potential is considered as constant in time, also see chapter 9.
Use of matrices to solve the system of simultaneous equations

The principle of finite element analysis is based on the minimisation of the functional for the problem with respect to each variable quantity or property, at each of the nodes. This results in a system of simultaneous equations, the solution of which determines the value of each of the unknown properties at the nodes. Once the node values of the parameters have been determined they can be substituted into the chosen expression and the value of the property calculated at any point within the element.

In the construction of the system of simultaneous equations to be solved the solution region is first considered as being made up of lots of separate, disconnected, elements. The node values of each element have been considered for that element individually. The way in which the nodes are connected together must be known in order to change to considering a system of connected simultaneous equations. In the system of connected equations the value of a parameter at any node is calculated to take full account of that node’s influence on, and by, each separate element that it is part of. In the disconnected matrix each node is only considered as a local node of a particular element. In the connected matrix each node has a global number to indicate its position within the whole solution region.

5.3 Requirements definition - Hardware

5.3.1 Financial and Time constraints

The research project was supported by EPSRC, DTI and National Power PLC. The project required the broad objectives of the research proposal to be completed within 3 years, i.e. by end of March 1996, and within the budget submitted in the proposal. No additional funds could be made available.

5.3.2 Hardware

The model is implemented on a Pentium90 with 32 Mbytes of RAM running under Windows 3.1 with 2 hard disk drives. Within the financial constraints the choice was between a high powered PC or a small unix-based workstation. The PC was the platform suggested by National Power PLC, one of the sponsors of
the project, as it was felt that it may be easier for their representative to make use of the program directly, although this was not a stated requirement.

The use of a Pentium 90 MHz processor with 32 Mbytes of RAM offered the best compromise between processor speed and size of RAM. The virtual memory is set up to use a permanent swap file of approximately 80 Mbytes on the second hard disk. A permanent swap file can be accessed more quickly than a temporary one. Dedicating a separate hard disk for use by the swap file maximises the size of the swap file. Windows 3.1 has not been designed to use RAM above 16 Mbytes efficiently, however, the use of 32 Mbytes allows finer grids to be used even if the memory is no longer used as efficiently as might be possible.

There are a variety of scientific software packages available for the PC. The development of the iterative procedure was being undertaken using MAPLEV, see section 5.6.3, on a separate PC. Building the model on a PC allowed an easy interface between the two machines which reduced the development time for the model and facilitated the incorporation of enhancements to the basic iterative procedure on which the model was based.

The model is written in MATLAB see section 5.6.3, which handles the memory management transparently to the user. This maximises development time for the construction of the FE model itself. See also section 5.4.2.

It would be possible to port the existing code, with some adaptations, to a workstation running UNIX. If the model is to be used to simulate more complicated geometries, using finer meshes it is expected that this would significantly reduce the running time, particularly through the more effective use of memory. The feasibility of this is discussed in chapter 9.

5.4 Design - high level

5.4.1 Principles of program design

There are several different methodologies for structured programming. Mostly these concentrate on the division of the problem into smaller and smaller steps that can be dealt with in turn. This is known as the ‘Top-Down’ approach. The
'Bottom-up' approach is the reverse method, where the lowest level functions are identified then combined by the use of higher level calling functions. Another technique that can be used in conjunction with the 'top-down' approach is the organising of the program code into separate procedures or modules that are called by a controlling program. This is known as the modular program approach and it is described more fully in [29].

5.4.2 Consideration of Object Oriented Programming
The interface program, see section 5.6.3.1, to convert the output from FEMGEN, the grid generation package, into the format required by the MATLAB program, was written in C++ using Object Oriented Programming techniques, OOP. The base class 'matrix' was built with member functions to create, access and update elements in a matrix. The matrix could be of type integer, float or short. OOP was chosen for this program as an investigation into whether OOP could be utilised for the construction of the model. Some initial work was done to identify objects within the model. This work is summarised in [7].

OOP is a popular method for building programs which aim for reusability with ease of maintenance and updating. It is considered that the objectives of the model are compatible with the ethos of OOP. Shammas, [57] was identified as having suitable source code that could be used for handling matrices within an OOP version of the model. To build an OOP model OOD, Object Oriented Design, would itself have to have been studied. There are texts, e.g. [13], and courses available in OOD, however the time needed to acquire OOD and OOP skills were not available within the time scale of the project. A commercially available package, such as MATLAB, has functions for standard matrix operations e.g. transpose and inversion, already available. The advantage of using such a package is that the research time could then be focused on developing the program to effectively use the analytical expressions already available and meet the objectives of the model.
5.4.3 Flow chart for the Iterative solution

The starting point for the design of the model is the iterative procedure detailed in Table 5-1. A control-flow structure to the model was chosen as this can be matched closely to the iterative procedure, and changes in the procedure could therefore be readily incorporated into the structure of the model. A 'Top-down' approach was used for the initial design of the model based on the flow chart in Figure 5-2. As additional features and details were incorporated then a 'Bottom-up' approach was usually employed.

The flow chart for the implementation of this procedure and the relationship to numbered steps of the iterative procedure is shown in Figure 5-2.
grid and boundary data Solve Laplace's Equation
Set field at coronating nodes
Set initial small space charge (zero at non-coronating discharge electrode nodes)
Start iterative procedure
Solve Poisson's equation
Set space charge at coronating nodes
Solve current continuity
set space charge to current continuity solution
Has solution converged?

Yes
Stop

No

Results from Laplace's equation

Solve Laplace's Equation

Results of this iteration

Start

Equivalent steps in the iterative procedure

step 1

step 2 without dust

step 3

step 1

step 4

step 5

step 6

step 7

step 8

Figure 5-2 Flow chart of the iteration process
The finite element model as described in [36] gives 8 stages in the iterative procedure. This includes the initial background charged dust. The present implementation of the model in MATLAB does not have background dust therefore the equation to be solved first is Laplace's rather than Poisson's. The solution of Laplace's equation gives the field components at the nodes; i.e. the field magnitude and direction to be used in determining which nodes are coronating.

5.5 Design - low level

To use the program for any geometry, general routines have been constructed that use data input files, that have been generated for a specific grid, to construct matrices that represent the way that the global nodes and their associated unknowns are connected to each other. Separate matrices of this type are required for Poisson and current continuity. General routines have also been written to collapse the matrix and vector for connected nodes to remove rows and columns that relate to the knowns. A reverse, vector expansion, routine is also available to construct a vector containing a full solution, e.g. for the solution to Poisson's equation the expanded vector contains the potential and field components for all nodes in the solution region.

To solve the initial Laplace’s equation, the matrix representing the simultaneous equations is constructed element by element taking into account whether any face or node(s) of the element are on an electrode boundary. Different expressions, derived from the appropriate functionals, are selected according to the properties of the individual element. In the variational method implicit boundary conditions are used but imposition of the appropriate zero field components at such boundaries improves accuracy and reduces the number of unknowns that have to be calculated (although more sophisticated pre-processing is required). A vector is derived to incorporate the known boundary conditions, i.e. the applied potentials on the inner and outer electrodes and the field components that have been set to zero to impose the symmetry boundaries. This vector also includes the constant terms that result from the derived expressions for curved surface electrode elements. This matrix and vector are
then collapsed to represent the system of simultaneous equations for all the unknowns. Multiplication of the resulting matrix and vector gives a vector containing these required unknowns. This vector is expanded to obtain the full solution. Figure 5-3 shows the flow chart for the operation converting the Laplace connected matrix into the Laplace collapsed matrix.

A similar procedure is followed for the solution of the Poisson and current continuity equations in the iterative procedure. For Poisson's equation the implementation of the boundary conditions for nodes on the discharge electrode requires the comparison of the initial Poisson solution field to the Peek-type fixed field expression, as described above. For a coronating node the field magnitude is fixed at the Peek field, in the direction as calculated for the initial Poisson solution. For a non-coronating node the space charge is fixed at zero. These boundary conditions are maintained for all future iterations. In the current continuity stage of the iteration the discharge electrode boundary space charge is set to zero for non-coronating nodes and for coronating nodes to the value calculated by the Poisson stage of the iteration. This boundary value therefore changes as the iteration proceeds and homes in on the actual value.
Figure 5-3 Flow chart for collapsing of Laplace connected matrix
The MATLAB program is designed to predict potential, field and space charge density for any geometry. The design of the grid is described in section 7.7. The FEA method requires the solution of a large system of simultaneous equations. This system is established by considering each individual element in turn and calculating the coefficients for each unknown within that element. This is done for all the elements. This ‘disconnected’ matrix must then be converted to a ‘connected’ matrix. By taking account of the connection of each element to neighbouring elements a ‘connection’ matrix is produced, which when operated on with the ‘disconnected’ matrix gives a further matrix which represents the coefficients of the global unknowns. The operations required to produce this matrix are described in Appendix A. This ‘connected’ matrix then requires further operations to remove the rows and columns that relate to known values, e.g. a node potential that is fixed because it is on an electrode. A similar procedure is required to remove rows from the boundary value vector. Manipulation of the collapsed connected matrix and the collapsed boundary vector gives the solution for the unknowns, as a vector. This is then expanded to include the known boundary values i.e. to give the full solution vector. This solution vector contains the potential, electric field components and space charge for every node and the mid-point potential for every element face. This same procedure is followed for solving Poisson’s equation and Current Continuity.

To summarise this procedure the principle matrices are defined in Table 5-2.
Matrix/Vector for Laplace | Purpose | Equivalent for Poisson | Equivalent for Poisson | Equivalent for Current Continuity
--- | --- | --- | --- | ---
matdis | Disconnected matrix of coefficients - each element considered individually | p_matdis | e_matdis |
conul | Connection matrix relating local nodes of each element to globally number nodes of solution region | conup | conuc |
imat | Connected matrix of coefficients - global numbering of nodes | pmat | cmat |
lmat | Collapsed matrix of coefficients - rows and columns relating to known values removed | pmat | cmat |
vk_kns | Vector of known node values, and constant terms | pois_kns | chg_kns |
uk_sol | Vector of calculated value of unknowns | uk_sol | uk_sol |
lp9_sol | Vector of all node values | pois9_sol | cc9_sol |

Table 5-2 Summary of matrices and vectors required by the program.

5.5.1 Reusable functions

The design of functions for handling matrices and vectors in solving Laplace’s equation is then used to build similar functions for use in solving Poisson and Current Continuity. The function for collapsing the connected matrix has been shown in Figure 5-3. The same design, with the addition of the copying of the row and column for the scaling factor, k, is used for collapsing the Poisson connected matrix. To collapse the connected matrix for current continuity also uses the same design, but here it is less complicated as there are no face nodes and there is only one parameter at each node. This reusability of design was carried forward into the reusability of code, as the function for collapsing the Poisson connected matrix was written by copying the related function for Laplace and then adapting it, rather than having to write it from the design. This enabled new features to be rapidly included.
5.5.2 Use of Global Variables

Constants that remain unchanged through the program are declared as global variables. The initial values of these variables may be from data files or calculated within the program. In addition the disconnected matrices for Laplace, Poisson and current continuity are also declared as global. The values of the elements in these matrices are changed through the iteration procedure but they are declared as global to avoid passing them into functions as variables. In MATLAB functions the variables are copied when the function is called, and this would use more memory, and therefore slow down the prediction program.

5.6 Implementation

5.6.1 Development of Structure Diagrams

Structure diagrams for implementation of the low level design in MATLAB, see section 5.6.3, are shown separately for the 1D field dependent mobility model in chapter 6, and for the 3D constant mobility model in chapter 7. The structure diagrams are different because of the increase complexity of the 3D model, e.g. more stages are required in the construction of the disconnected matrices, rather than because of the different treatment of mobility.

5.6.2 Imposition of boundary conditions

To solve the governing differential equations the known boundary conditions must be imposed for each set of equations. The boundary conditions dictate which parameters at which boundary nodes are ‘knowns’.

The boundary conditions are shown in Table 5-3.
Differential Equation | Boundary Condition
--- | ---
Laplace | applied potentials at discharge electrode (plane electrodes only) and collecting electrode
| The field direction at the electrodes is fixed at perpendicular to the surface normal, by means of a data file giving the cosine of the angle of the surface normal to each of the axes

Poisson | applied potentials at discharge electrode (plane and curved) and collecting electrode
| for coronating nodes the field magnitude is fixed at the critical field, in the direction calculated by Laplace

Current continuity | for coronating nodes the space charge is fixed at the value calculated by Poisson
| for noncoronating nodes the space charge is fixed at zero

Table 5-3 Boundary Conditions for the Differential Equations to be solved in the iterative procedure.

The setting of these boundary conditions as part of the iterative loop is shown in 5.6.2. The determination of the magnitude of the critical field has been explained in section 1.2.6. The use of the variational functional for Laplace and Poisson means that the field is implicitly set along the grid boundary. In 1D this ensures that symmetry boundaries are set automatically. In 3D, to improve accuracy and reduce computation time, the field components that are zero for nodes along any grid boundary are explicitly set at zero. The Galerkin residual method does not set symmetry boundary conditions implicitly. In the 3D model this is partly corrected by the use of cyclical boundary conditions or 'wrapping', connecting nodes on the upper plane of the grid to nodes on the lower plane, as explained in section 8.3.4.

5.6.2.1 Implementation of the fixed field injection law

The phenomena of charge injection is explained in section 1.2.1. Mathematical representations of charge injection are reviewed by Budd and Hare in [11] and considered in section 1.2.9.

The setting of the additional boundary conditions for the nodes on the discharge electrode for solving Poisson's equations and current continuity depends on
whether the node is coronating or not. For each node on the discharge electrode the magnitude of the Laplacian field must be examined. The critical field at the node is determined having reference to the local radius of curvature at this point. If the Laplacian field is greater than the critical field then the node is considered to be coronating.

Having calculated the solution to Laplace’s equation the calculated values of potential on the vertex and face nodes on the discharge and collecting electrodes become part of the imposed boundary values for the solution of Poisson’s equation.

For Poisson’s equation:

- At coronating nodes: field magnitude is fixed to the critical field for that node, in the direction of the Laplacian field.
- At non-coronating nodes: field components are unknowns.

For current continuity:

- At coronating nodes: space charge is set to a small initial value. This initial value depends linearly on the difference between the Laplacian field and the critical field. For further iterations the space charge is fixed at the present value multiplied by the scaling factor.
- At non-coronating nodes: space charge is set to zero.

For the 3D model the small initial values of space charge at the discharge electrode nodes are set in a linear relationship to magnitude of the Laplace field over the critical field at each node, see section 7.6.

5.6.3 Use of commercial software packages

To develop the quasi-electrostatic simulation program to predict the potential, electric field, space charge and current density, for general discharge electrode geometries in electrostatic precipitators several high level software packages have been employed.

MATLAB, [62], is high level numerical manipulation and data visualisation package. It is designed for the efficient manipulation of matrices - its basic data
type is the matrix. MATLAB incorporates functions for many standard matrix operations e.g. inverse and transpose and it will also handle sparse matrices. The 3D prediction program has been written in MATLAB. MATLAB is also used to plot results.

MAPLEV, [12], is a powerful symbolic computation package. This was primarily used to derive the Hermite cubic representation of potential and linear representation of space charge. From these expressions the Variational functionals and weighted Galerkin residuals are formulated in MAPLEV and converted, using a ‘C’ program, to MATLAB functions.

FEMGEN/FEMVIEW, [27], is an interactive pre- and post-processor for FEA. FEMGEN is used for grid generation, see section 7.7. The FEMGEN output file is interfaced to MATLAB via a ‘C++’ program which converts the generated grid of prisms to Tetrahedra and presents the data in a form that can be input directly to MATLAB.

The interaction between these software packages is represented in Figure 5-4.
The model was developed symbolically using MAPLEV to produce the general symbolic form for a finite element. The use of Maple V, which was used to as
late a stage as possible in the model development, greatly reduced the opportunity for the occurrence of software errors. The reasons for this are:

- The symbolic formulation of the model is a mathematically correct expression of the initial equations and approximation scheme.
- The optimised code for implementing the final symbolic formulation of the model is generated automatically as output from MAPLEV using the worksheet containing this formulation. The symbolic approach to the model reduced computation in the numeric implementation whilst maintaining accuracy and generality.

The general symbolic formulation can be applied to a large number of problems and can be built on to tackle more complex problems. Exactly soluble problems were used for initial testing. The procedure allows modifications even down to the basic model structure to be developed quickly and incorporated. The use of symbolic methods allows possible extensions of the model to be accommodated in a clear and structured manner. The design of the program therefore requires an implementation of the general solution method, using the expressions derived analytically using MAPLE V, which can be used for any discharge electrode geometry.

5.6.3.1 Convert FEMGEN output in MATLAB data file format
MATLAB can load data directly from ASCII files, provided that it is in the form of a matrix, which may have only one row or column - a vector, or a single element. The FEMGEN output file, see section 7.7.2, contains most of the grid information required by the program but in a form that can not be read directly. An interface program was written in C++, using Object Oriented Programming, to reading the FEMGEN data file, convert the grid from prisms to tetrahedrals and write the resulting matrices to separate files.
5.6.3.2 Convert optimised C code into MATLAB function format

MAPLEV includes the facility to produce optimised C code. This is used to generate individual files of the coefficients of the expressions that are to be evaluated to construct the disconnected matrix. A 'C' program has been written to convert each of these files into MATLAB functions that are then called in turn to construct the disconnected matrix for the required grid and applied potentials.

5.7 Testing

As much testing as possible was undertaken during the construction of the model. The model is complicated and the testing of individual functions as they were coded was necessary to trap possible errors that would be difficult to locate at a later stage. The more difficult aspects to test were the introduction of new features when the main structure of the model was completed. The main aspect of testing at this stage was the printing out to screen, or storing in data files, of the variables that would be changed by the new feature and checking that the changes were as expected. This is a time consuming method of testing. A debugger that tracks the values of target variables, such as that included in the developers environment for Microsoft Visual C++ would be an advantage if the model was converted to a 3GL. Testing is also required each time a new grid is used.

5.7.1 Testing during coding

MATLAB allows the direct calling of functions from the run-time environment, as well as calling from a controlling program. Data files were loaded into the environment and the required variables declared as global. Individual functions were coded and called to test for syntax errors and correct operation. In the initial construction of the program this testing was carried out as functions were designed and coded.

The functions for collapsing the connected matrices and vectors, and expanding the vector of unknowns to the full solution, were tested by using dummy vectors and matrices. The elements of the dummy were integers, the value of which
reflected their place in the input matrix. The elements in the output matrix or vector are then examined to ensure that elements have been moved, inserted or discarded correctly.

Once the early version of the main controlling program, contained in a script file, was complete all the functions could be tested together. The key matrices and vectors were stored as ASCII files to be examined individually in the case of errors; additionally their size is output to the screen for checking as the program was running. The storage requires the writing of data to the hard disk which significantly increases the running time of the program. As stages of the program were checked the instructions to store the matrices and vectors were ‘commented out’, so that they could readily be used again if new features necessitated further testing. MATLAB includes the command ‘keyboard’ that can be included in the script or function files. Once this command is reached the operator can enter additional commands via the command window to examine the state of variables local to the current function.

When the expressions derived from the functional for equipotential were available to be incorporated the functions to create the disconnected matrices were redesigned and coded. This was tested using the plane-plane geometry but setting the input data files to show that the electrodes are curved. The changed size of the matrices and vectors was monitored on screen. The prediction from the program was checked; it should be the same as for using the plane electrode expressions, to within the numerical accuracy of the computer and MATLAB.

When a program has run the complete script, or the program has crashed, the global variables can still be examined via the command window.

3.7.2 Checking the Laplace solution

The first stage of the program is the calculation of the solution to Laplace’s equation. This part of the program was coded first. The solution vector is stored as a data file. Additionally the Laplace solution is stored as iteration 0 in the data file which stores the output of each iteration of Poisson’s equation and current continuity. The Laplace solution data file, called lp9_sol.dat, is easily accessed from within MATLAB. lp9_sol.dat lists the vertex node potential and
field components; x, y and z; for each node in global number order and the face potentials. In addition to showing whether the correct answer has been calculated it is examined to check for possible errors in the input data files. The aspects considered are:

- correct applied potentials at the electrodes
- monotonically changing potential
- monotonically changing field components
- zero field components along symmetry boundaries where specifically set
- symmetry in the node values where this would be expected for a specific grid.

In the case of a wire in a duct the field magnitude on the wire at the node closest to the collecting plate shown be greater than that at the node furthest from the plate. Nodes in between should have a monotonically changing field magnitude.

The final test for the Laplace solution is that it closely matches the analytical solution. There will be some error due to the coarseness of the grid and the success, or otherwise, of the matching of the equipotential surface to the electrodes.

5.7.3 Checking the Poisson solution

In normal operation the program will consider the magnitude of the Laplace field at each node on the discharge electrode surface. If the Laplace field is greater than the critical field then the field is set to the critical field. If the Laplace field is smaller than the critical field then the field components are recalculated in the Poisson stage of the iteration. For the plane-plane geometry the charge injection law is simulated by setting the field at one of the electrode surfaces to half the Laplace field. To test the implementation of the Poisson functionals the code is temporarily adapted to set the field at all the nodes on the discharge electrode boundary to the Laplace field. The space charge scaling factor should then be calculated to be zero. This gives zero space charge which
is the Laplace condition. For plane-plane grids aligned along an axis the scaling factor is calculated to be between $10^{10}$ and $10^{12}$, for the general orientation plane-plane grids the scaling factor is of the order of $10^9$ and for the simple cylindrical grid the scaling factor is calculated to be $10^4$.

5.7.4 Comparison to analytical solutions
For plane plane geometry and cylindrical geometry the solution of Laplace's equation and the predictions for the full ion-drift solution are compared to analytical solutions. The derivations of these analytical solutions are reported in [35] and the results of the comparison, with accuracies achieved, are shown in chapter 8.

5.7.5 Problems that were difficult to solve
During the building of the program there were two particular problems that were difficult and time consuming to identify. These are described below and a suggestion for identification of such problems is given.

5.7.5.1 The missing volume factor
As explained in section 5.2.1, this program was developed as part of an on going research program and many of the required details of the program only became known during it's construction. Much of the analytical work in deriving the cubic expression for potential and the functionals and residuals was undertaken by a colleague. It had initially been the intention to use the Galerkin weighted residual method to solve both Poisson's equation and current continuity. During the early part of the investigation it was decide to develop, in parallel, the variational functional method for Poisson. In each case local co-ordinates were used to simplify the expressions. The expressions required to solve Laplace's equation were derived first to enable a simple comparison the two methods. It was found that the imposition of the symmetry boundary conditions in the Galerkin method would be very complicated and consequently the variational functional method was chosen. This was implemented in 3D and accurate results obtained for the plain-plain geometry, using the test grid called the 'Toblerone'. However, correct results could not be obtained for a cylindrical
geometry. Considerable time was expended in trying to find the cause of this problem. Since the program could produce the correct prediction for the plain-plain geometry it was thought that the difficulty was connected to the matching of the potential to the curved inner and outer electrode. It was subsequently found that results for the plain-plain geometry were correct by chance; the expressions had been incorrectly derived. The integration in local co-ordinates required the use of a volume conversion factor, so that the resulting expressions would be equivalent to those which would have been obtained if Cartesian co-ordinates had been used. The ‘Toblerone’ grid, see section 8.3, uses elements of equal volume, so that the error cancelled out in the solution of the simultaneous equation. The expressions for the variational functional method had by then also been completed independently by a colleague. The mistake was found only by detailed comparison between the two derivations. This mistake lead to the following schedule of testing:

- ‘Toblerone’ aligned along the x axis, with elements of equal volume
- ‘Toblerone’ aligned along the y axis, with elements of unequal volume
- ‘Toblerone’ aligned along the z axis, with elements of equal volume.

For the grid aligned along an axis many terms in the coefficients go to zero, as at least one face in each element is perpendicular to one of the axes. Also several ‘Toblerones’ were combined to obtain a rectangular grid, 1 element deep, results from which are shown in section 8.3.4. Additional testing with the ‘Toblerone’ grid was undertaken to ensure there was no directional bias that might be hidden by these terms becoming zero. Bias may arise through incorrect derivation of the cubic potential or terms being omitted from the integration. Orientations of the grid used were:

- ‘Toblerone’ in the x-y plane, with elements of equal volume
- ‘Toblerone’ in a general orientation, with elements of equal volume.

These test grids were used to check the implementation of new features of the model as they were implemented. The identification of this particular error was
primarily due to the comparison of the two derivations made by different people. A similar process identified an error in the handedness of the grid elements.

5.7.5.2 Right-handed Tetrahedra

It is important that all the elements of the finite element grid have the same handedness. This means that the local numbering of the 3D elements should always be clockwise, or anti clockwise. They should all be the same as the integration over the surface will be calculated with the wrong sign for those elements that are numbered in the opposite sense. Similarly with the 3D tetrahedral elements for the integration over a volume. A right-handed tetrahedral is one where local node 1 can be imagined at the Cartesian origin, local node 2 then lies in the direction of the x axis, local node 3 in the direction of the y axis and local node 4 in the direction of the z axis, see Figure 5-5.

For elements numbered in the opposite sense the integration over an element will give the same magnitude but opposite sign. In the matrix manipulation required to convert the disconnected matrix to the connected matrix these opposite signs will result in the incorrect calculation of some of the entries in the connected matrix.
The grids generated by FEMGEN, [27], all use right-handed elements. In converting a FEMGEN grid, see section 7.7.3, care is taken to ensure that this right-handedness is preserved.

Of the four vertex nodes in a tetrahedral a maximum of three can be on an electrode boundary. The matrix 'elem' contains the global node numbers for each of the local nodes in each element. To simplify the identification of the correct functional to use for each node, 'elem' is sorted so that nodes on an electrode are only in local node positions 1, 2 or 3. Local node 4 is therefore always a bulk node and bulk expressions will always be appropriate. This sorting must ensure that the right-handedness of the tetrahedral is maintained.

The first version of the sorting routine, 'sortelem.m', was only required to consider elements having a face on an electrode. In such an element the only bulk node was identified and the nodes rotated so that the bulk node was in the position of local node 4. For example

if the boundary electrode element has, in global numbering, the following nodes

\[ 26810 \]

where local node 1 has global number 2 etc. and global node 6 is the bulk element, then the numbering becomes

\[ 81026 \]

In this case the handedness has been maintained as the node numbering had been rotated through 2 places. By chance, the grids in use at the time this routine was developed all had the bulk node of an electrode surface element in local node position 2 or position 4. The error was in thinking that the right-handedness was maintained if the rotation of the numbering was through 1 or 3 places. For example, in the same element

\[ 26810 \]

if global node 8 is the bulk node and 'sortelem' rotates the node numbering to

\[ 10268 \]

but the tetrahedral is now left-handed.
This mistake was identified at the time the bulk expressions for the field on the electrode surfaces were introduced. These expressions were used for nodes that touched an electrode surface, as well as for nodes that are part of a face on an electrode. The sorting routine was adapted to identify elements that contain any nodes on an electrode and to renumber the nodes so that local node 4 is always a bulk node. Incorrect predictions were obtained but no errors in the derivation of the new expressions or the use of them in the program could be found. The new expressions had been derived by a colleague using MAPLEV. To check further the implementation of the expressions in the 3D model The MAPLEV code was adapted to try to reproduce the disconnected matrix for a simple grid. In this case the ordering of the nodes within an element was not changed. In comparing the numbers in the disconnected matrix produced by the two methods it was noticed that for most elements the numbers were the same, but for some the sign was changed. Those elements where the sign was changed were identified as those where the ordering of the nodes had been rotated by 1 or 3 places. In these cases an additional swap of nodes was also required to restore the right-handedness. For example the element having nodes

\[2 \ 6 \ 8 \ 10\]

where node 8 is the bulk node is rotated 1 place and then local nodes 1 and 2 are swapped to become

\[2 \ 10 \ 6 \ 8\]

The element sorting function was rewritten and called 'srt2elem.m'.

This is further example of how a particular feature of a simple grid has allowed the program to appear to be operating correctly when there is a error. In each case the problem was identified by cross checking between this program and the MAPLEV code used by a colleague for the derivation of the functionals and residuals. MAPLEV itself was not suitable for the building of the full 3D program because it is much, up to 10 times, slower in carrying out the matrix operations. It is also more difficult to prepare data files for input to MAPLEV; detailed formatting with brackets and commas is required. In MATLAB matrices and vector are input using simple ASCII files containing the elements
of the matrix/vector and having the same name as the matrix with an extension 
'.dat'.

5.7.6 Typical run-time errors
Each time a new grid is used the Laplace solution should be examined closely as 
explained in section 5.7.2. In addition many possible errors in the input data 
files will be evidenced by error messages during run-time. Some example are 
given below.

5.7.6.1 Duplicate node numbers in an element
If any element has a node repeated then this an element of zero volume, in the 
case of 3D, or zero length , in the case of 1D. The MATLAB generated message 
"Warning: divide by zero" is displayed on the screen. The error may be found by 
inspection. In the case of larger grids the matrix generating routine is amended 
to output to screen the number of each element as calculations are made, so that 
the error is quickly located.

5.7.6.2 No coronating nodes
If no coronating nodes are identified the first iteration for Poisson’s equation 
will be completed but a null vector will be generated as the vector of ‘knowns’ 
for current continuity. The MATLAB generated error message “Inner matrix 
dimensions must agree” will be displayed on the screen.

5.7.6.3 Inconsistencies in defining node types
The 3D model uses 12 separate input data files, see section 7.9, to define the 
grid and the properties of it’s nodes and elements. At present there is no 
mechanism for checking that the information in the separate files is consistent. 
If in one file a node is specified as having a fixed potential, but in a separate file 
is specified as being on a curved electrode surface, for which the potential is an 
‘unknown’, then the row relating to this node potential at in the disconnected 
matrix will contain zeros, and the connected matrix will be singular. The 
MATLAB generated message “ Matrix is singular to working precision” will be 
displayed on screen.
A user interface to the model, with checking of the input data and graphical display of the predictions, is considered as possible further work in chapter 9.
6. IMPLEMENTATION OF 1D MODEL WITH FIELD DEPENDENT MOBILITY

6.1 Variation of ion mobility with high electric field

This chapter describes the extension of the 1D model described in [36], see Appendix C, to include a simple relationship between the field strength and the ion mobility, (section 2.5). For the simple cylindrical geometry [9] has shown that for an applied voltage of -300 kV the field strength near to the discharge electrode is of the order of 5 MV/m. At this magnitude the ion mobility is unlikely to be independent of field although the dependence of the mobility on the field magnitude is not fully understood.

The standard ohmic (i.e. constant mobility) model assumes that the magnitude of the drift velocity is much less than the thermal speed of the carriers so that the electric field only has a small effect on the distribution of thermal velocities. As the field strength increases, the energy gained between collisions will also increase, and the average drift velocity will increase until it is no longer negligible compared to the thermal speed of the gas ions. Cobine, [14], gives data that shows \( \mu \) for positive ions to be constant up to a critical \( \frac{E}{p} \), where \( E \) is the field strength and \( p \) is the gas pressure after which \( \mu \) increases linearly with \( \frac{E}{p} \). Loeb, [44], quotes several sets of experimental data where the mobility of ions at high fields have been investigated. The results are inconclusive; in some case \( \mu \) increases as \( E \) increases, in some it increases to maximum and then decreases in a hyperbolic manner. In section 2.5 it is assumed that the drift velocity is much smaller than the thermal speed.
Thomson and Thomson, [63], states that if the thermal speed is large compared to the drift velocity then the drift velocity is proportional to $\frac{E}{p}$, and the total velocity, $v$, will be of the form

$$ v = c \frac{E}{p} $$

Equ. 6-1

where $c$ is a constant so that:

$$ \mu = \text{constant} $$

Equ. 6-2

This is the dynamic equilibrium case considered in section 2.5.1.1.

If the thermal speed of an ion is small compared to the drift velocity, which may be the case at very high fields (or low pressures), then the drift velocity is proportional to $\sqrt{\frac{E}{p}}$, and the total velocity, $v$, would be of the form

$$ v = a \sqrt{\frac{E}{p}} $$

Equ. 6-3

where $a$ is a constant so that

$$ \mu \propto \sqrt{\frac{1}{Ep}} $$

Equ. 6-4

This is the high field case considered in section 2.5.1.2.

In Equ. 6-1 $\mu$ is independent of $E$ but in Equ. 6-3 $\mu$ is dependent on $E$.

Experimental evidence in [63] shows that the effect of this dependence can not easily be quantified, possibly because the state of the ion changes during its passage through the field and measurements are an average of its behaviour during these different states.
More recent papers have presented expressions to represent the relationship between ion mobility and field strength. Abdel-Salam [1] gives the ion mobility, in dry air, related to the distance travelled, d, from the discharge electrode of radius $R_0$.

$$\mu_d = \mu_0 \exp \left( -\frac{1}{\alpha} \frac{d^2}{E} \right)$$

where $\alpha = 4 \times 10^{-5} \text{m}^2 \text{V}^{-1}$ and $\mu_0$ is the ion mobility averaged over the ionisation zone, $= 4 \times 10^{-4} \text{m}^2 \text{V}^{-1} \text{s}^{-1}$. This value is supported by Hayashi et al, [33], where the measured mobility, for zero field, at atmospheric pressure for O$_2$ is $2.05 \times 10^{-4} \text{m}^2 \text{V}^{-1} \text{s}^{-1}$. Over the range of $E/p$ 10 to 100 Vm$^{-1}$Torr$^{-1}$, i.e. for fields in the range 7850 Vm$^{-1}$ and 78500 Vm$^{-1}$ at atmospheric pressure the mobility decreases slightly from 2.05 to $1.8 \times 10^{-4} \text{m}^2 \text{V}^{-1} \text{s}^{-1}$. The data shown by Hayashi is plotted on a log scale. Visual inspection of the plot suggests a power law of the form $\mu \propto |E|^{-0.8}$, which indicates that mobility is almost independent of field.

Since mobility $\mu$ is no longer considered constant an expression for the relationship between mobility and field strength must be determined and then used to derive the Galerkin residual for current continuity. For the purposes of investigating whether the model design produced in section 5 can be extended to take account of field dependent mobility a simple expression for this relationship will be used and implemented in 1D.

A simple relationship is chosen first to test the derivation of the residual and the implementation of this in the 1D model. The feasibility of other relationships is considered in section 6.2. The chosen representation of the mobility in terms of field magnitude is linear:

$$\mu = A|E| + B$$

where A and B are constants.
The chosen expression is not intended to reflect accurately the physics of ion mobility at high fields but to test the design of the model. The two constants in this expression will be chosen by reference to experimental data, see above, although it is not expected that any physical conclusions can be drawn since the data does not relate directly to the field magnitudes present in an electrostatic precipitator.

6.2 Derivation of the Galerkin Residual

The standard Galerkin residual, [36], is given by:

\[ \text{Residual} = \int_V \nabla(\sigma E) dV \]

Starting from Kirchhoff’s Law and Ohm’s Law in vector form:

\[ \nabla \cdot J = 0 \]
\[ J = \sigma E \]

therefore

\[ \nabla(\sigma E) = 0 \]

using a vector identity, for \( \sigma = \text{constant} \),

\[ \sigma \nabla E + (\nabla \sigma) E = 0 \]

but \( \sigma = \rho, \mu \) where \( \rho = \text{space charge} \).

An expression for \( \mu \) in terms of \( E \) is required. Using the linear expression Equ. 6-6, and remembering that \( \rho = \text{constant} \) so that:

\[ \sigma = \rho (A|E| + B) \]

and this gives

\[ \rho (A|E| + B) \nabla E + \nabla (\rho (A|E| + B)|E|) = 0 \]
but

\[ \mathbf{E} = -\nabla \phi, \quad |\mathbf{E}| = |\nabla \phi| \quad \text{and} \quad \nabla \cdot \mathbf{E} = \nabla^2 \phi \]

therefore

\[ \text{Equ. 6-14} \quad -\rho (|\nabla \phi| + B) \nabla^2 \phi - (\nabla \rho (|\nabla \phi| + B)) \nabla \phi = 0 \]

again using vector identity

\[ \text{Equ. 6-15} \quad -\rho (|\nabla \phi| + B) \nabla^2 \phi - (\rho \nabla (|\nabla \phi| + B) + (\nabla \rho (|\nabla \phi| + B)) \nabla \phi = 0 \]

Equ. 6-15 gives a general expression for \( \nabla (\sigma \mathbf{E}) \), in any number of dimensions, which can be integrated to give the Galerkin Residual. In this expression the difficult term to integrate is \( |\nabla \phi| \).

### 6.3 The Galerkin Residual for 1D with cylindrical symmetry

For 1D with cylindrical symmetry Equ. 6-15 becomes

\[ -\rho \left( \frac{d^2 \phi}{dr^2} + B \left( \frac{d \phi}{dr} + \frac{1}{r} \frac{d \phi}{dr} \right) \right) \left( \nabla \rho (|\nabla \phi| + B) + (\nabla \rho (|\nabla \phi| + B)) \nabla \phi \right) = 0 \]

which can be rearranged to give

\[ \text{Equ. 6-16} \quad -\rho \left( \frac{d^2 \phi}{dr^2} \left( \frac{d \phi}{dr} + A \frac{d \phi}{dr} + \frac{B \phi}{dr} \right) \right) - \left( \rho \frac{d \phi}{dr} - \frac{d \phi}{dr} \right) + \frac{d \phi}{dr} + (\nabla \rho (|\nabla \phi| + B)) \nabla \phi = 0 \]

If the terms involving \( \frac{d \phi}{dr} \) can be integrated then Equ. 6-16 can be integrated over each 1D element. In the 1D case of cylindrical symmetry the form of the function \( \phi(r) \) is known and therefore \( |\nabla \phi| \) can be integrated. This is illustrated in Figure 6-1 to Figure 6-3. This would not be the case in 3D as the gradient of \( \phi(x,y,z) \) can vary in each direction and the appropriate limits of the integration in each direction can only be determined by examination of each
point within the solution region, rather than being established for the general case.

In this case $\frac{d\phi}{dr}$ can be integrated as $\frac{d\phi}{dr}$.
6.4 Implementation of 1D field dependent mobility

The derivation of the Galerkin residual and the Poisson variational functionals is carried out in MAPLEV, as explained in Figure 5-4 and the expression for the calculation of each element of the disconnected matrix then converted into C code using the MAPLEV conversion functions and then converted into the form required to be MATLAB functions.

For the simple 1D grid of 4 nodes, i.e. 3 elements, the connected matrix is calculated directly, rather than creating the disconnected matrix and the connection matrix and then using matrix manipulation, see Appendix A.

6.5 Structure of 1D Model

The structure of this 1D program, shown in Figure 6-4, is derived Figure 5-2. This is because the changes required for the field dependent mobility are at the analytical stage, i.e. in the symbolic formation of the expression to generate the matrices, rather than in the way the matrices are constructed or manipulated.

The method for handling the imposition of boundary conditions is the same, as is the method for collapsing the matrices, in both Poisson and current continuity, to remove matrix positions that relate to known values. The method of expanding the solution vector of unknowns to include the knowns, and therefore become the full solution vector is also the same. This illustrates the general applicability of the matrix handling routines that have been developed.
The general procedure for the solution of Laplace's equation, Poisson's equation and current continuity is the same. This is illustrated in the structure diagram of the routine to solve Laplace's equation which is shown in Figure 6-5.
Figure 6-3 Structure diagram of functions to solve Laplace's equation

Figure 5-3 shows the general procedure for collapsing the connected matrix to remove the rows and columns relating to known values of parameters. The structure diagram to implement this in 1D is shown Figure 6-6.
The structure diagram for collapsing the Poisson connected matrix and the current continuity matrix is similar to that for Laplace shown in Figure 6-6.

6.6 Testing of the 1D FDM Model
In addition to using the general testing methods described in section 5.7 the 1D field dependent model was tested by setting the mobility to be independent of field and comparing the results to the field independent mobility (FIμ) solution. In each case the number of iterations was chosen to ensure than the space charge scaling factor was 1 for at least 2 iterations before the program terminated.

6.6.1 Comparison to constant mobility model
If the constants are set to A=0, B=1 then the model is assuming mobility to be independent of field. An applied potential of -300kV is set at the inner electrode.
and 0 kV at the outer electrode. The Laplace analytical solution, see [35], for this applied potential shows field strengths of approximately 6000 kV/m at the inner electrode and 1250 kV/m at the outer electrode. The results are shown in Figure 6-7 to Figure 6-12.
Figure 6-7 Potential, blue line is calculated value, red line is FIμ value.

Figure 6-8 Electric field, blue line is calculated value, red line is FIμ value.

Figure 6-9 Charge density, blue line is calculated value, red line is FIμ value.

Figure 6-10 Percentage error in calculated potential.

Figure 6-11 Percentage error in calculated field.

Figure 6-12 Percentage error in charge density.
The errors are calculated as a percentage of the mean of the exact field independent mobility (FIμ) value of the parameter over the solution. It is therefore expected that the %age error will be greater near the inner electrode than near the outer electrode, as the value of the parameters is greater at the inner electrode. The errors of less than 0.5% in potential, 2% in electric field and 6% in charge density were achieved with 7 iterations. It is to be expected that the error in charge density will be greater than that in potential and electric field since the approximation for charge over an element is linear, compared with the cubic approximation of potential. For the coarse grid in use, 3 elements and 4 nodes, the accuracy achieved is good.

6.7 Results from 1D Model

The model has been used to investigate the effect of two different values for zero field mobility (i.e. constant B in Eqn. 6-4, see section 6.1. For one zero field mobility value the predictions are compared between mobility being independent of field, increasing with field and decreasing with field. For the second zero field mobility value predictions for two rates of increase in mobility are compared. The chosen values for A and B are shown in Table 6-1.

<table>
<thead>
<tr>
<th></th>
<th>B zero field mobility m(^3)V(^{-1})s(^{-1})</th>
<th>A rate of change of mobility with field m(^3)V(^{-2})s(^{-1})</th>
<th>Results section</th>
</tr>
</thead>
<tbody>
<tr>
<td>mobility independent of field</td>
<td>2.22*10(^{-4})</td>
<td>0</td>
<td>6.7.1.1</td>
</tr>
<tr>
<td>mobility increases with field</td>
<td>2.22*10(^{-4})</td>
<td>3*10(^{11})</td>
<td>6.7.2</td>
</tr>
<tr>
<td>mobility decreases with field</td>
<td>2.22*10(^{-4})</td>
<td>-3*10(^{11})</td>
<td>6.7.2</td>
</tr>
<tr>
<td>mobility decreases with field</td>
<td>2.05*10(^{-4})</td>
<td>10(^{11})</td>
<td>6.7.3</td>
</tr>
<tr>
<td>mobility increases with field</td>
<td>2.05*10(^{-4})</td>
<td>3*10(^{11})</td>
<td>6.7.3</td>
</tr>
<tr>
<td>mobility increases with field</td>
<td>2.05*10(^{-4})</td>
<td>10(^{10})</td>
<td>6.7.3</td>
</tr>
</tbody>
</table>

Table 6-1 Constants chosen to test the 1D field dependent mobility model
The effect on mobility of these constants for the range of field magnitude in the solution region, for an applied potential of -300kV, is shown in Figure 6-13 and Figure 6-14.

Figure 6-13 Zero field mobility = 2.22 \times 10^{-4} \text{ m}^2\text{s}^{-1}\text{V}^{-1} (black), the rate of increasing mobility (blue) is 3 \times 10^{-11} \text{ m}^3\text{V}^2 \text{s}^{-1} and the rate of decreasing mobility (red) is -3 \times 10^{-11} \text{ m}^3\text{V}^2 \text{s}^{-1}.

Figure 6-14 Zero field mobility = 2.05 \times 10^{-4} \text{ m}^2\text{s}^{-1}\text{V}^{-1} (black), the rate of increasing mobility is 10^{-11} \text{ m}^3\text{V}^2 \text{s}^{-1} (blue), 3 \times 10^{-11} \text{ m}^3\text{V}^2 \text{s}^{-1} (red) and 10^{-10} \text{ m}^3\text{V}^2 \text{s}^{-1} (green)
6.7.1 Mobility independent of field

Figure 6-15 Potential, blue line is calculated value, red line is $F_l\mu$ value

Figure 6-16 Electric field, blue line is calculated value, red line is $F_l\mu$ value

Figure 6-17 Charge density, blue line is calculated value, red line is $F_l\mu$ value

Figure 6-18 Percentage error in calculated potential

Figure 6-19 Percentage error in calculated field

Figure 6-20 Percentage error in charge density
Using a realistic value for constant mobility rather than $B=1 \text{ m}^2\text{V}^{-1}\text{s}^{-1}$ as in the testing stage gives the same predicted values for potential, field and charge density, see Figure 6-15 to Figure 6-20. This is expected because when mobility is a constant it cancels from each term in the residual and therefore its actual numerical value has no effect.

### 6.7.2 Comparison of increasing to decreasing mobility

Figure 6-21 to Figure 6-26 shows the predictions for increasing mobility with field. Figure 6-27 to Figure 6-32 shows the predictions for decreasing mobility with field. In both cases the zero field mobility is 0.00022. In all cases 9 iterations were made.

<table>
<thead>
<tr>
<th>Mobility</th>
<th>Potential</th>
<th>Electric Field</th>
<th>Space Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>Increase with field</td>
<td>± 1.4%</td>
<td>± 4 %</td>
<td>± 12 %</td>
</tr>
<tr>
<td>FIGURES 6-21 AND 6-24</td>
<td>FIGURES 6-22 AND 6-25</td>
<td>FIGURES 6-23 AND 6-26</td>
<td></td>
</tr>
<tr>
<td>Decrease with field</td>
<td>± 0.5%</td>
<td>± 2.5 %</td>
<td>± 14 %</td>
</tr>
<tr>
<td>FIGURES 6-27 AND 6-30</td>
<td>FIGURES 6-28 AND 6-31</td>
<td>FIGURES 6-29 AND 6-32</td>
<td></td>
</tr>
</tbody>
</table>

*Table 6-2 Comparison of errors for predictions with increasing and decreasing mobility.*
A = 3 \times 10^{-11} \text{ m}^2 \text{V}^{-2} \text{s}^{-1} \quad B = 2.22 \times 10^4 \text{ m}^2 \text{s}^{-1} \text{V}^{-1}

Figure 6-21 Potential, blue line is calculated value, red line is $F_{\text{I}}\mu$ value

Figure 6-22 Electric field, blue line is calculated value, red line is $F_{\text{I}}\mu$ value

Figure 6-23 Charge density, blue line is calculated value, red line is $F_{\text{I}}\mu$ value

Figure 6-24 Percentage error in calculated potential

Figure 6-25 Percentage error in calculated field

Figure 6-26 Percentage error in charge density
A = $-3 \times 10^{-11}$ m$^2$V$^{-2}$s$^{-1}$ B = $2.22 \times 10^{-4}$ m$^2$V$^{-1}$s$^{-1}$

**Figure 6-27** Potential, blue line is calculated value, red line is $F_{\mu}$ value

**Figure 6-28** Electric field, blue line is calculated value, red line is $F_{\mu}$ value

**Figure 6-29** Charge density, blue line is calculated value, red line is $F_{\mu}$ value

**Figure 6-30** Percentage error in calculated potential

**Figure 6-31** Percentage error in calculated field

**Figure 6-32** Percentage error in charge density
6.7.3 Comparison of different increases in mobility

Figure 6-33 to Figure 6-38 show the results for a rate of increase of mobility with field of $10^{11}$ and Figure 6-39 to Figure 6-44 show the results for a rate of increase of $3*10^{11}$. The errors are summarised in Table 6-3.

<table>
<thead>
<tr>
<th>rate of increase</th>
<th>potential</th>
<th>field</th>
<th>space charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{11} \text{m}^3\text{V}^{-2}\text{s}^{-1}$</td>
<td>$\pm 0.6%$</td>
<td>$\pm 2.5%$</td>
<td>$\pm 4%$</td>
</tr>
<tr>
<td>$3*10^{11} \text{m}^3\text{V}^{-2}\text{s}^{-1}$</td>
<td>$\pm 3%$</td>
<td>$\pm 3%$</td>
<td>$\pm 10%$</td>
</tr>
</tbody>
</table>

Table 6-3 Comparison of errors for predictions with 2 rates of increasing mobility

The errors in field are not significantly different, but the $10^{11} \text{m}^3\text{V}^{-2}\text{s}^{-1}$ rate increase shows smaller errors in potential whilst $3*10^{11} \text{m}^3\text{V}^{-2}\text{s}^{-1}$ shows smaller errors in space charge.

Using the values $A=10^{10} \text{m}^3\text{V}^{-2}\text{s}^{-1}$ and $B=2.05*10^9 \text{m}^3\text{s}^{-1}\text{V}^{-1}$ the program becomes unstable with such a large rate of increase in mobility with field, and the solution does not converge.
A = 10^{-11} \text{ m}^3 \text{ V}^{-2} \text{ s}^{-1} \quad B = 2.05 \times 10^{-4} \text{ m}^2 \text{ s}^{-1} \text{ V}^{-1}

Figure 6-33 Potential, blue line is calculated value, red line is $F_{\mu}$ value

Figure 6-34 Electric field, blue line is calculated value, red line is $F_{\mu}$ value

Figure 6-36 Percentage error in calculated potential

Figure 6-37 Percentage error in calculated field

Figure 6-35 Charge density, blue line is calculated value, red line is $F_{\mu}$ value

Figure 6-38 Percentage error in charge density
A = 3 \times 10^{-11} \text{ m}^3 \text{V}^{-2} \text{s}^{-1} \quad B = 2.05 \times 10^{-4} \text{ m}^2 \text{s}^{-1} \text{V}^{-1}

Figure 6-39 Potential, blue line is calculated value, red line is $F_1$$\mu$ value

Figure 6-40 Electric field, blue line is calculated value, red line is $F_1$$\mu$ value

Figure 6-42 Percentage error in calculated potential

Figure 6-43 Percentage error in calculated field

Figure 6-41 Charge density, blue line is calculated value, red line is $F_1$$\mu$ value

Figure 6-44 Percentage error in charge density
6.7.4 The effect of different zero field mobility values

For each of the zero field mobility values chosen, 0.000222 and 0.000205 m$^3$s$^{-1}$V$^{-1}$, the predictions are compared for increasing mobility at a rate of $3 \times 10^{-11}$ m$^3$V$^{-2}$ s$^{-1}$ with field. The errors are shown in Table 6-4.

<table>
<thead>
<tr>
<th>Zero field mobility m$^3$s$^{-1}$V$^{-1}$</th>
<th>Potential</th>
<th>Field</th>
<th>Space Charge</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000222</td>
<td>± 1.4%</td>
<td>± 4%</td>
<td>± 12%</td>
</tr>
<tr>
<td>0.000205</td>
<td>± 1.6%</td>
<td>± 3%</td>
<td>± 10%</td>
</tr>
<tr>
<td>Constant mobility</td>
<td>± 0.5%</td>
<td>± 2.5%</td>
<td>± 6%</td>
</tr>
</tbody>
</table>

Table 6-4 Comparison of errors in predictions for constant mobility, and different zero field mobility with the same rate of increasing mobility.

6.7.5 Summary

At high fields such as those in a precipitator the relationship between the field strength and mobility is not clearly understood. The excited state of the ion may change over the duct and measurements are an average over the different states. The investigation using the 1D model with field dependent mobility gives the smallest errors in the predictions of field, potential and space charge. This is possibly because a linear relationship does not represent the actual relationship closely enough. Other possible relationships are considered in section 6.8.

6.8 Considering other mobility-field relationships

The effect of choosing the linear relationship between mobility and field can be seen in Eq. 6-16. The following terms involving $\frac{d\phi}{dr}$ must be integrated:

$$\frac{d^2 \phi}{dr^2}, \frac{d\phi}{dr}, \frac{d\phi}{dr} \left( \frac{d\phi}{dr} \right)^2 \text{ and } \frac{dp}{dr} \frac{d\phi}{dr}$$

If other relationships between mobility and electric field are to be considered the terms that are to be integrated must be investigated. For example if the relationship suggested by Eq. 6-3, Thomson and Thomson, is considered:

$$v = a \frac{|E|}{\sqrt{p}}$$
so that

\[ \frac{v}{E} = \frac{a}{\sqrt{Ep}} \]

therefore

\[ \mu \propto \frac{1}{\sqrt{E}} \]

so that the terms to be integrated are:

\[ d^2 \phi \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right), \quad d\phi \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right), \quad d\frac{1}{\sqrt{\frac{d\phi}{dr}}} \quad \text{and} \quad d\rho \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right) \]

Alternatively if the power law possibly suggested by the data in Hayashi [33] is considered the terms to be integrated are:

\[ d^3 \phi \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right)^{-0.05}, \quad d\phi \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right)^{-0.05}, \quad d\frac{1}{\sqrt{\frac{d\phi}{dr}}} \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right)^{-0.05} \quad \text{and} \quad d\rho \left( \frac{1}{\sqrt{\frac{d\phi}{dr}}} \right)^{-0.05} \]

In the present version of the 1D model a cubic representation of \( \phi(r) \) has been used. The integration method required for either of the above suggestions will depend on the representation chosen, but it is unlikely that an analytical integration will be possible. If a numerical method of integration over an element is used this would have to be included in the iterative loop as different techniques may be appropriate as the node parameters vary. In that case the advantage of the present model, that the expressions remain in a symbolic form until specific grid data is used, is invalidated.
6.9 Conclusions

The use of a linear field dependent mobility has allowed the feasibility of including field dependent mobility in the model to be considered. Section 6.2 considers whether it is possible to develop this in 3D and concludes that it would not always be possible to retain the analytical formulation of the integration as knowledge of the behaviour of $|\mathbf{\nabla} \cdot \mathbf{\phi}|$ over an element is required to decide how to proceed with the integration. Similarly section 6.8 considers the use of other relationships between mobility and field strength and concludes that numerical techniques may be required for the integration.

A primary objective of the research is to build a model that can be used for many geometries. If numerical methods are employed the generality of the model is not maintained.

The design and implementation of the model has also been tested by extending it to include field dependent mobility. The general functions to handle the construction and manipulation of the matrices have not been changed to include this enhancement. This shows that the model is sufficiently general so as to be able to develop it in other ways, e.g. the inclusion of dust, without changing the basic design.

From the plots of calculated space charge, Figures 6-17, 6-23, 6-29, 6-35 and 6-41, it can be seen that the effect of introducing a field dependence for mobility, at least in this geometry, makes little difference to the calculated results.

For the 3D model explained in chapter 7 constant mobility is assumed.
7. THE 3D CONSTANT MOBILITY MODEL

This chapter describes the low-level design and implementation for the 3-D constant mobility model. The choice of the appropriate expressions, derived from the functionals and residual described in chapter 5, and subsequent construction of the disconnected matrix, is explained and illustrated with a flow chart and structure diagram. The manipulation required to convert the disconnected matrix to the connected matrix is described in Appendix A. Structure diagrams are also used to explain the procedure for collapsing the connected matrix and using this to obtain the solution to Laplace's equation. The imposition of boundary conditions for the 3D model is clarified.

The generation of the finite element grid is explained and the input data files to define the grid and its properties are specified. The results from the 3D model, and the possible improvements to the model that were identified, are described in chapter 8.

7.1 Overview of the 3D model

The 3D model uses the iterative procedure, Functionals and Galerkin residual reported in [36], see Appendix C, and described in section 5.2.3. The purpose of this model is to implement the analytical formulation in a general geometry, for a constant mobility, including the equipotential functional. The model will allow predictions to be made for any geometry, by simply providing data about the grid to be used and the properties of the grid.

In 3D the model must be capable of constraining the potential along the electrode surface to an equipotential. [36] reports a functional that can be used for nodes on the electrode surface and this is given as Equ. 7-3. This functional uses a constant term in VE, the potential applied at the electrode. The coefficients have a contribution to the boundary conditions and are input to a separate vector, bound1. bound1 is then added to the existing vector of
unknowns. Apart from the changes to the construction of the disconnected matrices, the use of this functional requires only one additional line of code.

The field at the electrode must also be constrained to be in the direction of the normal to the surface of the electrode. For this the Poisson functional for variation of potential can be used but must be rewritten so that the partial differentials are in terms of the field magnitude and direction in relation to the Cartesian axes, rather than in terms of the field components in each of the Cartesian directions.

This new functional and revised functional were made available for the implementation of this model. The functionals and residuals used are:

Poisson functional for variation of $\varphi$

$$F(\varphi) = \frac{1}{2} \left( \nabla \varphi \right)^2 - \rho \varphi dV$$  
(Eq. 7-1)

Poisson functional for variation of $\rho$

$$F(\rho) = \frac{1}{2} \rho^2 + \varepsilon \nabla \rho dV$$  
(Eq. 7-2)

functional for equi potential surface

$$F(\varphi) = \int_V \varphi^2 - 2\varphi V_e dV$$  
(Eq. 7-3)

$V_e$ is the applied electrode potential

Galerkin weighted residual

$$\int_V \left( \rho \nabla^2 \varphi + \sum_{i,j} \frac{\partial}{\partial x_i} b_i^e \varphi \right) dV$$  
(Eq. 7-4)

$b_i^e$ defines the coefficients for the element $e$, with vertices $\zeta$
7.2 Potential and space charge approximation within an element

A requirement of the model is that the potential, electric field and space charge at any point within the solution region can be predicted. In FEA the solution region is divided into elements. An expression is chosen to represent the required physical parameter within that element. The choice of expression depends on the level of accuracy that is required and the computation time available, e.g. a linear expression is the simplest choice, but will give less accurate results than a higher order expression such as parabolic or cubic. It is often possible to use a coarser grid with higher order expressions so that accuracy is improved without prohibitive increases in computation time.

The representation of potential within an element must be stated in terms of the node co-ordinates of that element. For example a general linear expression in 1D, \( f(x) = Ax + B \), requires an element with 2 nodes and one parameter at each node to determine the constants \( A \) and \( B \) uniquely. For higher order expressions more parameters and/or more nodes are needed. For the 1D iterative method described in chapter 6 a cubic expression was used for potential. The elements were in 1D having 2 nodes and the parameters were the potential and electric field, (minus 1st differential of potential).

In 3 dimensions the computation of the constant coefficients in a quintic expression is prohibitive. A cubic was chosen as achieving a favourable balance between accuracy of ability to manipulate the expressions in MAPLEV. A 3D cubic has 20 constant coefficients. The element shape was chosen to be a tetrahedral as this gives 4 corner nodes for which potential and electric field components (in each of x, y and z directions) are considered together with the potential at the mid-face nodes. This gives 20 parameters to be used to express the 20 constants in the cubic.

If a cubic representation of potential is chosen then it follows that field, first derivative, will be represented by a quadratic. The second derivative of potential
becomes the space charge and it would be physically reasonable to represent space charge by a linear function.

The space charge was also chosen to be expressed as a linear function because the Galerkin residuals required to solve for current continuity are more complex than the Variational Functionals for solving Poisson and substitution of a higher order expression for space charge into the residuals would result in prohibitively large equations to be solved.

Tetrahedra are particularly suitable for the present application because they can be fitted to a variety of geometries and they allow the use of the Hermite approximation.

7.3 Design of MATLAB program to incorporate complex discharge electrode geometries

For the simpler 1D model described in chapter 6, the connected matrix was constructed directly. In the 3D model each element is initially considered in isolation. For solving Laplace's and Poisson's equations it is necessary to include in that consideration whether any of the nodes of the element are touching an electrode. If no nodes are touching an electrode then the element is a bulk element and all the bulk expressions are used to generate the section of the disconnected matrix for that element. If any node is touching an electrode then it must be determined whether:

1. a face of the element is on the electrode or a corner or edge is touching the electrode
2. any node on the electrode is in a coplanar electrode region or a curved electrode region.

Depending on these two conditions the different expressions for planar electrodes or curved surface electrodes must be used to construct the disconnected matrix. To facilitate these procedures the table of nodes in each element is arranged so that any node within the element that is on an electrode is
in local positions 1, 2 or 3. Node 4 is therefore always a bulk node, see section 5.7.5.2 for the description of how this achieved.

Section 5.6.2 explains the implementation of the boundary conditions. Section 7.6.4 explains how the cyclical boundary conditions are simulated. This requires that the field is forced in the correct direction at the edge of the grid which involves the use of the field magnitude and direction expressions denoted by the prefix \( f_{\text{m}} \). For either coplanar, curved electrode surface nodes or nodes on a cyclical boundary it is necessary to know the dominant direction of the surface normal to the electrode at that point, i.e. is it mainly in the direction of the x, the y or the z axis. The dominant direction determines the position in the disconnected matrix of the coefficients of the specific for that particular node.

The different groups of expressions are shown in Table 7-1 and the method of selection of the appropriate expression is shown in Figure 7-1.

<table>
<thead>
<tr>
<th>node parameter</th>
<th>prefix of functions for coefficients</th>
<th>related functionals</th>
</tr>
</thead>
<tbody>
<tr>
<td>potential expressions for bulk node</td>
<td>( p_l )</td>
<td>Equ. 7-1</td>
</tr>
<tr>
<td>field expressions for bulk node not on cyclical boundary</td>
<td>( p_l )</td>
<td>Equ. 7-1</td>
</tr>
</tbody>
</table>
| field expressions for bulk node on cyclical boundary | \( f_m \) if node 1
\( f_m \) if node 2
\( f_m \) if node 3 | Equ. 7-1 |
| field expressions for electrode (curved or coplanar) | \( f_m \) if node 1
\( f_m \) if node 2
\( f_m \) if node 3 | Equ. 7-1 |
| potential expressions for curved surface | \( g_l \) | Equ. 7-3 |
| potential expressions for coplanar electrode surface | \( n_l \) | |
| space charge expressions | \( p_k \) | Equ. 7-2 |

Table 7-1  Types of expressions used for construction of disconnected matrix
The 3D program uses the procedure shown in Figure 7-1 and implemented within function m8_lmd and its subroutines lmd8_n1, lmd8_n2 and lmd8_n3, see structure diagrams in Figure 7-4 and Figure 7-6, to call the correct functions to calculate the coefficients for local nodes 1, 2 and 3. Local node 4 is arranged to be a bulk node and pl expressions are used unless the cyclical boundary condition is required, in which case fm expressions are used for the field magnitude and direction.
Figure 7-1 Flow chart for determining appropriate expressions to construct the disconnected matrix for a single element

The use of the fm expressions to simulate the cyclical boundary conditions was introduced at a late stage in the development of the model. fm expressions were
only available for local nodes 1, 2 and 3. It is possible that an element having a
face on an electrode surface, local nodes 1, 2 and 3, also has node 4 on a
cyclical boundary. The fm expressions have cyclical symmetry, because of the
symmetry of the expressions for potential and space charge. The fm2 expression
was therefore used instead of an fm4 expression, having first rotated the node
co-ordinates, for this row in the disconnected matrix only. If this model is to be
extended or developed it is recommended that the fm4 expression is derived and
used in place of this adaptation.

7.4 Structure diagrams of the 3D model

To implement the iterative procedure, described in section 5.2.3.1, the flow
chart shown in Figure 5-2 is used as the basis for the structure diagram in. This
shows the initial stage of solving Laplace’s equation, followed by the iterative
procedure for solution of Poisson’s equation and current continuity. The ‘Top-
level’ MATLAB script is constructed from this structure diagram and is called
ci3d9.
Figure 7-2 BS structure diagram of c3d9, the top level MATLAB program. Function names are shown underlined.
Ip9 is the MATLAB function which takes the grid data, disconnected matrices and vectors prepared in ci3d8 and processes them to obtain the solution to Laplace's equation. The structure diagram is shown in Figure 7-3. In Figure 7-2 the functions g_npots, g_fpots, get_exs, get_eyes and get_eyes are simple procedures for extracting from the solution vector the vertex node potentials, face potentials, x field component, y field component and z field components respectively. They will not be explained further here.

**START**

- convert the disconnected matrix to a connected matrix
- **lp_kns9**
  - set up boundary sector for applied potentials and zero field components
- convert the disconnected vector of constant terms to a connected vector
- add the applied boundary vector and constant terms vector to get complete boundary vector
- **collmlp9**
  - collapse the connected matrix of unknowns' coefficients i.e. remove rows and columns relating to known node values
- **collvlp9**
  - collapse the boundary vector
- obtain solutions of unknowns:
  - (inverse of collapsed matrix) collapsed boundary vector
- **expvlp9**
  - obtain the full Laplace solution: expand the calculated vector of unknown by including the applied boundary values

**STOP**

*Figure 7-3 Structure diagram of ip9, the MATLAB function for the solution of Laplace's equation*
7.4.1 Structure diagrams for construction of disconnected matrix

The disconnected matrix represents the coefficients of the unknowns by reference to their local node number in an individual, isolated element. The connected matrix represents the coefficients of the unknowns by reference to the global numbering scheme. The structure diagrams to construct the disconnected matrix for Laplace are shown in Figure 7-4 and Figure 7-5. M8_lmd, together with sub-routines lmd8_n1, lmd8_n2 and lmd8_n3, is the MATLAB function that constructs the disconnected matrix of coefficients for each unknown.

The elements of the grid are considered as separate. However, the global position of an element's local nodes, in relation to the discharge and collection electrodes, determines the required analytical expression to calculate the correct coefficient. Use is therefore made of the input data concerning the type of each individual node: is it a bulk or electrode surface node; if surface node is it coplanar or non-coplanar with nearest neighbours; if coplanar is the surface normal to the electrode in the x, y or z axis direction at this point.
For number of elements

If is a bulk element - for surface 123

THEN

bulk expression

ELSE

if coplanar with both neighbouring surfaces

THEN

do nothing

ELSE

face node - variable potential surface expression

for surfaces 234, 341, 412 use bulk expressions

$\text{Imd}_8 \_n_1$ for local node 1

Calculate coefficients using appropriate expressions

$\text{Imd}_8 \_n_2$ for local node 2

Calculate coefficients using appropriate experiments

$\text{Imd}_8 \_n_3$ for local node 3

Calculate coefficients using appropriate expressions

For local node 4 use bulk expressions

Figure 7.4 Structure diagram of m8_Imd
Figure 7-5 Structure diagram of lmd8_n1, lmd8_n2, lmd8_n3

The function for the solution of Laplace's equations is lp9, and similarly pois9 for solving Poisson's equations and curcon9 for solving current continuity. Lp9.m uses the global variables l_matdis and conul, the disconnected matrix and the connection matrix to construct the connected matrix, lmat, see Appendix A. The matrix lmat is then passed to the function collmpl9 which removes the rows and columns relating to node parameters that are knowns. This is achieved by reference to the global variables nodetype and facetype that contain the properties of the vertex nodes and face nodes respectively. Figure 7-6 shows the structure diagram of collmpl9.
create temporary sparse matrix
nrows = 20 * elems - number of known node parameters
ncols = 20 * elems

For number of nodes
  get node type
  copy appropriate rows from disconnected matrix
to temporary matrix
  (see note below)

create connected matrix (sparse)
nrows = 20 * elems
ncols = 20 * elems

For number of nodes
  get node type
  copy appropriate rows from temporary matrix
to connected matrix
  (see note below)

STOP

Figure 7-6 Structure diagram of function collmplp9

Note: which rows or columns are copied from one matrix to another depends on whether the related node parameter is 'known' or 'unknown'. If 'known' the row or column is not copied, if 'unknown' then it is copied. The vector 'nodetype' contains the information about which parameters are 'known', see Table 7-7. Figure 7-6 is derived from the flow chart in Figure 5-3.
7.5 Convergence

The number of iterations is determined by a convergence criterion based on the maximum relative change in the components of the solution vectors. The physical problem has a real solution, but this may not be a stable solution. It is possible, under certain conditions, for the calculated solution not to converge and therefore the program is set to perform a maximum of 20 iterations. Examples of conditions which may inhibit convergence are:

- use of too coarse a grid
- badly spaced nodes on the grid.

The convergence algorithm was developed for use with the simple geometries model, and has been implemented in MATLAB for the 3D program. The change between each iteration of the node and face potentials, the field magnitudes and the space charge are tested until the change from the last iteration is less than a predefined maximum difference. The algorithm is shown in Appendix B.

7.6 Boundary Conditions

The boundary conditions have been described in general terms in section 5.6.2. The implementation of these boundary conditions in the 3D model is described here. The imposition of the boundary conditions for Laplace at the vertex nodes is controlled by the input data in the vector nodetype, see section 7.9. At the face nodes the imposition of the boundary condition is controlled by the vector facetype which is generated by reference to the input data file nle_type.dat, see section 7.9. Since the boundary conditions for Poisson are, in part, derived from the Laplace solution the values representing the node properties for nodes on the discharge electrode, contained in the global variables nodetype and face type, are updated in the function 'rev_nt'.
7.6.1 Field magnitude and direction at the discharge electrode

Figure 7-7 shows an extract from the function sort_in which demonstrates the setting of the Poisson boundary values in the vector ci_field. This function is also used for the testing of the Poisson implementation by setting the boundary field to equal that calculated by Laplace, and to set the Poisson field at half the Laplace field for simulating charge injection in plane-plane geometry. In each of these cases the field must be fixed at all the nodes on the electrode and this is achieved by setting the critical field at half the field magnitude at a particular node, rather than commenting out the if-else-end structure.

```matlab
function [inner_c,inner_nc,ci_field]=sort_in(exs,eys,ezs)

declarations

nb=length(inner_b);
for a=1:nb
    n=inner_b(a);
    Ex=exs(n);
    Ey=eys(n);
    Ez=ezs(n);
    Enorm=dirfield(Ex,Ey,Ez);
    E=emag(Ex,Ey,Ez);
    Ec=get_ec(n);
    E<r=.5*E;  
    if(E >= Ec) %force all nodes to coronate
        inner_c(countc)=n;
        %force at Laplace field
        fixe=fixedfield(Enorm,Ec);
        %fix at half Laplace field
        fixe=fixedfield(Enorm,E/2);
        for b=1:3
            ci_field(countc,b)=fixe(b);
        end
        countc=countc+1;
    else
        inner_nc(countnc)=n;
        countnc=countnc+1;
    end
end

for a=1:length(inner_c)
    num=inner_c(a);
    nodetype(num)=100;
end
```

Figure 7-7 Extract from function sort_in.m
7.6.2 Space charge at the discharge electrode
The boundary conditions for the solution of current continuity are set according
to which nodes on the discharge electrode are coronating, by reference to vector
inner_c, see Figure 7-7. For coronating nodes the space charge is set to the
value calculated in the latest iteration of Poisson. At non-coronating nodes the
space charge is set to zero. This procedure is followed in the function chg_kns9.

7.6.3 Symmetry boundary conditions
Symmetry boundary conditions are imposed by setting the required field
components to zero. This requires that the grid be positioned in the x, y z co­
ordinate system so as to place the maximum number of symmetry boundaries
along, or parallel to, a co-ordinate axis. For example, if an edge of the grid is
placed along the x axis then the field components for nodes along this edge are
zero in the y and z directions. These node parameters, FY and FZ, are then
‘knowns’ and this property is specified in the input data file nodetype.dat, see
section 7.9.

7.6.4 Cyclical boundary conditions
Cyclical boundary conditions are those which match node values at one part of
the grid to those at another, because of the cyclical symmetry of the solution
region. Section 8.3.4 shows the implementation of these conditions by use of a
further input data file, nodepair.dat see section 7.9, which matches nodes on
parallel planes, either the upper and lower edge planes in the z direction or
parallel sides of the grid in the x or y directions. For cylindrical grids the parallel
upper and lower planes may be matched in this way but the sides of the grid are
no longer parallel. To impose cyclical boundary conditions in this case requires
the field to be constrained in the direction of the edge of the grid. This is
achieved by the use of the fmn expressions (field magnitude and direction rather
than x, y and z components) for the appropriate nodes, in the construction of the
disconnected grid, this is explained in section 7.3.
7.7 Grid Generation

7.7.1 Element definition
The element shape for the grid was chosen to be a tetrahedral with 4 vertex nodes and 4 mid-face nodes see section 7.2. The potential within each element is represented by a cubic. This has 20 constant coefficients which are expressed in terms of the potential and x, y and z field components at the vertex nodes and the potential at the mid face node. The space charge over an element is chosen to be linear, which has 4 constant coefficients expressed in terms of the charge at each of the vertex nodes.

Figure 7-8 Tetrahedral element showing the four corner nodes.

7.7.2 FEMGEN
FEMGEN, see section 5.5, is used to generate the basic grid data. FEMGEN is an interactive FEA pre-processor which generates files of grid data in a variety of formats suitable for many commercial FE solvers. It can also generate files in a ‘Neutral’ format which can be used by other solvers. The neutral format output file, an ASCII file, is passed to the MATLAB prediction program via a C++ program. FEMGEN output gives the node and element numbering, with node co-ordinates and lists the global number of local nodes for each element.

7.7.3 Convert grid of prisms to Tetrahedra.
FEMGEN does not use Tetrahedra in grid definition. To overcome this the grid was generated using prisms and then each prism was divided into 3 Tetrahedra.
A C++ program was written to extract the required information from the
FEMGEN output file to convert the prisms to Tetrahedra and rewrite it in the format required for the MATLAB program. This produces the input files coor.dat and elem.dat, see Table 7-2.

7.7.4 Grids designed by hand
Simple grids such as the 'Toblerone', described in 8.3.1 and used for testing plane-plane geometry, were designed by hand and the data files constructed manually.

7.3 Data files to define the grid and it's properties
The prediction program, as well as needing to know the applied potentials at each electrode, requires further information about the grid:

- the element number of any element having a surface on an electrode.
- the node numbers of nodes on an electrode boundary
- whether a node on an electrode is on a curved or planar section of the electrode
- the node numbers of nodes on symmetry boundaries and which field components are zero at that node
- the direction of the unit normal at nodes on the electrode surfaces.
This information is provided to the prediction program by means of a set of input data files that are summarised in Table 7-2.

<table>
<thead>
<tr>
<th>Data file</th>
<th>Format +</th>
<th>Purpose</th>
<th>How generated</th>
</tr>
</thead>
<tbody>
<tr>
<td>initial</td>
<td>vector</td>
<td>number of vertex nodes</td>
<td>C++ program using FEMGEN output file</td>
</tr>
<tr>
<td></td>
<td>4 elements</td>
<td>number of elements</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>applied potential-discharge electrode</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>applied potential-collecting electrode</td>
<td></td>
</tr>
<tr>
<td>coor</td>
<td>nrows=elems ncols=3</td>
<td>Cartesian co-ordinates of each vertex node</td>
<td>C++ program using FEMGEN output file</td>
</tr>
<tr>
<td>elem</td>
<td>nrows=elems ncols=4</td>
<td>global node number of the 4 local nodes in each tetrahedral element</td>
<td>C++ program using FEMGEN output file</td>
</tr>
<tr>
<td>bo elems</td>
<td>vector</td>
<td>the number of each element having a surface on the collecting electrode</td>
<td>manually by inspection</td>
</tr>
<tr>
<td>bi elems</td>
<td>vector</td>
<td>the number of each element having a surface on the discharge electrode</td>
<td>manually by inspection</td>
</tr>
<tr>
<td>inner b</td>
<td>vector</td>
<td>the number of each node on the discharge electrode</td>
<td>manually by inspection</td>
</tr>
<tr>
<td>outer b</td>
<td>vector</td>
<td>the number of each node on the collecting electrode</td>
<td>manually by inspection</td>
</tr>
<tr>
<td>nodetype</td>
<td>vector</td>
<td>specifies boundary conditions applicable to each node</td>
<td>manually by inspection</td>
</tr>
<tr>
<td></td>
<td>nrows=nodes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>n4e type</td>
<td>vector</td>
<td>specifies bulk or electrode node, if electrode whether on curved or flat surface.</td>
<td>manually by inspection</td>
</tr>
<tr>
<td></td>
<td>nrows=nodes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>nodepair</td>
<td>matrix</td>
<td>specifies that matching of nodes for imposition of cyclical boundary conditions</td>
<td>manually by inspection</td>
</tr>
<tr>
<td></td>
<td>nrows=2 ncols=no of matched nodes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>edge</td>
<td>vector number of nodes of cyclical boundary</td>
<td>specifies nodes, not on an electrode, that are on cyclical boundary for which field direction is to be fixed</td>
<td>manually by inspection</td>
</tr>
<tr>
<td></td>
<td>number of cyclical boundary</td>
<td></td>
<td></td>
</tr>
<tr>
<td>nodecurv</td>
<td>matrix</td>
<td>cols. 1 2 3 specify the cosine to the x, y, z axis of the electrode at this point</td>
<td>manually by inspection</td>
</tr>
<tr>
<td></td>
<td>nrows=elems ncols=5</td>
<td>cols. 4 5 radius of electrode at this point</td>
<td></td>
</tr>
<tr>
<td></td>
<td>ncols=number of columns</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>nodes = number of nodes</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**nrows=number of rows**

**ncols=number of columns**

**elems = number of elements**

**nodes = number of nodes**

*Table 7-2 Input data files for the 3D prediction program*

The details of each data file are given in section 7.9.
7.9 Grid data input files

This section specifies the input data files to define the grid and the electrodes.

**initial.dat**

Column vector; number of rows = 4.

<table>
<thead>
<tr>
<th>nodes</th>
<th>number of nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>elems</td>
<td>number of elements</td>
</tr>
<tr>
<td>vi</td>
<td>applied voltage discharge electrode</td>
</tr>
<tr>
<td>vo</td>
<td>applied voltage plate electrode</td>
</tr>
</tbody>
</table>

*Table 7-3 initial.dat data file specification*

**coor.dat**

Matrix: number of rows = nodes, number of columns = 3.

x, y, z co-ordinates for each of the nodes, in global node number order.

<table>
<thead>
<tr>
<th>X1</th>
<th>Y1</th>
<th>Z1</th>
</tr>
</thead>
<tbody>
<tr>
<td>X2</td>
<td>Y2</td>
<td>Z2</td>
</tr>
<tr>
<td>X3</td>
<td>Y3</td>
<td>Z3</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td>:</td>
<td>:</td>
<td>:</td>
</tr>
<tr>
<td>X(nodes-1)</td>
<td>Y(nodes-1)</td>
<td>Z(nodes-1)</td>
</tr>
<tr>
<td>Xnodes</td>
<td>Ynodes</td>
<td>Znodes</td>
</tr>
</tbody>
</table>

*Table 7-4 coor.dat data file specification*

**elem.dat**

Matrix: number of rows = elems, number of columns = 4 (4 local nodes per tetrahedral element).

Global node numbers of the local nodes of each element (row number = element number).
<table>
<thead>
<tr>
<th>ln1 of e1</th>
<th>ln2 of e1</th>
<th>ln3 of e1</th>
<th>ln4 of e1</th>
</tr>
</thead>
<tbody>
<tr>
<td>ln1 of e2</td>
<td>ln2 of e2</td>
<td>ln3 of e2</td>
<td>ln4 of e2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ln1 of e(elems-1)</td>
<td>ln2 of e(elems-1)</td>
<td>ln3 of e(elems-1)</td>
<td>ln4 of e(elems-1)</td>
</tr>
<tr>
<td>ln1 of e(elems)</td>
<td>ln2 of e(elems)</td>
<td>ln3 of e(elems)</td>
<td>ln4 of e(elems)</td>
</tr>
</tbody>
</table>

In = local node, e = element

Table 7-5 elem.dat data file specification

**bi elems.dat and bo elems.dat**

Row or column vector.

Number of elements = number of elements having face on discharge electrode or collecting electrode in ascending numerical order.

**inner b.dat and outer.dat**

Row or column vector.

Number of elements = number of nodes on discharge electrode or on collecting electrode in ascending numerical order.

**edge.dat**

Row or column vector.

Number of elements = number of nodes on a cyclical boundary and not on an electrode, in ascending numerical order.

**nodepair.dat**

Matrix: number of rows = number of pairs, number of columns = 2.

Node numbers in column 1 are the major nodes, that other nodes are paired to. Nodes in column 2 must be in ascending numerical order. Nodes may appear only once in column 2. In column 1 nodes may appear more than once as several nodes may be paired with each 'major node'.
n4e_type.dat

Vector: number of rows = nodes

Defines, for each global node, the node type that is used in selecting the correct set of expressions to use in constructing the disconnected matrix, see section 7.3. There are three sets of expressions that can be used:

- *pi* expressions for potential and field expressions for bulk nodes
- *fm* expressions for field components for nodes on electrodes, or cyclical boundaries, use *fm1* for field at local node 1, *fm2* for local node 2 and *fm3* for local node 3, together with dummy expressions for components in non-dominant direction.
- *gl* expressions for potential for nodes on a curved electrode surface

<table>
<thead>
<tr>
<th>Type</th>
<th>Meaning</th>
<th>Expressions</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>bulk node</td>
<td>pl or fm1/fm2/fm3</td>
</tr>
<tr>
<td>11</td>
<td>plane electrode, surface normal predominantly in x direction</td>
<td>fm1</td>
</tr>
<tr>
<td>12</td>
<td>plane electrode, surface normal predominantly in y direction</td>
<td>fm2</td>
</tr>
<tr>
<td>13</td>
<td>plane electrode, surface normal predominantly in z direction</td>
<td>fm3</td>
</tr>
<tr>
<td>21</td>
<td>curved electrode, surface normal predominantly in x direction</td>
<td>fm1 and gl</td>
</tr>
<tr>
<td>22</td>
<td>curved electrode, surface normal predominantly in y direction</td>
<td>fm2 and gl</td>
</tr>
<tr>
<td>23</td>
<td>curved electrode, surface normal predominantly in z direction</td>
<td>fm3 and gl</td>
</tr>
</tbody>
</table>

*Table 7-6 node types used in the construction of the disconnected matrix*
nodecurv.dat

Matrix: number of rows = nodes, number of columns = 5,
column 1 = cosine of surface normal to x axis,
column 2 = cosine of surface normal to y axis,
column 3 = cosine of surface normal to z axis,
column 4 = smallest radius of curvature,
column 5 = largest radius of curvature.

nodetype.dat

Vector: number of rows = nodes

The ‘type’ of each node indicates which parameters at the node are fixed as
boundary conditions. this is indicated by a type number which is defined in
Table 7-7.
Position of node  | Field boundary conditions  | Type number
---|---|---
discharge electrode (vi is fixed)  | Ex!0 Ey!=0 Ez!=0  | 1
  | Ey!=0 Ez!=0  | 2
  | Ey!=0  | 3 or 4
  | Ex!=0 Ez!=0  | 5
  | Ex!=0  | 6 or 7
  | Ex!=0 Ey!=0  | 8 or 9
plate electrode (vo is fixed)  | Ex!=0 Ey!=0 Ez!=0  | 11
  | Ey!=0 Ez!=0  | 12
  | Ey!=0  | 13 or 14
  | Ex!=0 Ez!=0  | 15
  | Ex!=0  | 16 or 17
  | Ex!=0 Ey!=0  | 18 or 19
non-electrode (node in bulk or on a curved electrode so that potential is an unknown)  | Ex!=0 Ey!=0 Ez!=0  | 50
  | Ex!=0 Ey!=0  | 21 or 22
  | Ey!=0 Ez!=0  | 23
  | Ex!=0 Ez!=0  | 24
  | Ex!=0  | 32 or 34
  | Ey!=0  | 31 or 33
  | null point in field  | 35 or 36
discharge electrode, coronating node  | field magnitude fixed by charge injection law, field direction fixed by Laplace solution  | 100

vi = discharge electrode voltage, vo = collecting electrode voltage

Table 7.7 Possible values in nodetype.dat and their meaning

7.10 Improvements to the model

To test the model comparisons are made to analytical solutions for plane-plane and cylindrical geometries. The grids used for these tests, the results and improvements made to the model in the light of these results are explained in chapter 8.
7.10.1 Pre-processor
At present mistakes in the input data files are identified when errors occur during the running of the program. For example:
- a matrix becomes unexpectedly singular
- an operation is carried out on a vector or matrix of inappropriate size.

The result of solution of Laplace's equation is incorrect, either by comparison to analytical solution or more obviously by the prediction of positive potential or field components pointing in the wrong direction. This means that mistakes in the data files have to be identified, corrected and the program restarted.

A user-interface could be designed to check that the input data from the 11 data files currently required is self-consistent. Possible errors are then reported to the operator before computation time has been used.
8. RESULTS AND IMPROVEMENTS TO THE 3D MODEL

8.1 Introduction
This chapter presents the results from testing the model in plane-plane and cylindrical geometry. Predictions for the full ion-drift problem are obtained for plane-plane geometry. Predictions for Laplace in cylindrical geometry are obtained and compared for several grids. The difficulties in predicting the full ion-drift solution are discussed. From the results of this testing several improvements to the model are identified.

8.1.1 Cyclic boundary conditions
The use of cyclic boundary conditions, in the case of cylindrical geometry this requires the forcing of the field direction at nodes on a cyclic boundary, has been explained in sections 7.6.4 and 7.3 as this affects the choice of expressions used to construct the disconnected matrix. Further cyclic boundary conditions may be applied via the input data files. This is called ‘wrapping’ and is explained in section 8.3.4.

8.1.2 Symmetric grid
Section 8.4.1 shows the results for plane-plane electrodes with sides of the grid non-parallel, both without a symmetrical grid and with a symmetrical grid. Subsequent grid designs for testing in the cylindrical geometry were chosen to be symmetric.

8.2 Visualisation of the results
The final solution can be viewed in an ASCII output data file, (section 8.2.2). To plot the results MATLAB is used to calculate the potential, field and space charge along a line in the solution region from discharge electrode to collecting plate electrode. For example in cylindrical geometry the line is chosen along a radius and the result compared to the analytical solution.
8.2.1 Post processor

A post processor would be desirable. A generalised plotting routine has not been developed in MATLAB; MATLAB is unable to produce vector plots. The data could be transferred to a plotting package such as AXUM. Several types of plots could be used, plots of parameters along a chosen line in the region, plots over a surface such as the collecting plate electrode and vector plots of the field in a plane over the whole solution region.

8.2.2 Output data file format

The output data file is called DATAOUT.TXT and the format is shown in Table 8-1. The format is repeated for each iteration:

| Number of vertex nodes, number of elements |
| Applied potential on discharge electrode |
| Applied potential on collecting electrode |
| Number of iterations completed (0 = Laplace Solution) |
| Calculated node potentials in global node number order |
| Calculated x field component |
| Calculated y field component |
| Calculated z field component |
| Calculated field magnitude |
| Calculated space charge (Poisson) |
| K, the scaling factor |
| Current continuity space charge density solution (proportional to) current density |

The data file is opened to store the results from one iteration and then closed. This ensures that if the program fails or is interrupted the output data file contains the results from the program so far.
8.3 Results for plane-plane geometry

The derivation of the analytical ion drift solution for plane-plane geometry is given in [35].

8.3.1 Grid for testing

The grid consists of a triangular prism, a 'Toblerone-like' solution region, the plane parallel ends representing the discharge and collecting electrodes. The distance between the electrodes measures 12 cm and nodes are spaced evenly 4 cm along each edge. The height of the isosceles triangles that forms the electrode is 2 cm and the base is 2 cm. This results in a grid of 9 tetrahedral elements, 3 tetrahedra from each of the 3 prisms, with 12 vertex nodes. This is the simplest grid used for testing. The potential applied at the discharge electrode is -300 kV (for comparison with cylindrical geometry), or -60kV (as a practical voltage used on the laboratory rig), and 0 kV at the collecting electrode.

![Schematic representation of the solution region, each prism is divided into three Tetrahedra](image)

*Figure 8-1  Schematic representation of the solution region, each prism is divided into three Tetrahedra*
8.3.2 Plane-plane geometry using only bulk elements

Figure 8-2 to Figure 8-4 shows the calculated potential, field magnitude and space charge obtained using a simple grid for plane-plane geometry. The grid is aligned in the x direction. The field components in the y and z directions are all set to zero. The calculated values are compared to the analytical solution for plane-plane geometry. To simulate the presence of coronating nodes the field at the discharge electrode is fixed at half the calculated Laplace field. The iterative loop is repeated six times and the Figures show maximum errors of 0.15% in potential, 0.2% in field magnitude and 10% in space charge. Errors are calculated as a %age of the analytical value of the parameter at each point. The larger error in space charge is to be expected since a linear representation is used within each element, compared with the cubic representation of potential.

![Figure 8-2 Analytical (blue) and FEM calculated (green) potential along an edge of the solution region with percentage errors. The calculated values overlay the analytical solution](image)
Figure 8-3 Analytical (blue) and FEM (green) calculated field magnitude along an edge of the solution region with percentage errors. The calculated values overlay the analytical solution.

Figure 8-4 Analytical (blue) and FEM calculated (green) space charge along an edge of the solution region with percentage errors.

These results indicate that high levels of accuracy can be achieved with only a small number of iterations on a coarse grid. Houlgreave, Bromley and Fothergill [36], see Appendix C, reports errors of only 0.003% for potential, 0.04% for field magnitude and 4% for space charge on a grid of 33 nodes and 30 elements.
for 10 iterations. In this case the errors are calculated in the same way. For later comparison purposes the errors associated with the predictions in Figure 8-2 to Figure 8-4 are recalculated as a %age of the mean of the analytical of the parameters. These errors are a maximum of 0.17% in potential, 0.8% in field magnitude and 22% in the charge density.

8.3.3 Plane and curved electrode elements

The implementation of the expressions for curved electrodes were first tested in plane-plane geometry. These expressions use the data file nodecurv.dat to obtain the direction of the field at the node on the curved electrode. To test this the Toblerone was placed in a general orientation, i.e. not aligned with the Cartesian axes. The results are shown in Figure 8-5 to Figure 8-10. Errors are calculated as a %age of the mean of the analytical value over the whole region.

Figure 8-5 Potential, blue is analytical, green is calculated value

Figure 8-6 Error in potential
Figure 8-7 Field magnitude, blue is analytical, green is calculated value

Figure 8-9 Error in field magnitude

Figure 8-8 Charge density, blue is analytical, green is calculated value

Figure 8-10 Error in charge density
Table 8-2 shows the comparison of errors, calculated as a % age of the mean, for the predictions made using only bulk expressions or using the equipotential expressions on the electrodes and bulk expressions elsewhere. The errors are similar, as would be expected for plane-plane simple geometry. This demonstrates that:

- the curved electrode expressions are being correctly selected in the construction of the disconnected matrix
- the equipotential over the plane electrode is being correctly calculated
- the field direction is being correctly determined.

### 8.3.4 Introduction of cyclical boundary conditions

The implementation of cyclical boundary conditions by choosing appropriate expressions to construct the disconnected matrix has been described in section 7.6.4. The need to match nodes from the top of the grid to corresponding nodes on the bottom of the grid was identified from the following results, and is called ‘wrapping’. The implementation of ‘wrapping’ using a look-up table, supplied via an input data file is described. The name ‘wrapping’ was used since it requires 2 or more nodes to be ‘tied together’, i.e. to have equal values for all their node parameters.
The test grid described in section 8.3.1 was used for further testing by adapting it in several ways:

1. reoriented to be aligned along the y axis,
2. rotated about the z axis and then about the y axis,
3. amalgamated with 1 other 'Toblerone' to form a square ended box,
4. amalgamated with 3 other 'Toblerones' to form a rectangular ended box.

The predictions from 1 and 2 were as expected. The solution was duplicated exactly, within the numerical computational limit of the computer, but now reoriented in the same way that the grid had been reoriented. The results from the rectangular box were particularly interesting. The grid used is known as rectbox2 and is shown in Figure 8-11 and the calculated node values from this grid are shown in Table 8-1. From these results the requirement for 'wrapping' was identified.

![Figure 8-11 The test grid known as rectbox2.](image)
The analytical potentials are -60, -40, -20 and 0 kV at x = 0, 4, 8 and 12 cm respectively. The analytical field components are -500000 V/m in x direction and 0 V/m in y and z direction.

Table 8-3 Rectbox2 results without ‘wrapping’. Nodes that are in one element only are highlighted.

Table 8-3 shows the co-ordinates of each vertex node on the grid together with the calculated values of each node parameter. The results from this grid, when compared to the analytical solution shown in [35] revealed that the potential/field magnitude was generally accurate but nodes at the near upper left hand corner and the far lower right hand corner of the grid showed much greater inaccuracies. These nodes are unusual in the grid in that they are in only one element, i.e. they are in an element which has one face on the end of the box, one face on a side and one face on the top or bottom of the grid. These nodes and calculated values are highlighted. This means that the node parameters are determined only in connection with the other nodes within that individual element and are not connected to any other element. These parameters at the
corners are less well defined than at other points on the grid. From this was devised the idea of 'wrapping' or connecting the nodes on the top of the grid to those on the bottom of the grid. Although the actual number of global nodes remains the same, the number of unknowns to be found is halved, but each unknown is more well defined. In the case of this grid, which has a high degree of symmetry, it is also possible to connect the sides to each other so that the parameters to be calculated are those at the nodes marked with the dots, see Figure 8-12.

![Figure 8-12 The grid rectbox2, parameters may be calculated for only nodes marked with dots](image)

This feature required the revision of the functions to create the connection matrix, and of the functions to collapse the connected matrix and vector and to expand the vector of calculated node values. The result is a reduction in the size of the connection matrix but not of the disconnected matrix. The collapsed vector and matrix are also smaller and this can result in a reduced computation time, although on this size of grid the reduction is not significant. The improvement in the accuracy of the predictions are shown in Table 8-4.
With full ‘wrapping’ the predicted results matched the analytical results exactly to 7 significant figures. For most grid designs it is only possible to wrap top to bottom and not possible to wrap side to side. Nodes can only be wrapped together when their parameters match.

The improved accuracy with top to bottom wrapping is significant in reducing errors, especially for grids having only 1 element in height. The small errors in predictions for plane-plane geometry on a more complicated grid are further confirmation of the validity of the program in handling the different node properties and constructing and manipulating the matrices and vectors.

8.4 Results for Cylindrical geometry

An early test of the 3D program was the comparison of the predictions of the Laplace solution for cylindrical geometry. The derivation of the analytical solution is shown in [35]. The prediction along a radial of the 3D cylindrical grid was compared to the analytical solution.

8.4.1 Checking for symmetry

The testing on the plane-plane grid resulted in the introduction of ‘wrapping’ the nodes on the top layer of the grid to those on the bottom layer. Although the curved electrodes expressions had been used in testing on the rectbox2 grid (see section 8.3.4) further tests were required on a near cylindrical grid. The edges of such a grid between the discharge and the collecting electrode would no longer be parallel but would lie along the radial of a circle. The axis of symmetry was arranged along each of the co-ordinate axes in turn, as shown in Figure 8-13.

<table>
<thead>
<tr>
<th>maximum error percentage</th>
<th>no wrapping</th>
<th>top to bottom wrapping</th>
<th>top to bottom and side to side wrapping</th>
</tr>
</thead>
<tbody>
<tr>
<td>potential</td>
<td>1.16</td>
<td>.33</td>
<td>0 to 7 sig. fig.</td>
</tr>
<tr>
<td>field magnitude</td>
<td>48.0</td>
<td>10.7</td>
<td>0 to 7 sig. fig.</td>
</tr>
</tbody>
</table>

Table 8-4 Effect on error of partial and full wrapping
From the discharge electrode, looking along the axis of symmetry, the faces are arranged as shown in Figure 8-14.

It was expected that the field components would be a mirror image across the symmetry plane and would be independent of the orientation. The results were obtained without the implementation of the cyclical boundary conditions described in section 7.6.2 and are shown in Table 8-5, Table 8-6 and Table 8-7.
### Table 8-5 node values of near cylindrical grid, aligned along x axis

<table>
<thead>
<tr>
<th>Variable</th>
<th>Radial</th>
<th>Node distance along radial in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.03</td>
</tr>
<tr>
<td>potential</td>
<td>y-ve</td>
<td>-298122.74</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>-299702.33</td>
</tr>
<tr>
<td></td>
<td>y+ve</td>
<td>-298220.18</td>
</tr>
<tr>
<td>field magnitude</td>
<td>y-ve</td>
<td>6214857.79</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>5377361.71</td>
</tr>
<tr>
<td></td>
<td>y+ve</td>
<td>5887735.84</td>
</tr>
<tr>
<td>x field component</td>
<td>y-ve</td>
<td>-589593.17</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>-537376.71</td>
</tr>
<tr>
<td></td>
<td>y+ve</td>
<td>-5585596.65</td>
</tr>
<tr>
<td>y field component</td>
<td>y-ve</td>
<td>1965310.60</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y+ve</td>
<td>-1861865.55</td>
</tr>
<tr>
<td>field component</td>
<td>y-ve</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y+ve</td>
<td>0.00</td>
</tr>
</tbody>
</table>

### Table 8-6 node values of near cylindrical grid, aligned along y axis

<table>
<thead>
<tr>
<th>Variable</th>
<th>Radial</th>
<th>Node distance along radial in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.03</td>
</tr>
<tr>
<td>potential</td>
<td>x+ve</td>
<td>-298122.74</td>
</tr>
<tr>
<td></td>
<td>x=0</td>
<td>-299702.33</td>
</tr>
<tr>
<td></td>
<td>x-ve</td>
<td>-298220.18</td>
</tr>
<tr>
<td>field magnitude</td>
<td>x+ve</td>
<td>6214857.79</td>
</tr>
<tr>
<td></td>
<td>x=0</td>
<td>5377361.71</td>
</tr>
<tr>
<td></td>
<td>x-ve</td>
<td>5887735.84</td>
</tr>
<tr>
<td>x field component</td>
<td>x+ve</td>
<td>-589593.17</td>
</tr>
<tr>
<td></td>
<td>x=0</td>
<td>-537376.71</td>
</tr>
<tr>
<td></td>
<td>x-ve</td>
<td>-5585596.65</td>
</tr>
<tr>
<td>y field component</td>
<td>x+ve</td>
<td>1965310.60</td>
</tr>
<tr>
<td></td>
<td>x=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>x-ve</td>
<td>-1861865.55</td>
</tr>
<tr>
<td>field component</td>
<td>x+ve</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>x=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>x-ve</td>
<td>0.00</td>
</tr>
</tbody>
</table>

8-14
<table>
<thead>
<tr>
<th>Variable</th>
<th>Node distance along radial in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0.03</td>
</tr>
<tr>
<td>potential</td>
<td></td>
</tr>
<tr>
<td>x+ve</td>
<td>298122.74</td>
</tr>
<tr>
<td>x=0</td>
<td>299702.33</td>
</tr>
<tr>
<td>x-ve</td>
<td>298220.18</td>
</tr>
<tr>
<td>field</td>
<td></td>
</tr>
<tr>
<td>magnitude</td>
<td></td>
</tr>
<tr>
<td>x+ve</td>
<td>6214857.79</td>
</tr>
<tr>
<td>x=0</td>
<td>5373761.71</td>
</tr>
<tr>
<td>x-ve</td>
<td>5887735.84</td>
</tr>
<tr>
<td>x field</td>
<td></td>
</tr>
<tr>
<td>component</td>
<td></td>
</tr>
<tr>
<td>x+ve</td>
<td>-1965310.60</td>
</tr>
<tr>
<td>x=0</td>
<td>0.00</td>
</tr>
<tr>
<td>x-ve</td>
<td>1861865.55</td>
</tr>
<tr>
<td>y field</td>
<td></td>
</tr>
<tr>
<td>component</td>
<td></td>
</tr>
<tr>
<td>x+ve</td>
<td>0.00</td>
</tr>
<tr>
<td>x=0</td>
<td>0.00</td>
</tr>
<tr>
<td>x-ve</td>
<td>0.00</td>
</tr>
<tr>
<td>z field</td>
<td></td>
</tr>
<tr>
<td>component</td>
<td></td>
</tr>
<tr>
<td>x+ve</td>
<td>-5895931.79</td>
</tr>
<tr>
<td>x=0</td>
<td>-5373761.71</td>
</tr>
<tr>
<td>x-ve</td>
<td>-5585596.65</td>
</tr>
</tbody>
</table>

Table 8-7 node values of near cylindrical grid, aligned along z axis

These tables show the calculated values of the node parameters; potential, x, y, and z field components; and the field magnitude calculated from these. A higher degree of symmetry had been expected. To investigate further the grid was adapted so that the elements were rearranged symmetrically about the axis of symmetry.

Figure 8-15 Re-arrangement of element faces on the discharge electrode, dotted line shows symmetry plane

Table 8-8 shows the recalculated node parameters on the simple cylindrical symmetrical grid aligned in the z direction. The highlighted section relates to the highlighted section in Table 8-7. The symmetrical pattern was repeated for alignment along the x axis and y axis. This shows that with a symmetrical grid the calculated node values for the field components are reflected about the symmetry plane.
<table>
<thead>
<tr>
<th>Variable</th>
<th>Radial</th>
<th>Node distance along radial in mm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>0.03</td>
</tr>
<tr>
<td>potential</td>
<td>y -ve</td>
<td>-298134.81</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>-299696.37</td>
</tr>
<tr>
<td></td>
<td>y +ve</td>
<td>-298134.81</td>
</tr>
<tr>
<td>field magnitude</td>
<td>y -ve</td>
<td>6172569.98</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>5301039.14</td>
</tr>
<tr>
<td></td>
<td>y +ve</td>
<td>6172569.98</td>
</tr>
<tr>
<td>x field component</td>
<td>y -ve</td>
<td>-1951938.01</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y +ve</td>
<td>1951938.01</td>
</tr>
<tr>
<td>y field component</td>
<td>y -ve</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>0.00</td>
</tr>
<tr>
<td></td>
<td>y +ve</td>
<td>0.00</td>
</tr>
<tr>
<td>z field magnitude</td>
<td>y -ve</td>
<td>-5855814.04</td>
</tr>
<tr>
<td></td>
<td>y=0</td>
<td>-5301039.14</td>
</tr>
<tr>
<td></td>
<td>y +ve</td>
<td>-5855814.04</td>
</tr>
</tbody>
</table>

Table 8-8 node values of simple symmetric cylindrical grid, aligned along z axis.

All subsequent grids were designed to be symmetrical to avoid introducing errors into the predictions as a result of the non-symmetry of the grid.

### 8.4.2 Effect of angle of grid on Laplace solution

To test the model in cylindrical geometry the grid was designed by adapting the symmetric rectbox2 grid, to a simple cylindrical geometry, shown in Figure 8-16. This grid has 24 nodes and 36 elements and is called ‘cyl_sim’. There are 4 nodes along each radial, giving a spacing of 3 elements between the electrodes.

![Figure 8-16 Rectbox2 grid converted to cylindrical geometry](image)

The angle made by the 2 outer edges, extended to the centre of the circle, will affect the accuracy of the predictions made using this grid. The grid was arranged to have, first, an angle of approximately 12° and, secondly, 8°. Thirdly
the number of nodes along the radial of the grid having angle 8° was increased to 6, giving 5 elements. The inner radius is 3 cm and the outer radius is 15 cm. The potential applied at the inner electrode is -300 kV and at the outer electrode is 0 kV. The choice of these values ensures that all the nodes on the inner electrode are coronating. The Laplace predicted values of potential and field magnitude are compared to the analytical solution see Figure 8-17 to Figure 8-28.
8.4.2.1 Grid with 4 radial nodes, angle of 24°

Figure 8-17 Potential, red line is analytical value, blue line is calculated value

Figure 8-19 Error in potential, as percentage of mean true potential

Figure 8-18 Field magnitude, red line is analytical value, blue line is calculated value

Figure 8-20 Error in field magnitude as percentage of mean true field.
8.4.2.2 Grid with 4 radial nodes and angle of $8^\circ$
8.4.2.3 Grid with 6 radial nodes and angle of 8°

Figure 8-25 Potential, red line is analytical value, blue line is calculated value.

Figure 8-27 Error in potential as percentage of mean true potential

Figure 8-26 Field magnitude, red line is analytical value, blue line is calculated value

Figure 8-28 Error in field magnitude as percentage of mean true field
8.4.2.4 Summary

The accuracy of the 3 grids above is compared in Table 8-9.

<table>
<thead>
<tr>
<th>Angle of grid, °</th>
<th>Number of nodes along radial</th>
<th>Maximum %age error</th>
<th>Potential</th>
<th>Field magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>4</td>
<td>2.4</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>4</td>
<td>0.3</td>
<td>8</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>6</td>
<td>0.06</td>
<td>1.2</td>
<td></td>
</tr>
</tbody>
</table>

*Table 8-9 Comparison of errors in field magnitude and potential for changes in node spacings*

The accuracy is improved by use of a finer grid. This is expected - the disadvantage is the increase in running time. From the comparison above it was decided that the wider angle grid was not suitable. If, at a later stage the model is to be used for predictions in a wire-duct geometry then the accuracy achievable will depend on the design of the grid. The design could be such that the grid is finer closer to the electrode, i.e. in the region of greatest change of the variables. The grid design could be tested first on a 1/4 cylinder grid. Figure 8-29 shows the calculated field vectors for a simple wire-duct grid, adapted from the rectbox2 grid described in section 8.3.4. The field magnitude on the wire nearer to the plate is greater than the field magnitude on the wire away from the plate. This is as would be expected.
8.4.2.5 Effect on space charge calculations

The values of potential and field obtained from the solution of Poisson’s equation are used as the starting point for the solution of current continuity. It has been shown in section 8.3.3 that this procedure works well for plane-plane geometries where the errors are small and the variation of space charge between the electrodes is relative small. For cylindrical geometries section 8.4.2 shows that the angle of the grid and the spacing of the radial nodes are highly significant in the accuracies achievable. If early iterations of Poisson’s equation calculate unrealistic values of space charge, the coarseness of the grid and the linear approximation for space charge limits the current continuity solution in converging to the correct solution. Additionally if the calculated values of space charge are unrealistic this feeds back to the solution of Poisson’s equation. The program will then either oscillate or not approach convergence. For realistic discharge electrode diameters, e.g. 5mm, the spacing close to the electrode must be such that the order of change in a parameter over an element is similar for all elements.

Figure 8-29 Field vectors for Laplace on a simple wire-plate grid
8.4.2.6 Non-convergence of iterative solution

The cylindrical grid has been used to test the accuracy of predictions for Laplace, and the effect on this accuracy of the design of the grid and the spacing of the nodes. The 8° grid was then used to test the Poisson solution, as explained in section 5.7.3. A scaling factor of $10^{-4}$ was obtained. The model was then run for the full ion-drift problem. The space charge scaling factor is output to the screen and from this it appeared that the iteration was proceeding satisfactorily. After 8 iterations it could be seen that the value of the scaling factor was oscillating between 0.9945 and 1.2327. This indicates that the calculated values of space charge are increasing and the solution is not converging. Examination of the data file showed that at 8 iterations the space charge on the electrode was a factor of 10 too large. A similar pattern was observed for the grid with 6 radial spacings and again for a lower applied voltage (-200kV) where the field suppression is less and therefore the variation of space charge over the region is smaller.

The testing of the Poisson solution by fixing the field to the values calculated by Laplace indicates that the program is formulated correctly. It appears that, for the coarseness of grid, the model is unable to home in on the correct space charge at the boundary and a solution cannot be obtained. Finer grids are required to match closely to smaller discharge electrode radii and also to allow more nodes along a radial and hence reduce the variation of space charge over an element. The size of the grid then exceeds that which can be handled by the present hardware and operating system.

8.5 Comparison of the model’s predictions to experimental data

Whilst the model can be tested for plane-plane geometries and cylindrical geometries against the analytical solution no such solutions are available to compare with predictions for more realistic geometries e.g. square or cylindrical wire discharge electrode in a duct with flat plate collecting electrode. In this case predictions can be compared to experimental data, such as [28]. Chapter 9
discusses the memory management and running time limitations of the program and identifies possible solutions so that wire-duct geometries can be modelled. The predictions should be plotted in a similar form to the experimental data to facilitate comparisons.

In cylindrical geometry the radius of the inner electrode was chosen as 3cm. The larger the radius the fewer the number of elements required close to the electrode. To obtain a V-I curve for a practical discharge electrode of diameter say, 5mm, in cylindrical geometry, would require a larger grid than can be handled on the present platform. For illustration purposes Figure 8-30 shows a simulated V-I curve obtained using the plane-plane geometry. From inspection of Figure 1-4 the corona onset voltage is approximately -40kV. At this voltage the Laplace field is 271186 V/m. This is chosen as the corona onset field and used to simulate charge injection at higher potentials.

![Simulated VI curve](image)

*Figure 8-30 Simulated VI curve, inner electrode radius 2.5mm, outer electrode distance 15cm.*

One of the aims of the model was to not rely on semi-empirical data which does not take account of the variations over the discharge electrode. It had been intended to use the full analytical model to predict V-I curves but this is not feasible at present.
There are other factors that can affect the corona onset such as the surface roughness of the electrode and the temperature and humidity in the duct. Whilst constructing this model the laboratory precipitator used to obtain the results in [28] was being constructed and operated. The hiss of the corona could easily be heard in the laboratory and in the dark the corona could clearly be seen. The laboratory has a glass roof and, at constant applied voltages, changes in the corona hiss could be heard as clouds passed overhead, the light incident on the precipitator was reduced and the temperature dropped. To improve the model predictions for practical discharge electrodes the relative importance of these effects need to be considered with the aim of planning their inclusion in the model.

8.6 Summary
The accuracy achieved for plane-plane and cylindrical geometry demonstrates that the appropriate functionals have been used, the equipotential surface is matching sufficiently closely to the electrode so that the field is not distorted. The memory management of the program needs to be improved before finer grids, with greater numbers of nodes and elements, can be used. It would be helpful if the running time could be reduced. The ways of achieving these improvements are considered in chapter 9.

Since finite element analysis allows the value of the parameters to be calculated at any point, the potential, electric field and charge density can be determined for the whole region, or for a particular area of interest, e.g. over the collecting plate electrode. A graphical post-processor would facilitate the interpretation of the predictions.
9. CONCLUSIONS AND FURTHER WORK

The model has laid the foundations of a computer simulation of the effects of small scale variations in the discharge electrode geometry on the electric field, potential and space charge density within a precipitator. The research objectives in section 1.5 are stated as:

1. build a model that can easily be adapted to include new features
2. model the detailed geometry of a discharge electrode
3. develop an improved design technique for discharge electrodes.

9.1 A model that can be adapted to include new features

Section 5 shows the development of the broad specification of the model. A key factor in the design is that it should be easily adapted to include new features as other areas of the research work identified new requirements. During the building of the model the need for the equipotential functional was identified.

The inclusion of these expressions required the functions for the construction of the disconnected matrix to be changed. The generality of the overall design allowed these changes to be made without further changes to other parts of the code. Additionally the equipotential expressions include a constant which is the applied potential at the electrode. Outside of the functions to construct the disconnected matrix the inclusion of this constant required only one line of code.

9.1.1 Background dust

A possible extension of the 3D model would be the inclusion of a background dust, for which a new functional would be required. The inclusion of dust in 1D is reported in [9], see Appendix C. The use of any new functional would require the adaptation of the functions to create the related disconnected matrix.

Dust can be considered not to contribute to the current within the precipitator because dust has a low mobility compared to the ions. Its presence will contribute to the overall charge density and hence change the electric field. The
construction of the Laplace and Poisson disconnected matrices would be adapted to include expressions derived from the new functional. This new functional also includes a constant term which could be placed in a new vector. Again the generality of the model would be unaffected; the conversion to the connected matrix, collapsing of the matrix and obtaining the solution to Laplace, Poisson and current continuity would remain the same.

9.1.2 Time varying potential
The present model uses a constant applied potential. Currently there is much interest in pulsed energisation of precipitators. A possible extension to the model would be the application of a time varying potential. This would require the use of the time dependent form of the Laplace and Poisson functionals. A related project within the group is to build a switched mode high voltage power supply. If the model could be extended to include the time variation of applied potential then comparison could be made between the model predictions and experimental measurements on the existing laboratory rig using the prototype pulsed power circuit. It is possible that another method other than FEA, might be more appropriate.

9.1.3 Field dependent mobility
The 1D model, with cylindrical symmetry, has already been developed to include a linear field dependent mobility relationship. This required the derivation of a new formulation of the Galerkin residual, and therefore new expressions were used in the construction of the current continuity disconnected matrix. No other changes were required. The new feature was included in the analytical formulation of the residual, rather than by major changes to the model. The possibility of extending the field dependent mobility to 3D and other possible dependencies of mobility upon field were discussed. It was concluded that the advantage of the symbolic nature of the underlying expressions that allow the model to remain unchanged for different grids would be lost if this route for development were followed. Constant mobility matches the exact field independent solution more closely than any of the illustrated linear relationships. The inclusion of field dependent mobility in 1D illustrated the
generality of the model and the inclusion of new features within the existing model design.

9.2 Detailed modelling of discharge electrode geometry

This model demonstrates the principles of the detailed modelling of the geometry of the discharge electrode. Most previous simulations model a barbed or spiked electrode using a cylindrical wire with an 'equivalent radius'; the equivalent radius having been determined by examination of the VI characteristic. This model demonstrates that the fitting of elements to plane and curved surfaces can be built up to fit any electrode geometry. The use of the local radii of curvature, based on the Peek expressions [51], is reported in [37], see Appendix C. Input data files and global variables are the means of incorporating the information about the discharge electrode into the model, by specifying for each node separately:

- the field direction and radii of curvature
- whether the node is on a curved electrode, on a plane electrode or in the bulk of the solution region
- the known parameters at each vertex node.

Further global variables are then derived, whether a face node is on a plane electrode, on a curved electrode or in the bulk of the region.

The use of data files allows the local geometry and the properties of the electrodes to be passed to the prediction program. The program uses this information to select the appropriate expressions for an element in the disconnected matrix and set the vector of unknowns. The model handles this information for any combination of curved or plane electrode nodes without changes to the code.

9.2.1 User interface

At present the code must be run by someone who was directly involved in the design and construction of the program. It was suggested that a user-friendly pre-processor, that prompts the operator for the required information and
automates much of the data input, would be useful. A post-processor for graphical visualisation of the predictions would also make the application more user friendly.

9.2.2 Practical discharge electrodes

The grids currently make use of all the symmetry planes to reduce the number of nodes necessary to make a prediction. To use a quarter section of a discharge electrode would assume that the duct has reflective symmetry about the plane midway between the discharge electrodes perpendicular to the plate and about the plane of the discharge electrodes. To consider some practical electrodes these reflection planes may not be applicable. For spiked electrodes the spikes give rise to plumes of corona discharge. Plumes from neighbouring electrodes can interfere, the stronger plume deflecting the weaker plume. To simulate this it may be necessary to include at least 2 electrodes with the boundary conditions set up so that the coronating regions are not identical at the electrodes.

9.2.3 Corona fluctuations

Recent experimental work [28] has shown that corona is variable in both time and spatially. In a laboratory precipitator the corona points were observed to move over the discharge electrode. For a square wire the corona occurred along the corner edge, in tufts which moved. It seemed that at some points the corona appeared for longer, or was more like to reappear at the same place sooner. This may be due to irregularities or dirt on the surface of the electrode. For the round wire the corona moved over most of the discharge electrode surface whereas on the square wire the corona could mostly be seen on the sharp edge of the electrode. The model will predict the average current density at the collecting plate and this can be compared to time averaged experimental data.

To simulate the moving tufts of corona, stochastic variation of the corona location could be introduced into the model. The full iterative solution must be obtained for one corona arrangement and then repeated for other corona arrangements, e.g. using Monte Carlo techniques. The distribution of the results could then be constructed. A number of arrangements would be needed to get a
good range of results. This idea would be more practicable if the running time of the model could be reduced.

9.3 Improved design technique for discharge electrodes

The need for a simulation that can predict the electric field and charge density within a duct precipitator had been identified. In particular the effects of the small scale variations in discharge electrode geometry are of interest. If these effects can be predicted then different electrodes can be compared; either to evaluate the suitability of existing electrode design for particular priorities, e.g. collection of very small particles, or to investigate novel electrode designs. Before the present model can be developed to make the predictions required for such detailed studies several improvements are required.

9.3.1 Limitations of the model and further work

The fundamental design, implementation and testing of this model have been completed. The limitations of the present model are in the long running time and the memory management. Typical semi-conductor device models have the order of $10^6$ elements, do not use higher order expressions, do not require an iterative solution and take several days to run. There are several small amendments to the code in the present model that would give minor improvements in the running time. For example, greater use of global variables would reduce the memory overhead, and hence reduce swap file operations, and some functions that are called many times could be examined to determine more efficient methods of computation, perhaps by implementing them in assembler language. A change of operating system could also be considered as Windows 3.1 does not efficiently use more than 16 Mbytes of RAM.

To model realistic wire duct geometries the grids would be larger, both having more layers and with finer spacing. Finer spacing is especially important around any curved surfaces of the discharge electrode. If such grids were used the running time would be prohibitive - especially if comparisons at different voltages were required. The model was developed for a PC because, primarily, this met the financial constraints of the project and allowed the purchase of
several software packages that assisted in the development of the model to the present level within the time available.

9.3.2 Change of operating system
Use of a PC operating system other than Windows 3.1 may be an improvement. Systems such as 'Windows NT' or 'OS/2 Warp' could be considered. Windows NT would itself required additional hard disk space and memory space. Although OS/2 Warp is advertised as running programs that will run under Windows 3.1, the compatibility of MATLAB with another operating system must first be investigated. If an alternative version of MATLAB were to be used then the compatibility of the existing program with the alternative MATLAB would need to be assured.

9.3.3 Convert to run on a UNIX based workstation
If the model is to be used to simulate practical electrodes in precipitator geometries then an alternative hardware platform to the PC should be considered. MATLAB 4.2c runs on a UNIX based workstation such as a Sun SparcStation. The model, which uses standard MATLAB functions, could be ported to run on such a workstation with only minor alterations to the code required. Typically a Sun SparcStation has 32 Mbytes of RAM which can be increased to 128 Mbytes or more. Like a PC, virtual memory or a swap file is also used. UNIX addresses the RAM more efficiently than DOS and the memory management limitations inherent in DOS would not apply.

9.4 Summary
A 3D model, to use the symbolic formulation of the finite element functionals and residuals, has been developed to predict potential, field and space charge. The use of the analytical form of the integrals allows the model to be easily used for a variety of geometries. The generality of the design allows new features to be included. This adaptability has been demonstrated and will proved a useful, and unusual, aspect as the model is developed further.
The model has demonstrated the use of

- plane electrode nodes, with potential fixed or on an equipotential,
- curved electrode nodes, potential on an equipotential,
- elements having a face on an electrode,
- elements touching an electrode,
- nodes on a cyclical boundary,
- nodes on symmetry boundaries,
- bulk nodes.

From these a grid can be designed to model a variety of geometries.

Further work is required to improve the efficiency of the model and to develop a user-interface. On more powerful computer hardware, using a sufficiently large grid, discharge electrodes having spikes or barbs could be modelled, and new electrode designs could be simulated. This is the foundation of a new design tool for the design testing of novel discharge electrodes.
10. APPENDICES

APPENDIX A MATRIX MANIPULATION

The matrix [NEW_ELEM] contains the information about the global number of each local node within all the elements. To determine the relationship between the local nodes of an element and the global node numbering within the solution region a 'connection' matrix is constructed.

In this prediction program the matrices for Laplace, Poisson and Current Continuity are similarly named, but include an L P or C to designate which part of the iterative procedure they relate to. The disconnected matrix of coefficients is known as [MATDIS]. It is constructed element by element. For Laplace there are 20 unknowns in each element, and therefore 20 coefficients in the expression for each unknown. The part of [MATDIS] that relates to each element therefore has 20 rows and 20 columns. The full matrix consists of one of these 20 by 20 sections for each element along the diagonal of the matrix. This results in a very large matrix, size (20*number of elements, 20*number of elements), of mainly zero elements.

The connection matrix, as described above, consists of the same number of rows as the disconnected matrix. the number of columns is the same as the number of global variables. The matrix is all zeros except for ones in the positions that relate a disconnected coefficient to its global numbered coefficient e.g. if local node 1 of element 1 has the global number of 10 then, remembering that there are 4 variables at each node, there will be a 1 in row 1, column 37; row 2 column 38; row 3, column 39 and row 4, column 40. This matrix is known as [CONU]

The connected matrix of coefficients is known as [MAT]. Once this has been collapsed, to remove the rows and columns that relate to variables already set by boundary conditions, it is the 'collapsed connected matrix' and is known as [CMAT].
To convert [MATDIS] to [MAT] is not a simple operation as [CONU], which represents the relationship between them, is not a square matrix. The matrix manipulation that is therefore required is given below.

[MATDIS] is a matrix such that

\[ [MATDIS] \cdot [UDIS] = [ZERODIS] \]

where [UDIS] is the vector of disconnected unknowns and [ZERODIS] is the associated zero vector

and [CONU] is such that

\[ [UDIS] = [CONU] \cdot [UCON] \]

where [CONU] is obviously not square

It is required to find the matrix [MAT] where

\[ [MAT] \cdot [UCON] = [ZEROCON] \]

where [UCON] is the vector of connected unknowns and [ZEROCON] is the associated zero vector

Firstly it is necessary to calculate [CONNECT_U] such that

\[ [UCON] = [CONNECT_U] \cdot [UDIS] \]

It is known that

\[ [UDIS] = [CONU] \cdot [UCON] \]

therefore

\[ [CONU]^T \cdot [UDIS] = [CONU]^T \cdot [CONU] \cdot [UCON] \]

where \([A]^T\) is the transpose of the matrix \([A]\)

The product \([CONU]^T \cdot [CONU]\) is a square matrix therefore can take the inverse

\[ ( [CONU]^T \cdot [CONU] )^{-1} \cdot [CONU]^T \cdot [UDIS] = [UCON] \]

ie

\[ [CONNECT_U] = ( [CONU]^T \cdot [CONU] )^{-1} \cdot [CONU]^T \]
now using
\[ \text{MATDIS} \cdot \text{UDIS} = \text{ZERODIS} \]
we have
\[ \text{MATDIS} \cdot \text{CONU} \cdot \text{UCON} = \text{ZERODIS} \]
\[ \text{CONNECT, U} \cdot \text{MATDIS} \cdot \text{CONU} \cdot \text{UCON} = \text{CONNECT, U} \cdot \text{ZERODIS} \]
\[ \text{CONNECT, U} \cdot \text{MATDIS} \cdot \text{CONU} = \text{ZEROCON} \]
ie
\[ \text{MAT} = \text{CONNECT, U} \cdot \text{MATDIS} \cdot \text{CONU} \]
therefore
\[ \text{MAT} = (\text{CONU}^T \cdot \text{CONU})^{-1} \cdot \text{CONU}^T \cdot \text{MATDIS} \cdot \text{CONU} \]
The potential at the boundaries are represented in a vector BOUND. The value in BOUND are calculated from the relevant coefficients in the matrix MAT and the applied potentials.
MAT includes the coefficients for the known values that have been included in BOUND. MAT is collapsed to CMAT by removing from MAT those rows and columns that relate to the known values.
The solution vector SOLUTION is found from
\[ \text{CMAT} \cdot \text{SOLUTION} = \text{BOUND} \]
SOLUTION contains the determined values for potential, field and space charge for each of the nodes. The order of these values within the vector SOLUTION depends on the order of the coefficients in the matrices, but the vectors POTENTIAL, E_FIELD and S_CHARGE are extracted from SOLUTION which together with the applied potentials at the boundary nodes are the full solution.
APPENDIX B CONVERGENCE

At the end of each iteration loop, the present and previous solution vectors for potential, field components and space charge at the nodes are compared to find if the solution vectors have all converged. To do this, a vector of the absolute normalised differences between the present and previous values of the solution components is calculated for each variable. Taking potential as an example, the vector of differences is found as follows.

Let \( \mathbf{p}^{\text{new}} \) be the vector of the latest values for the node potentials, and \( \mathbf{p}^{\text{old}} \) be the vector of the previous values. Let \( N \) be the size of these vectors. The magnitude of \( \mathbf{p}^{\text{new}} \) is

\[
\text{mag}(\mathbf{p}^{\text{new}}) = \left( \sum_{n} (p_n^{\text{new}})^2 \right)^{\frac{1}{2}} \tag{Equation 1}
\]

and the r.m.s. value is

\[
\text{rms}(\mathbf{p}^{\text{new}}) = \frac{\text{mag}(\mathbf{p}^{\text{new}})}{N^{\frac{1}{2}}} \tag{Equation 2}
\]

If \( \text{mag}(\mathbf{p}^{\text{new}}) \) is not zero, a vector of absolute normalised differences is constructed with entries

\[
\text{diff}(\mathbf{p}^{\text{new}}, \mathbf{p}^{\text{old}})_i = \frac{|p_i^{\text{new}} - p_i^{\text{old}}|}{\text{rms}(\mathbf{p}^{\text{new}})} \tag{Equation 3}
\]

Such a vector of differences is constructed for each variable that is not identically zero at all nodes. A tolerance \( \text{maxdiff} \) is defined (e.g. \( \text{maxdiff} = 0.0001 \)), and the solution vectors are said to have converged if the maximum entry in all the vectors of differences is less than \( \text{maxdiff} \), and any identically zero solution vector was also identically zero after the previous iteration. An upper limit is also put on the number of iterations (this is normally set at 20).
APPENDIX C PUBLICATIONS

The following publications are associated with this work. Those marked X are bound with this thesis.


Bromley KS, 1994, *Development of a computer model to predict the electric potential, field and space charge for an electrostatic precipitator using finite element analysis*. Interim report for SERC research grant GR/J10044.


X Houlgreave JA, Bromley KS and Fothergill JC, 1996, *An electroquasistatic finite element model of electric fields and currents generated by coronating electrodes in an electrostatic precipitator*. 3rd Int. Conf. on Computation in Electromagnetics, IEE Conf. Pub. 420, 121-126


Abstract. A finite element based computer model is being developed to estimate electric potential, field, and charge and current densities in an electrostatic precipitator. It uses an efficient iterative procedure to solve the ion drift problem which requires no empirical assumptions about space charge at the injecting surface or the effects of space charge on flux paths. The development process takes advantage of the algebraic and numeric mathematical languages available on PCs. Initial results in one dimension are presented which verify the solution procedure. The anticipated approach in three-dimensions is summarised.

Introduction

Electrostatic precipitators are widely used to remove dust particles from gas flows such as those in the boiler chimneys of electricity generating stations. The gas is drawn between earthed collecting plates, past high voltage corona discharge electrodes which ionise gas molecules and hence charge the dust particles. The particles are then electrostatically attracted to the earthed collecting plates. Software is being developed to implement an accurate electroquasistatic model to predict the effects of new discharge electrode geometries on electrical conditions within an electrostatic precipitator. The work is part of a research programme aimed at producing improved techniques for designing discharge electrodes. This programme has parallel modelling and experimental components, enabling the full model to be tested against purpose designed experiments as well as published results. The experimental work, which will not be described here, uses a well-instrumented laboratory rig having parallel 1.5m x 2.7m plates with variable spacing and which allows different discharge electrode geometries and spacings to be introduced.

Methodology

Problem Definition: The problem that the model will solve is to find reasonable approximations to the spatial distributions of potential and mobile ionic space charge that simultaneously satisfy the Poisson and current continuity equations over a given gaseous region containing suspended charged dust. This region has symmetry boundaries and geometrically complex conducting boundaries. The potentials on the conducting boundaries
are fixed, and there is charge injection from ionisation processes in regions with sufficiently high field - these high field regions are close to highly-curved parts of the conducting boundaries.

The aim is to model the effects of electrode geometry on the important electrical parameters affecting precipitator performance - the electric field, current density and ionic space charge distributions. Only those factors having the most significant effect on these parameters are being included in the model at present. The model currently being developed is purely electroquasistatic, that is the coupled fluid dynamic (i.e. electrohydrodynamic) effects are being ignored. Dust particle charging and migration are not being modelled at this stage; but dust space charge effects, which are very important, are being incorporated by allowing an arbitrary background space charge distribution in the model. This will enable electrode characteristics to be predicted for a range of space charge distributions, ranging from typical to extreme, taken from experiments and other sources.

The model will enable the approximate characteristics of given electrode designs under a range of conditions and constraints to be compared in terms of space averaged values of quantities such as ionic space charge density (important in determining dust charging rates). Detrimental effects of phenomena such back ionisation and electric wind can be minimised by having near uniform current distributions and maximum current densities as design criteria. Performance could be further enhanced by varying electrode design along a precipitator based on expected levels of collection and re-entrainment. The model will have the advantage that new electrode designs can be tested quickly and at low cost, even if the approximations used imply that the tests are not exhaustive. Only promising designs will be passed on for testing on a pilot plant. It will be possible to incorporate the techniques used in this model into a more complete model.

Overview of Solution Method: The problem is to be solved using a finite element based model. This approach was chosen because of the particular suitability of the finite element method (FEM) for dealing with complicated geometries. The fixed field charge injection law has been specified as it gives a good macroscopic approximation to charge injection from a corona discharge. For the model to be successful, the electric field, current density and space charge density must be estimated with sufficient accuracy to predict changes in levels of particle charging and the velocities with which the particles migrate towards the collecting electrodes, with changes in design. A Hermite cubic approximation [1] for potential and a linear approximation for space charge density over an element have been used to give good accuracy with small numbers of elements and to reduce discontinuities in the piecewise field and current approximations. A Hermite cubic approximation matches magnitude and gradient of potential at the element vertices, so each element vertex has the local values of potential and field components as parameters.

The variational and Galerkin weighted residual method [1] were used respectively to derive the desired set of equations from Poisson's equation and the current continuity equation. Current continuity leads to equations that are non-linear in the node parameters (node potential, field and space charge density), hence an iterative solution procedure is needed. The set of simultaneous equations can be solved using the direct iteration procedure summarised below.

1. Use general symbolic formulation, mesh information, dust space charge distribution and boundary conditions to form initial matrices. Set ionic space charge initially to be uniform and non-zero.

2. Obtain FEM solution to Poisson's equation with the following kept fixed: boundary
potentials, injection electric field, dust space charge distribution and shape of ionic space charge distribution. The FEM solution gives estimates for potential, electric field and scaling factor for ionic space charge.

3. Obtain FEM solution to current continuity equation with the following kept fixed: potential, electric field and discharge electrode injection current density (equivalent to fixing space charge at the discharge electrode since field is fixed). The FEM solution gives an estimate for ionic space charge. (Dust charging and migration are assumed to have negligible effect on the solution to current continuity).

4. Check for convergence. Repeat from step 2 if convergence criterion not met.

In the solution to Poisson's equation, ionic space charge density is assumed to have the form $k \rho(r)$ where $k$ is the scaling factor and $\rho(r)$ is the previous estimate for the ionic space charge density. The use of a scaling factor means that ionic space charge does not have to be fixed as a boundary condition at the charge injection point as is usually the case in such models, hence ionic space charge is predicted as a function of operating conditions, geometry and injection field only. For cylindrical geometries, the injection field at the discharge electrode surface is fixed according to Peek's empirical law [2] which has been derived theoretically for positive corona by Budd [3], or using the more exact expression due to Zaengl and Nyffenegger [4]. These fixed field laws are valid when discharge electrode diameters and corona thicknesses (typically 0.5 to 2.5 mm) are small compared to the outer cylinder diameter. More involved schemes are needed to fix the field with complicated geometries.

Algebraic Formulation Technique: As much as possible of the development of the finite element solution uses symbolic computation so that it is kept accurate and general, to reduce errors, speed up the development process and to largely automate the process of trying out different modelling ideas. The use of symbolic computation means that the complex algebraic expression inherent in using high order three dimensional elements can be incorporated into the model, and that exact polynomial integration can be used and performed once prior to any numeric code being implemented. This will increase the accuracy and speed of the final software.

Development Tools and Techniques: New “PC-type” computers have speeds and memory sizes which are comparable to those of many workstations, they have the advantage that they are widely used, and powerful software is available at competitive prices. These developments are being used to advantage in developing the computer model.

The first stage of the development cycle uses Maple V [5], a powerful symbolic and numeric computation software package. Maple V has been used to symbolically derive the chosen polynomial expressions for potential and space charge density and the relevant functional equations in terms of node parameters. Maple V incorporates a facility for outputting run-time optimised C code. Such code could be used as the basis of C functions to generate numeric values from any of the polynomial expressions. Instead, however, an interface program has been written to convert this C code into MATLAB [6] functions. The analytical expressions derived using Maple V are therefore efficiently passed to MATLAB. The numeric calculation for the model is undertaken in MATLAB. Numeric computation of a solution to the model, by implementing the iterative solution procedure for a very simple grid, can also be done for checking purposes using Maple V.

MATLAB is a high level software package designed to give high performance in numeric computation and data visualisation. MATLAB is designed for efficiently
manipulating matrices - its basic data type. The finite element method requires the construction and solution of simultaneous equations that can best be represented as matrices. MATLAB has therefore been chosen as an easy to use, efficient means for the numeric solution of these systems of equations. MATLAB is used for developing and implementing the iterative solution procedure which involves the solution of a sequence of sets of linear equations. MATLAB uses the function files based on the algebraic expressions derived using Maple V together with numeric grid data.

The mesh of the solution region is generated using C++ and FEMGEN/FEMVIEW [7], an interactive graphical pre- and post-processor for use with finite element packages. FEMGEN is used to generate a mesh of prism elements. The neutral output file format is interfaced to MATLAB via a C++ program which converts the generated grid of prisms to tetrahedrals and renumbers the elements. The resulting data file may be loaded directly to MATLAB.

Verification

Verification of the Iterative Procedure using a One Dimensional Model: The initial cycle of software development was using one-dimensional radial elements in a cylindrically symmetric model. That is, position in an element is described using a single co-ordinate, the radial distance from the axis of symmetry; hence the volume integrals used in the finite element approach were over the space between two concentric unit length cylinders corresponding. This cylindrical geometry was chosen so that an analytical solution, which is known to give a good representation of experimental results, could be easily obtained for the purpose of proving the technique. The figures show results obtained using from the one-dimensional model for a 5 mm diameter wire at a 300 mm diameter earthed cylinder, the first two figures are for -60 kV applied voltage. Figure 1 shows a set of graphs illustrating example results and errors. The lines in the left-hand graphs show the analytical results superimposed on the piecewise FE approximations after 7 iterations with 10 radial elements. The node values for the approximations are shown by the circles, and the dotted lines show the mean values over the cylindrical solution space. It can be seen that the approximations are very close to the analytical solutions (the curves are almost indistinguishable). The graphs on the right show absolute errors relative to the mean values. It can be seen that the only significant absolute errors are in values for field and current density in the region of rapidly changing field close to the discharge electrode: and it must be noted that these are in a region where true values are large compared to the mean.

Figure 2 shows a comparison of charge densities and current densities with and without a uniform background dust space charge (indicated by the curve labelled ‘dust’ in the left-hand graph). In both cases the curves with node values marked with circles are for no dust. In the left-hand graph, the curve labelled ‘ions’ shows the charge density of ions with dust present; the curve labelled ‘dust + ions’ shows the combined charge density of dust and ions. These graphs clearly show the corona suppressing effects of dust space charge. The circles on the curve in figure 3 show the results of running the model for a number of different applied voltages; this indicates how a V-I curve can be constructed from the model.

Extension of Iterative Procedure to Three Dimensions: Having been proved in one dimension, the model is being extended to three-dimensional geometries using tetrahedral elements. A Hermite cubic approximation is used for potential and a linear approximation is used for space charge requiring 20 and 4 node parameters respectively.
Figure 1: Results from 1-D model of ion drift between concentric cylinders
The main framework for the three-dimensional model is now complete. The grid generation and matrix handling routines have been successfully tested in solutions of Poisson's equation based on a variational formulation of the FEM using standard quadratic tetrahedral elements. The appropriate functional equations have been derived for modelling with Hermite cubic potential and linear space charge. Work is proceeding on imposing the desired boundary conditions.

Acknowledgements

We gratefully acknowledge support from EPSRC (project GR/J10044), DTI (ETSU), National Power plc and Lodge Sturtevant Ltd. and helpful discussion with Ken Parker, Martin Selby and Chris Budd.

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AN ELECTROQUASISTATIC FINITE ELEMENT MODEL OF ELECTRIC FIELDS AND CURRENTS GENERATED BY CORONATING ELECTRODES IN AN ELECTROSTATIC PRECIPITATOR

J A Houlgreave, K S Bromley & J C Fothergill
Department of Engineering, University of Leicester, LE1 7RH, UK

ABSTRACT
A three-dimensional finite element (FE) model is being developed to predict the effects of high-voltage corona discharge electrode geometry on charge injection, space charge distribution and electric field within an electrostatic precipitator. The motivation is to have a tool for improving the designing of discharge electrodes and enabling them to be custom-designed for specific applications. The problem which will be solved by the model is Poisson’s equation coupled with current continuity (i.e. the ion drift problem in air) with geometry dependent charge injection at the discharge electrode surface and an arbitrary static background space charge density (which is assumed not to contribute to the current) due to a charged airborne particulate.

Key features of the modelling include: the use of 3-D Hermite elements and use of symbolic computation in the model’s development.

BACKGROUND
Electrostatic precipitators are devices for removing entrained particulate from industrial gas flows e.g. fly ash from flue gases in coal-fired power stations. The gas flows through earthed metal ducts containing suspended high-voltage monopolar corona discharge electrodes. Electrons generated in the discharge close to the high-voltage electrodes quickly attach to electronegative gas molecules to form ions. These ions drift towards the earthed duct walls due to the electric field produced by the high voltage on the discharge electrodes. Some of the drifting ions impinge on the entrained particles thus charging them. This causes the particles to drift to the duct walls where they tend to adhere on contact. (The contribution to current flow from the motion of charged particulate is negligible due to its very low mobility). Typically, as the particles build up on the duct wall they form a cake which is then knocked off and caught in a hopper below.

Precipitators are difficult devices to model accurately: the electroquasistatic and fluid dynamic processes involved are complex in themselves, and the close coupling between them significantly adds to the complexity. This paper describes initial work on a new precipitator model which tackles the electroquasistatic problem of charge injection by monopolar corona and subsequent ion drift in isolation. Other major components of the model will include the dynamics of particle charging and particle transport in turbulent gas flow. A full-sized laboratory rig has been constructed to enable comparisons to be made with measured electrode characteristics. Thus there is provision for proving model developments against real measurements in addition to analytical solutions of simple cases.

To solve the electroquasistatic precipitator problem one must simultaneously solve Poisson’s equation and the current continuity equation subject to the appropriate potential, charge injection and space charge boundary conditions. If the applied voltage is constant in time and stochastic time variations due to corona are ignored, the appropriate equations are:

\[ \nabla^2 \phi = -\frac{Q}{\varepsilon} \]

\[ \nabla \cdot \left( \mu_d \nabla \phi \right) = -\nabla \cdot (\mu \nabla \phi) = 0 \]

i.e. \( \rho \nabla^2 \phi + \nabla \cdot \nabla \phi = 0 \)

(Mobility \( \mu \) is taken as constant). This coupled set of equations is non-linear since the current continuity equation involves products of terms involving potential \( \phi \) with ones involving space charge \( p \).

Charge injection is determined by the field close to the surface of the discharge electrodes, thus it is determined by electrode potentials, global geometry and global space charge distribution. Since the charge injection associated with a small region of surface depends on the local field, and field depends on space charge, it is clear that a coupled mechanism will be involved. It has been shown experimentally and theoretically that this “space charge limited charge injection” mechanism results in a field at the surface of a coronating electrode which is virtually independent of time and applied voltage (Peek (1), Budd (2), Zangwill and Nyffenegger (3)). This constant field is dependent on the local radius of curvature (2). Thus, to every point on the surface of an electrode there is an associated critical field dependent only on the local radius of curvature - the electrode voltage at which the critical field is reached is dependent on global geometry and space charge distribution. The field at the electrode surface will be prevented from exceeding this critical value by the production of electrons by a field-driven avalanche process and the consequent formation of space charge. The critical field is dependent on the local curvature because the field at all points along the approximately fixed length of an avalanche path must be
greater than the gas breakdown field strength, and the rate of change of field strength is higher close to more highly curved surfaces for a given surface field. Hence a higher surface field is required to produce corona near more highly curved surface regions.

Practical discharge electrodes can have complex shapes, often involving spikes or prongs or helices. Experimental measurements of electric fields and current distributions in typical precipitator geometries show that they are truly three-dimensional in nature and that their shape can change appreciably with parameters such as applied voltage. Two-dimensional models cannot represent these phenomena with sufficient accuracy, although with experimental data an equivalent 2D electrode geometry can be substituted so that such a model will give a good approximation to overall voltage-current characteristics.

Electrostatic precipitator performance, however, depends on the detailed rather than the average electrode characteristics. Further obtaining data to find these average characteristics necessitates building and testing proposed geometries which wastes resources at an early stage in the design process. Our model aims to meet the requirement to predict electrode performance based on geometry alone, allowing the elimination of many non-viable designs before pilot test. Thus it will go much further than models that provide insight into operation only after measurements have been made.

A FE approach was chosen because of its inherent ability to deal with complex geometries. FE modelling of systems with complex geometries and simple controlling equations is now routine. Much of the current thrust in research in FE methods is into dealing with complex non-linear systems.

The modelled physical quantities which are important in determining precipitator performance are electric field, current density and space charge density as they control how the dust will be charged and collected. The ability to predict accurately how these quantities are affected by electrode geometry, and to optimise them for given operating conditions and power dissipation, would facilitate the development of more efficient electrodes.

**FE MODEL**

The model uses Hermite cubic tetrahedral elements for potential and a linear approximation to space charge over the same elements. The use of higher order elements for potential allows electric field to be approximated more accurately, and the fixed field charge injection law, appropriate to corona discharge (1), (2), (3), to be implemented more readily.

The ion drift problem is solved by a direct iteration procedure with the following algorithm which is essentially the one reported for the one-dimensional prototype model (Bromley et al (4)).

1. Input grid data, electrode potentials, electrode radius of curvature at surface nodes and dust space charge distribution. Set ionic space charge distribution to be uniform and non-zero except at non-coronating surface nodes where it is set to zero.
2. Find the variational FEM solution to Poisson's equation for potential using dust space charge only; with the following fixed electrode potentials and dust space charge distribution.
3. Identify the coronating regions of electrode surface by finding nodes for which the Poisson solution field exceeds the surface curvature-dependent critical field.
4. Find the variational FEM solution to Poisson's equation for potential and ionic space charge scaling factor with the following fixed electrode potentials, field at coronating regions of electrode surfaces, dust space charge distribution and shape of ionic space charge distribution.
5. Set potential and ionic space charge scaling factor to the Poisson solution values, and change ionic space charge at coronating surfaces in accordance with the scaling factor.
6. Find the Galerkin FEM solution to current continuity equation for ionic space charge with the following fixed ionic space charge at coronating regions of electrode surfaces and potential. (The charging and subsequent motion of the particulate have negligible effect on current continuity and are hence ignored)
7. Set the ionic space charge to the current-continuity solution.
8. If solution has not converged then go to 2, else output ion drift solution.

The above solution technique has the advantage over many previous techniques that only the field needs to be fixed at the coronating regions of the electrodes as the solution algorithm homes in on the space charge level at the injecting boundary; it does not require empirical data such as the current for a given applied voltage when dealing with complex electrodes. The initial guess at the space charge distribution is chosen to be uniform since for a general geometry there will be no prior knowledge from measurements or analytical solutions. In the solution to Poisson's equation, ionic space charge density is assumed to have the form k . p (r) where k is the scaling factor and p (r) is the previous estimate for the ionic space charge density.

The variational approach is used in solving Poisson's equation. The appropriate functionals are (Jones (5)):  

$$F_1(\phi) = \int \frac{1}{2} \epsilon \nabla \phi ^2 - \phi \delta \phi \quad dV$$  

(3)  

$$F_2(p) = \int \frac{1}{2} \beta \nabla p ^2 + \epsilon \phi \delta p \quad dV$$  

(4)

for solution of Poisson's equation with variation of potential $\phi$ and space charge $p$ respectively. These functionals must be minimised by equating their partial
derivatives with respect to appropriate parameters to zero. \( F_1(p) \) is required for finding the ionic space charge scaling factor, and is in fact equivalent to the functional obtained by the least squares weighted residual method.

The current continuity equation is solved using the Galerkin-weighted residual method. Write space charge in the form:

\[
\rho'_{ij}(x,y,z) = \sum_{j=1}^{20} c_{ij} \phi_j^2
\]  

where \( \rho'_{ij} \) is the space charge at vertex \( j \), to define the coefficients \( c_{ij} \) for an element \( e \). The expressions used in applying Galerkin method, that are equivalent to partial derivatives of functionals over an element in the variational method, are:

\[
\int (\phi^2 \delta \phi + \sum_2 \delta \phi \delta \phi^2) \, dV
\]  

The boundary conditions at the discharge electrode are determined as follows. Initially Poisson's equation is solved for the fixed space charge due to the dust - this is to take account of global effects such as Faraday shielding. The field at each node on the discharge electrode is compared with that obtained from a Peek-type empirical formula based on local curvature (or with the breakdown strength of air for flat or concave sections of surface). If the Poisson solution field exceeds this then the field is constrained to the appropriate magnitude in the direction of the Poisson solution and said to be coronating. Non-coronating nodes do not have their fields fixed but the ionic space charge density is fixed to zero.

The electrode surface boundary condition of being an equipotential surface is imposed during the initial Poisson FEM solution by forcing surface potential parameters to minimise the variational functional

\[
F_3(\phi) = \int_{S_b} \left( \phi^2 - 24V_e \right) \, dS
\]  

over the electrode surface, where \( V_e \) is the applied electrode potential. (This functional is also equivalent to using the least squares weighted residual method).

The problem is typically solved over a region bounded by a high-voltage discharge electrode, a planar earthed duct wall and several symmetry planes. This solution region is divided into a grid of tetrahedral elements each having 4 corner nodes and 4 mid-face nodes.

**SYMBOLIC COMPUTATION**

Potential is represented by a complete cubic over a given tetrahedral element \( e \)

\[
\phi(x,y,z) = \sum_{i=1}^{20} c_i \phi_i
\]  

where the coefficients \( c_i \) are expressed in terms of the co-ordinates of the four vertices and the 20 node parameters for the element. The node parameters are \( \Phi_{1..20} \), \( E_{1..4} \), \( E_{1..4}^2 \), \( E_{1..4}^3 \), \( E_{1..4}^4 \), \( E_{1..4}^5 \) which are respectively the potentials at the element vertices and face centres, and the \( x, y \) and \( z \) components of electric field at the element vertices. This is a Hermite cubic approximation.

Space charge is linear over an element \( e \)

\[
\rho'_{ij}(x,y,z) = a_{ij} x + a_{ij} y + a_{ij} z + a_{ij}^2
\]  

where the coefficients \( a_{ij} \) are expressed in terms of the co-ordinates of the element vertices and \( P_{ij}^e \) the space charge at each of the vertices.

Symbolic expressions are derived for the coefficients \( c_{ij} \) and \( a_{ij} \). The symbolic forms of \( \phi' \) and \( \rho' \) with coefficients expressed in terms of node parameters are then substituted into the functionals \( F_1, F_2 \) and \( F_3 \) and these integrals are evaluated symbolically. The final step is symbolic differentiation of these functionals by the appropriate parameters and the symbolic evaluation of the expressions (6). The result of these operations is a set of very large expressions which it would be impractical to derive by hand. The expressions for the partial derivatives of \( F_1, F_2 \) and \( F_3 \) can be used directly as functions in software to calculate the entries of the sparse matrices used in the finite element model.

**SOFTWARE IMPLEMENTATION**

The model was developed symbolically using Maple V, a powerful symbolic and numeric mathematics software package, to produce the general symbolic form for a finite element. The use of Maple V, which was used to as late a stage as possible in the model development, greatly reduced the opportunity for the occurrence of software errors. The reasons for this are that: (i) the symbolic formulation of the model is a mathematically correct expression of the initial equations and approximation scheme; (ii) the optimised code for implementing the final symbolic formulation of the model is generated automatically as output from Maple V using the worksheet containing this formulation. The symbolic approach to the model reduced computation in the numeric implementation whilst maintaining accuracy and generality.

The general symbolic formulation can be applied to a large number of problems and can be built on to tackle more complex problems. Exactly soluble problems are
used for initial testing, and then more complex geometries for which experimental results exist can be used. The program allows modifications even down to the basic model structure to be developed quickly and incorporated. The use of symbolic methods allows the move to possible extensions to the model to be accommodated in a clear and structured manner. Symbolic methods mean that non-software specialists have immediate access to the model and can freely contribute to its development. The design of the program therefore requires implementation of the general solution method, using the expressions derived analytically using MAPLE V, which can be used for any discharge electrode geometry.

The program has been built using MATLAB which is a high performance 4th generation language for numeric computation and data visualisation. MATLAB is designed for efficient manipulation of matrices and is therefore suitable for coding finite element models based on systems of simultaneous equations represented in matrix form.

The grid data files that are required for input into the main part of the program are normally generated using FEMGEN/FEMVIEW. FEMGEN/FEMVIEW is an interactive pre- and post-processor package for Finite Element Analysis. It can produce an ASCII output file in 'neutral' format. A C++ program is then used to convert the output grid from prisms to tetrahedra and to reformat the data file for input to MATLAB. C and C++ have been used to build short interface programs to convert data files from FEMGEN/FEMVIEW format to MATLAB and to convert MAPLE V derived C code to MATLAB function format.

To use the program for any geometry, general routines have been constructed that use data input files, that have been generated for a specific grid, to construct matrices that represent the way that the global nodes and their associated unknowns are connected to each other. Separate matrices of this type are required for Poisson and Current Continuity. General routines have also been written to collapse the matrix and vector for connected nodes to remove rows and columns that relate to the knowns. A reverse, vector expansion, routine is also available to construct a vector containing a full solution, e.g. Poisson the potential and field components for all nodes in the solution region.

To solve the initial Poisson’s equation, the matrix representing the simultaneous equations is constructed element by element taking into account whether any face or node(s) of the element are on an electrode boundary. Different expressions, derived from the appropriate functionals, are selected according to the properties of the individual element. In the variational method implicit boundary conditions are used but imposition of the appropriate zero field components at such boundaries improves accuracy and reduces the number of unknowns that have to be calculated (although more sophisticated pre-processing is required). A vector is derived to incorporate the known boundary conditions, i.e. the applied potentials on the inner and outer electrodes and the field components that have been set to zero to impose the symmetry boundaries. This vector also includes the constant terms that result from the derived expressions for curved surface electrode elements and from the constant background space charge. This matrix and vector are then collapsed to represent the system of simultaneous equations for all the unknowns. Multiplication of the resulting matrix and vector gives a vector containing these required unknowns. This vector is expanded to obtain the full solution.

A similar procedure is followed for the solution of the Poisson and current continuity equations in the iterative procedure. For Poisson’s equation the implementation of the boundary conditions for nodes on the discharge electrode requires the comparison of the initial Poisson solution field to the Peek-type fixed field expression, as described above. For a coronating node the field magnitude is fixed at the Peek field, in the direction as calculated for the initial Poisson solution. For a non-coronating node the space charge is set to zero for non-coronating nodes and for coronating nodes to the value calculated by the Poisson stage of the iteration. This boundary value therefore changes as the iteration proceeds and homes in on the actual value.

The number of iterations is determined by a convergence criterion based on the maximum relative change in the components of the solution vectors. The final solution can be viewed in an output data file. For comparison with experimental measurements the current density over the collection plate must be calculated. The collection plate region is divided into a grid and for each point on the grid the field magnitude and charge density are calculated. From these a value proportional to the current density can be calculated and plotted. MATLAB can be used for plotting such 2D data. Alternatively the output matrix can be input to a data visualisation package.

RESULTS

The software implementation of the three-dimensional version of the model has reached the stage where a simple test case can be run to check that the ion drift problem can be solved. The geometry used for this is plane-plane using, for the results presented, a grid over a right triangular prism with the plane electrodes at the ends of the prism (see Figure 1). 30 elements and 33 nodes were used, 3 nodes on each of 11 planes parallel to the electrodes (two of these planes coinciding with the electrodes). The nodes were equi-spaced perpendicular to the planes. The cross-section of the prism is an
isosceles triangle with a base and height of 15 mm, the planes are 150 mm apart. A voltage of 60 kV is applied across the plate and it is assumed that charge is injected at the left-hand plate in such a way that the field is constrained to a magnitude of $2 \times 10^5$ V/m. This critical field level of half the Laplace solution was arbitrarily set to simulate a significant level of charge injection as the main purpose was to check the solution of the ion drift problem in the bulk of the region. There is no background space charge.

At present the geometry-dependent charge injection is not fully implemented and so realistic grids cannot be tackled.

![Diagram showing main features of grid used in example and one of the three tetrahedral elements located between two groups of three nodes.](image)

**Figure 1.** (a) Schematic showing main features of grid used in example. (b) One of the three tetrahedral elements located between two groups of three nodes.

![Graphs showing potential solution, electric field solution, and space charge density solution.](image)

**Figure 2.** Results from plane-plane geometry test case with current injection from the left plane.

The analytical solution for the field at position $x$ relative to the left-hand plate, when the left plate is negative with respect to the right, is

$$E(x) = - \sqrt{E_0^2 + \frac{2x}{\varepsilon}}$$  

(10)
where the constant current J is chosen to give the desired potential difference across the plates for the given critical field $E_c$.

Figure 2 shows plots of the solutions for potential, field and space charge between the planes obtained after five iterations.

The curves in figure 3 show that the solutions for potential and field show negligible errors. Relative errors in space charge are less than 0.01 (1%) for most of the solution region with maximum errors less than 0.04 (4%). The errors are displayed as a proportion of the mean value of the analytical solution over the region.

CONCLUSIONS

A 3D finite element model has been implemented which solves the ion drift problem in air using Hermite cubic approximation over tetrahedral elements. A scheme has been devised which uses the injected charge-free Poisson solution and an expression based on local curvature to fix surface field at coronating points and hence add charge injection for arbitrary discharge electrode geometries - implementation of this will be completed in the near future. Symbolic computation has proved invaluable in the models development.

ACKNOWLEDGEMENTS

We gratefully acknowledge support from EPSRC (project GR/J10044), DTI (ETSU) and National Power plc.

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INTRODUCTION

A three-dimensional finite element (FE) modelling method has been devised to allow the development of software for predicting charge injection, current distribution and electric field due to monopolar corona discharge in air from electrodes with complex geometries. Prototype software using this method has given promising results. The motivation for the modelling method was the prediction of the effect of discharge electrode geometries on the performance of electrostatic precipitators (ESPs) - devices that remove solid and liquid particles from industrial gas flows. Therefore the method also has provision for the inclusion of the effects of an arbitrary background space charge (since precipitators contain charged airborne particulate). This paper gives an overview of the physical problem and the FE method used to solve it.

FE approaches to systems governed by non-linear coupled sets of equations are not straightforward. They do however have an inherent ability to deal with geometrically complex solution regions and highly non-linear unknowns - they do not require a regular mesh of elements, so the mesh can be refined to follow complicated boundaries or in places where unknowns vary more rapidly.

To solve the electroquasistatic precipitator problem one must simultaneously solve Poisson's equation and the current continuity equation subject to the appropriate potential, charge injection and space charge boundary conditions. For the simplest particulate-free case, this non-linear coupled set of equations is:

\[
\nabla^2 \Phi = -\frac{\rho}{\varepsilon_0}
\]

\[
\nabla \cdot \mathbf{J} = -\nabla \cdot (\varepsilon_0 \mathbf{E}) = -\nabla \cdot (\varepsilon_0 \left( \mu_0 \nabla \Phi \right)) = 0
\]

i.e.

\[
\rho \nabla \Phi = \varepsilon_0 \nabla \cdot \mathbf{J} = 0
\]

which relate the potential \( \Phi \) and the space charge \( \rho \) due to the drifting ions (mobility \( \mu \) is taken as constant). These equations are solved subject to the appropriate boundary conditions for potential and charge injection. If the space charge \( \rho_p \) due to the particulate is to be included, then equation (1) becomes

\[
\nabla^2 \Phi = -\frac{\rho - \rho_p}{\varepsilon_0}
\]

The effects charged particulate on overall conductivity in equation (2) can be ignored because the current carried by the particulate is negligible in practical situations due to its low mobility. Hence the form of equation (2) remains unchanged.

A three-dimensional model is required because of the complexity of solutions for real situations which have important features that cannot be captured in lower dimensions. Practical ESP discharge electrodes can have complex shapes, often involving spikes or prongs or helices. Experimental measurements of electric fields and current distributions in typical precipitator geometries show that they are truly three-dimensional in nature and that their shape can change appreciably with parameters such as applied voltage (Fothergill and Houlgreave (1)). In practice, current flow is often restricted to ion 'plumes' following flux tubes from a number of isolated regions of electrode surface. The approximations used to simulate the boundary conditions at the corona discharge mean that an averaged solution is found, the solution ignores statistical variations and does not produce the discontinuities due to individual corona tufts.

EMPIRICAL LAW FOR THE CORONA FIELD

Charge injection is determined by the field close to the surface of the discharge electrodes, thus it is determined by electrode potentials, global geometry and global space charge distribution. It has been shown experimentally and theoretically that a 'space charge limited charge injection' mechanism is involved which results in a field distribution (at coronaing regions on the surface of a electrode) that is virtually independent of time and applied voltage (Peek (2), Budd (3), Zaengl and Nyffenegger (4)), and for which empirical formulae exist (2), (4). To a good approximation, this near constant field is entirely dependent on the mean local curvature of the electrode (3) provided the thickness of the discharge is negligible compared to the characteristic length of the geometry. (Curvature is defined as the reciprocal of radius of curvature and is zero for a plane). Thus, to every point on the surface of an electrode there is an associated critical field dependent only on the local curvature - the electrode voltage at which the critical field is reached locally is dependent on global geometry and space charge distribution. The field at the electrode surface is
prevented from exceeding this critical value by the production of electrons by a field-driven avalanche process and the consequent formation of space charge.

We have found that Peek's results (2) on corona fields can be fitted with a new empirical law:

$$E_{cor} = A \left( 1 + \sqrt{B \cdot \kappa} \right)$$  \hspace{1cm} (4)

where $\kappa$ is the mean local curvature, $A$ is the breakdown strength of air ($3.0 \times 10^6$ V/m for air at STP), and $B$ is a characteristic mean radius of curvature (2.01 x $10^5$ mm - the radius at which the corona field is twice the breakdown strength of air). Figure 1 compares this new law with those produced by Peek (2) for different standard electrode arrangements.

![Figure 1](attachment:image)

**Figure 1** Comparison between new empirical law (solid curves) and Peek's empirical laws (2) for corona field magnitude for sphere gaps (top) and concentric (bottom dashed) and parallel (bottom dotted) cylinders.

The general empirical law expressed in equation (4) allows us to define a critical field at any point on the surface of an arbitrarily-shaped electrode (flat and concave regions of the surface are said to have zero curvature). The mean curvature is stored as part of the grid data at each electrode node. It is taken as the average of the curvature in two perpendicular directions along the surface at the node.

**IONIC SPACE CHARGE DENSITY AT A CORONATING ELECTRODE**

We can rewrite equation (2) in the form:

$$E \cdot \nabla \rho + \rho (\rho - \rho_p) / \varepsilon_0 = 0.$$  

Therefore at a coronating surface where the field is fixed:

$$\frac{\partial \rho}{\partial t} = - \frac{\rho (\rho - \rho_p)}{\varepsilon_0 E_{cor}}$$

where distance $l$ is measured in the direction of the surface normal. Measurements show that $\rho_p$ is small compared with $\rho$ at a discharge electrode surface, so the equation becomes:

$$\frac{\partial \rho}{\partial t} = - \frac{\rho^2}{\varepsilon_0 E_{cor}}$$ \hspace{1cm} (5)

This can be integrated across the corona discharge close to the electrode to give:

$$\frac{1}{\rho_+} - \frac{1}{\rho_-} = \frac{\delta}{\varepsilon_0 E_{cor}}$$ \hspace{1cm} (6)

where $\delta$ is the thickness of the corona discharge, $\rho_-$ is the space charge density at the outer surface of the discharge and $\rho_+$ is its value at the electrode surface.

Within the discharge region there are two types of charge carrier: electrons with mobility $\mu_-$ and positive ions with mobility $\mu_+$. $\rho_-$ is entirely due to positive ions and $\rho_-$ is almost entirely due to electrons (since this is before electron capture by electronegative gas molecules takes place). The field within the discharge is approximately constant, hence by current continuity:

$$\rho_+ = \frac{\mu_- \rho_-}{\mu_+}$$

Therefore, since the mobility of the electrons is much higher than that of the ions, we can approximate equation (6) by:

$$\rho_+ = \frac{\varepsilon_0 E_{cor}}{\delta}$$ \hspace{1cm} (7)

Using equation (4) and the approximate proportionality $\delta \propto \kappa^{0.5}$ (3) we can produce an approximate proportionality between charge density at the injection surface and electrode curvature:

$$\rho_+ \propto \sqrt{\kappa} / B$$  \hspace{1cm} (8)

This proportionality which is linked to the physics of the injection mechanism (3) is used together with $E_{cor}$ in the FE solution method to vary injection realistically over an electrode surface.

**FINITE ELEMENT MODEL**

The key points behind the finite element method are:

• the solution region is divided into a number of elements of varying sizes (each containing a number of nodes);
• unknown functions are approximated by simple functions (dependent on node parameters) over each element;
• finding a function that solves a differential equation is equivalent to finding a function that solves a
minimisation problem (equating some appropriately chosen definite integral over the solution region to zero);

- the approximating functions are substituted into the definite integral which can then be equated to zero by varying the node parameters;

- a linear problem can be converted to a set of linear equations, expressed in matrix form, that can be solved by standard methods.

The three-dimensional problem is discretised using Hermite cubic approximations to potentials and linear approximations to space charge distributions over tetrahedral elements. In Hermite approximation fields as well as potentials are used as parameters and are matched at element nodes. The use of these higher order elements for potential allows electric field to be approximated more accurately, and the fixed field charge injection law, appropriate to corona discharge, to be implemented more readily.

The ion drift problem is solved by a direct iteration procedure with the following algorithm which is essentially the one previously reported for the one and three dimensional prototype models (Bromley et al. (5) and Houlgreave et al. (6)).

1. Input grid data, electrode potentials, radii of surface curvature at electrode nodes and dust space charge distribution.
2. Find the variational FEM solution to Poisson’s equation for potential using dust space charge only with the following fixed: electrode potentials and dust space charge distribution.
3. Identify the coronating regions of electrode surface by finding nodes for which the Poisson solution field exceeds the surface curvature-dependent critical field. Set ionic space charge distribution to an arbitrary uniform and non-zero value except at discharge electrode surface nodes. Set ionic space charge to zero at non-coronating discharge electrode nodes and in accordance with the proportionality in equation (8) for coronating nodes (mean value over coronating nodes equal to mean value in the bulk).
4. Find the variational FEM solution to Poisson’s equation for potential and ionic space charge scaling factor with the following fixed: electrode potentials, field at coronating regions of electrode surfaces, dust space charge distribution and shape of ionic space charge distribution.
5. Set potential and ionic space charge scaling factor to the Poisson solution values and change ionic space charge at coronating surfaces in accordance with the scaling factor.
6. Find the Galerkin FEM solution to current continuity equation for ionic space charge discharge electrode surfaces and potential.
7. Set the ionic space charge to the current-continuity solution.
8. If solution has not converged then go to 2, else output ion drift solution.

Note that only the field and the shape of the space charge distribution need to be fixed at the coronating regions of the electrodes, as the solution algorithm homes in on the space charge level at the injecting boundary. The initial estimate of the bulk space charge distribution is chosen to be uniform since for a general geometry there will be no prior knowledge from measurements or analytical solutions. In the solution to Poisson’s equation, ionic space charge density is assumed to have the form \( k \rho (x) \) where \( k \) is the scaling factor and \( \rho (x) \) is the previous estimate for the ionic space charge density. If only \( k \) is varied then the shape of the space charge distribution remains fixed.

The variational approach is used in solving Poisson’s equation. The appropriate functionals are (Jones (7))

\[
F_0(\phi) = \int \left[ \frac{1}{2} \nabla \phi \cdot \nabla \phi + \rho \phi \right] dV
\]

\[
F_p(\rho) = \int \left[ \frac{1}{2} \nabla \rho \cdot \nabla \rho + \rho \phi \right] dV
\]

for solution of Poisson’s equation with variation of potential \( \phi \) and space charge \( \rho \) respectively. These functionals must be minimised by equating their partial derivatives with respect to appropriate parameters to zero. \( F_p(\rho) \) is required for finding the ionic space charge scaling factor.

The current continuity equation is solved using the Galerkin weighted residual method. Writing the linear approximation to space charge in the form:

\[
\rho^e(x,y,z) = \sum_i b_i^e \phi_i^e (x,y,z) P_i^e
\]

where \( P_i^e \) is the space charge at vertex \( i \) defines the linear coefficients \( b_i^e \) for an element \( e \). These coefficients are used in the Galerkin method. The appropriate equations are

\[
\int \left( \rho \nabla \phi + \rho \nabla \phi \right) b_i^e dV = 0
\]

which are equivalent to equating partial derivatives of functionals to zero over an element in the variational method.

The boundary conditions at the discharge electrode are determined as follows. Initially Poisson’s equation is solved for the fixed space charge due to the dust - this is to take account of global effects such as Faraday shielding. The field at electrode surfaces is constrained to be in the direction of the surface normal (given as part of the grid data). The field at each node on the discharge electrode is compared with the value obtained.
from equation (4). If the Poisson solution field exceeds this critical value then the field is fixed to the appropriate magnitude constrained to the direction of the normal and the region of the node is said to be coronating. Non-coronating electrode nodes do not have their fields fixed but the ionic space charge density is set to zero to enforce zero charge injection.

The electrode surface boundary condition of being an equipotential surface is imposed during the initial Poisson FEM solution by forcing surface potential parameters to minimise the variational functional

$$F_I(\phi) = \int_{S} \left( \phi^2 - 2\phi V_e \right) dS$$

(13)

over the electrode surface, where $V_e$ is the applied electrode potential. (This functional is also equivalent to using the least squares weighted residual method). Field singularities at electrode surface nodes are avoided because the model "sees" a piecewise Hermite cubic equipotential surface as the electrode surface.

The problem is typically solved over a region bounded by a high-voltage discharge electrode, a planar earthed duct wall and several symmetry planes. This solution region is divided into a grid of tetrahedral elements each having 4 corner nodes and 4 mid-face nodes.

RESULTS

Initial tests of the method in a one-dimensional model of a cylindrically symmetric system, and later tests with a three-dimensional model of a plane-plane system with forced charge injection have been previously reported (5), (6). These models were solved with very low errors compared to the known analytical solutions of these geometries. The three-dimensional prototype software has since had curvature effects included using the approximations reported in this paper (equations (4) and (8)), so that general curved electrodes can now be modelled. Initial tests with cylindrical and wire-plate geometries have given promising results, and the effects of grid refinement are currently being investigated.

Examples of output from the prototype software models will be shown at the conference.

CONCLUSIONS

A method has been devised and implemented in prototype form for the prediction of the electrical effects of arbitrary 3D electrode geometries subject to corona discharge under constant dc conditions. The method uses the injected charge-free Poisson solution and expressions based on local curvature to realistically constrain charge injection at coronating points arbitrary discharge electrode geometries. The iterative solution method accurately homes in on the injection current due to a given fixed-field injection law - by the use of a scaling factor in the solution of Poisson's equation and by using the known shape of the space charge distribution on the electrode surface. The method has been implemented in 1D and 3D finite element prototype software which solve the ion drift problem in air using Hermite cubic approximation. The 3D prototype is possibly the first implementation of Hermite finite elements in a complex model.

During the course of the work a generalisation of empirical fixed field charge injection laws has been devised for arbitrarily curved surface regions. This law gives a good fit to data from standard electrode arrangements. We believed that this work is also the first to identify the approximate expression for the curvature dependence of space charge density at a coronating surface.

ACKNOWLEDGEMENTS

We gratefully acknowledge support from EPSRC (project GR/J10044), DTI (ETSU) and National Power plc.

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