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THETATRON, A TWO-DIMENSIONAL
MAGNETOHYDRODYNAMIC COMPUTER PROGRAMME,
PART I. GENERAL DISCUSSION

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THETATRON, A TWO-DIMENSIONAL MAGNETOHYDRODYNAMIC
COMPUTER PROGRAMME, PART 1. GENERAL DISCUSSION

by

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A B S T R A C T

The physical model used in the Thetatron programme is described. The basic differential equations and boundary conditions are defined and some discussion of numerical methods is given.

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1. INTRODUCTION

These series of reports discusses a two-dimensional magnetohydrodynamic programme called THETATRON, which is intended to follow the behaviour of a θ -pinch plasma in the (r,z) plane. The programme, which is written in Fortran II for the IBM 704, 709 or 7090, and in Sl-Fortran* for Stretch (IBM 7030), is a joint project of the Culham Laboratory and of the Institut für Plasmaphysik, Garching.

It is evident that in any real C.T.R. device, at least two dimensions are required to describe the behaviour of the plasma. This follows from the use of a (vector) magnetic field satisfying $\text{div } \underline{B} = 0$, combined with the finite size of the apparatus. For example in the linear z -pinch or θ -pinch, variables may depend on (r,z) only; in a toroidal device on (r,θ) and so on. Some success has been obtained with approximate one-dimensional calculations on plasma magnetohydrodynamics⁽¹⁾, in which functions are only allowed to depend on the radial co-ordinate r , their variation with the other co-ordinate being regarded as small and therefore neglected. But many phenomena are known which are strictly two-dimensional; for example end-loss, axial contraction or formation of closed field loops in the θ -pinch, and the operation of conical plasma guns. Again, in a toroidal device it may well be a poor approximation to neglect variation with the azimuthal co-ordinate θ , since even with (say) a 6:1 aspect ratio the magnetic pressure varies by a factor 2 across a diameter. Therefore it seems worthwhile to attempt to extend the numerical calculations to two-dimensional magnetohydrodynamics. This is especially so because the physical phenomena which occur in two dimensions are not so easy to understand intuitively or to calculate analytically as those in one dimension, and at the same time they are difficult to observe in the laboratory, so that useful information might be gained from 'numerical experiments' on a computer. (It may also be remarked that many plasma devices, and virtually all instabilities, involve all three space dimensions, and if these are ever to be tackled numerically it is obviously desirable to gain experience with two-dimensional problems first.

* Sl is a dialect of Fortran written for Stretch by A.E. Glennie and his co-workers at A.W.R.E., Aldermaston, in conjunction with IBM (United Kingdom).

Also phenomena governed by Vlasov's or Boltzmann's equation may involve from two to six dimensions in phase space.)

To make the first two-dimensional programme as simple as possible the linear θ -pinch was chosen, since this needs for its description only two field components (B_r, B_z) and two velocity components (v_r, v_z). In addition there is only a single current component j_θ , which is always transverse to \underline{B} so that only the transverse electrical resistivity is required*. The conical θ -pinch gun can be treated as a special case. (The cusp has the same field, velocity and current components, but would require the present programme to be re-written).

In formulating the calculation several physical and numerical problems arise, many of which are likely to appear in any two-dimensional magneto-hydrodynamic calculation. These problems and the limitations and possible extensions of the programme are discussed in this part of the report, which deals with the basic differential equations, boundary conditions and numerical methods which are employed. Subsequent parts will describe the difference equations and their programming in more detail and will discuss some results.

2. DIFFERENTIAL EQUATIONS

This section describes the basic differential equations which apply throughout the plasma. It is assumed that the region of interest is azimuthally symmetric about the z -axis, (cylindrical polar co-ordinates being denoted by (r, θ, z)), but its precise shape depends on the boundary conditions, which are discussed in section 3.

The plasma is supposed to be fully ionised. This is to some extent a practical limitation, since θ -pinches are sometimes operated with incomplete ionisation at the start of the main implosion, and also the ionisation is likely to remain incomplete in the two regions beyond the ends of the coil. But ionisation phenomena are very complicated and it would be unwise to

* Compare for example the toroidal pinch, with co-ordinates (r, θ, ϕ) . Although functions may depend only on (r, θ) , each vector $\underline{B}, \underline{v}, \underline{j}$ has all three components, and both parallel and perpendicular resistivities are needed.

include them here until they have first been studied with the one-dimensional partially-ionised programme which has been written at Culham.

We suppose that the plasma can be described by four variables, density ρ , total particle pressure p or temperature T , and velocity $\underline{v} = (v_r, v_z)$ and the magnetic field by two variables $\underline{B} = (B_r, B_z)$, i.e. six in all. All functions are to be independent of θ , and B_θ, v_θ are taken to be zero. Magnetic field lines and particle stream lines are thus confined to (r, z) planes.

To simplify the THETATRON programme as much as possible, ion and electron temperatures are taken to be equal, and no distinction is made between temperatures parallel and perpendicular to the magnetic field. The specific heat ratio is $\frac{5}{3}$ for both species. Heat conduction and energy loss by radiation and ionisation are ignored, (although an empirical formula for energy loss could be included if required).

In some θ -pinch situations it would indeed be desirable to distinguish between T_e and T_i , since they can be widely different, and to allow for energy exchange between them. This is not difficult and is done in the one-dimensional programme. In the two-dimensional case heat conduction by electrons along the magnetic field should probably be allowed for.

It is questionable whether one ought also to distinguish between parallel and perpendicular components of the ion temperature, $T_{\parallel, i}$ and $T_{\perp, i}$. All the radial shock and adiabatic heating goes into T_{\perp} , while motion along the lines of force depends on T_{\parallel} . Exchange of energy between these degrees of freedom by collisions is often quite slow so that one might expect T_{\perp} to be much larger than T_{\parallel} , but rapid relaxation may occur by some instability mechanism. The introduction of two ion temperatures would make the two-dimensional programme rather more elaborate, but it can easily be incorporated into the one-dimensional programme and this has recently been done by Fisher. Comparison with experiment may eventually show whether any rapid interchange of energy must be postulated, or whether the two temperatures are in fact quite different.

The basic differential equations used in THETATRON are therefore:

$$\frac{\partial \rho}{\partial t} + (\underline{v} \cdot \nabla) \rho = - \rho \nabla \cdot \underline{v} , \quad (2.1)$$

$$\rho \left\{ \frac{\partial \underline{v}}{\partial t} + (\underline{v} \cdot \nabla) \underline{v} \right\} = - \nabla p + \underline{j} \times \underline{B}, \quad (2.2)$$

$$\frac{\partial p}{\partial t} + (\underline{v} \cdot \nabla) p = - \gamma \nabla \cdot \underline{v} + (\gamma - 1) \mu \underline{j}^2, \quad (2.3)$$

$$\frac{\partial \underline{B}}{\partial t} = - \nabla \times \underline{E}, \quad \text{with} \quad \underline{E} + \underline{v} \times \underline{B} = \mu \underline{j}, \quad (2.4)$$

$$\nabla \cdot \underline{B} = 0, \quad (2.5)$$

where

$$\underline{j} = \nabla \times \underline{B}. \quad (2.6)$$

We note that

$$\underline{j} = (0, j_\theta, 0), \quad \text{where} \quad j_\theta = \frac{\partial B_r}{\partial z} - \frac{\partial B_z}{\partial r}. \quad (2.7)$$

In (2.2) and (2.3) certain artificial viscous terms, representing compressional and shear viscosity, have been omitted. These allow for shock heating and ensure numerical stability, and will be discussed in part II. Equations (2.1) - (2.6) are expressed in c.g.s. electromagnetic units, except for the current \underline{j} , (where a factor 4π has been omitted in equation (2.6)), and correspondingly the resistivity μ . Since only $j_\theta \neq 0$, all currents are transverse to \underline{B} , and it is appropriate to use Spitzer's formula for the transverse resistive diffusion coefficient

$$\mu = \frac{\eta_\perp}{4\pi} = \frac{1.29}{4\pi} \frac{\log \Lambda}{T^{\frac{1}{2}}} \times 10^{13} \text{ e.m.u.} \quad (2.8)$$

$\log \Lambda$ is taken to be 10, and T is in $^\circ K$ (2).

In equations (2.1) - (2.3) we use

$$\nabla \cdot \underline{v} = \frac{1}{r} \frac{\partial}{\partial r} (r v_r) + \frac{\partial v_z}{\partial z} \quad (2.9)$$

$$\underline{v} \cdot \nabla = v_r \frac{\partial}{\partial r} + v_z \frac{\partial}{\partial z}, \quad (2.10)$$

since there is no θ -dependence, and note that

$$\underline{j} \times \underline{B} = (j_\theta B_z, 0, -j_\theta B_r). \quad (2.11)$$

This gives the equations to be solved for ρ , \underline{v} and p . The magnetic field equations are obtained by eliminating \underline{E} from (2.4) and (2.6), and using (2.5), which gives

$$\frac{\partial \underline{B}}{\partial t} + (\underline{v} \cdot \nabla) \underline{B} = - \underline{B} (\nabla \cdot \underline{v}) + (\underline{B} \cdot \nabla) \underline{v} - \nabla \times (\mu \underline{j}) \quad (2.12)$$

or in components

$$\frac{\partial B_r}{\partial t} + v_r \frac{\partial B_z}{\partial r} + v_z \frac{\partial B_r}{\partial z} = - B_r \nabla \cdot \underline{v} - B_r \frac{\partial v_r}{\partial r} + B_z \frac{\partial v_r}{\partial z} + \frac{\partial}{\partial z} (\mu j_\theta) \quad (2.13)$$

$$\frac{\partial B_z}{\partial t} + v_r \frac{\partial B_z}{\partial r} + v_z \frac{\partial B_z}{\partial z} = - B_z \left(\frac{1}{r} \frac{\partial}{\partial r} (r v_r) \right) + B_r \frac{\partial v_z}{\partial r} - \frac{1}{r} \frac{\partial}{\partial r} (\mu r j_\theta) \quad (2.14)$$

Equation (2.12) implies

$$\frac{\partial}{\partial t} (\nabla \cdot \underline{B}) = 0 \quad (2.15)$$

if

$$\nabla \cdot \underline{B} = 0 \quad (2.16)$$

Therefore if (2.16) is satisfied initially it remains satisfied for all time. However it is not obvious that this will still be true when (2.12) is solved only approximately, by some difference scheme. This question is discussed in Part II.

3. BOUNDARY CONDITIONS ON THE MAGNETIC FIELD

In a real θ -pinch, the physics is complicated by the fact that magnetic lines of force run from the hot plasma inside the coil, along the tube into colder gas, and also through the insulating wall into the surrounding space. The plasma is therefore coupled, though perhaps only rather weakly, with cold partially-ionised gas beyond the ends of the coil, with the walls, and with a 'vacuum' magnetic field extending (in general) to infinity. This situation is difficult to make physically precise, and correspondingly awkward to treat mathematically.

The boundary conditions to be used for THETATRON therefore need rather careful discussion, and we shall find it convenient to use a physical model which is somewhat different from θ -pinches so far used in practice.

GENERAL PROBLEM

The general class of problem, of which THETATRON solves a special case, concerns the behaviour of a plasma in an apparatus which has azimuthal symmetry (so that it is consistent to assume that all functions are independent of θ), and in which moreover v_θ, B_θ are zero. This class includes for example

- (a) Linear θ -pinches, (with and without mirrors),
- (b) Conical θ -pinch plasma guns,
- (c) Cusps
- (d) Multistage compressional mirror machines.

As a matter of fact there is no reason why this type of calculation should not be extended further to include an azimuthal field B_θ , (linear pinch with electrodes, cusp with central rod), or even an azimuthal velocity v_θ , (rotating plasma), provided that all functions remain independent of the co-ordinate θ itself. But such extensions will not be considered in this report.

IDEAL APPARATUS

We first suppose that an ideal apparatus of this type contains plasma confined within an insulating tube I, whose inner wall is a surface of revolution about the z-axis $r=0$, defined by the function $r=r_w(z)$. (This function must be continuous but need not be single-valued, i.e. the tube wall might bend back on itself.) Outside this tube are placed one or more solid conductors C_i as indicated in Fig.1, each conductor being a solid of revolution. With each C_i there is associated an azimuthal e.m.f. $V_i(t)$ which may be an arbitrary function of time. The conductors are treated as perfect.

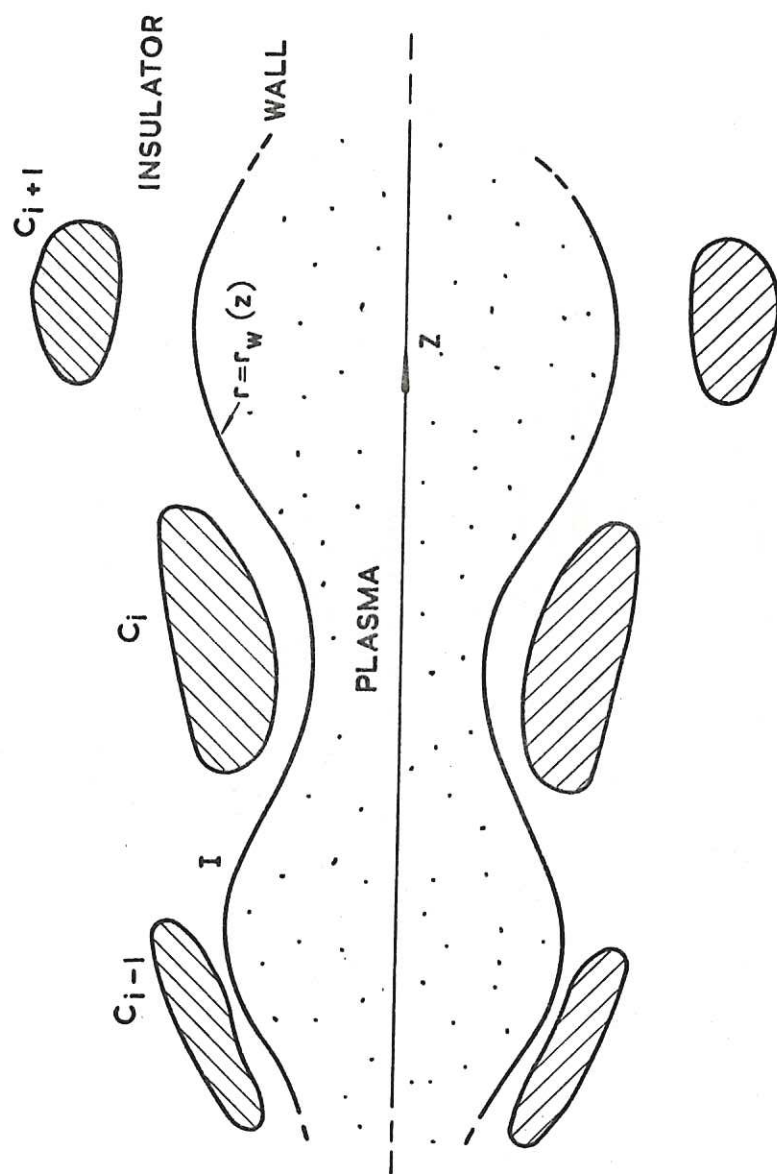
In practice, it is only possible to apply an azimuthal e.m.f. to one of these conductors by cutting a longitudinal slit in it, and connecting this slit via leads to a condenser bank for example. However, it is possible, by means of suitable conducting shields, to make the asymmetric effect of these leads on the magnetic field negligible in the physically-interesting region within the tube I, (although precautions of this type are not normally taken in present experiments), and so we may assume that our ideal azimuthally symmetric apparatus is logically consistent. Then each conductor C_i is equivalent to a single-turn coil which encircles a flux Φ_i , varying with time according to

$$\frac{d\Phi_i}{dt} = -V_i \quad (3.1)$$

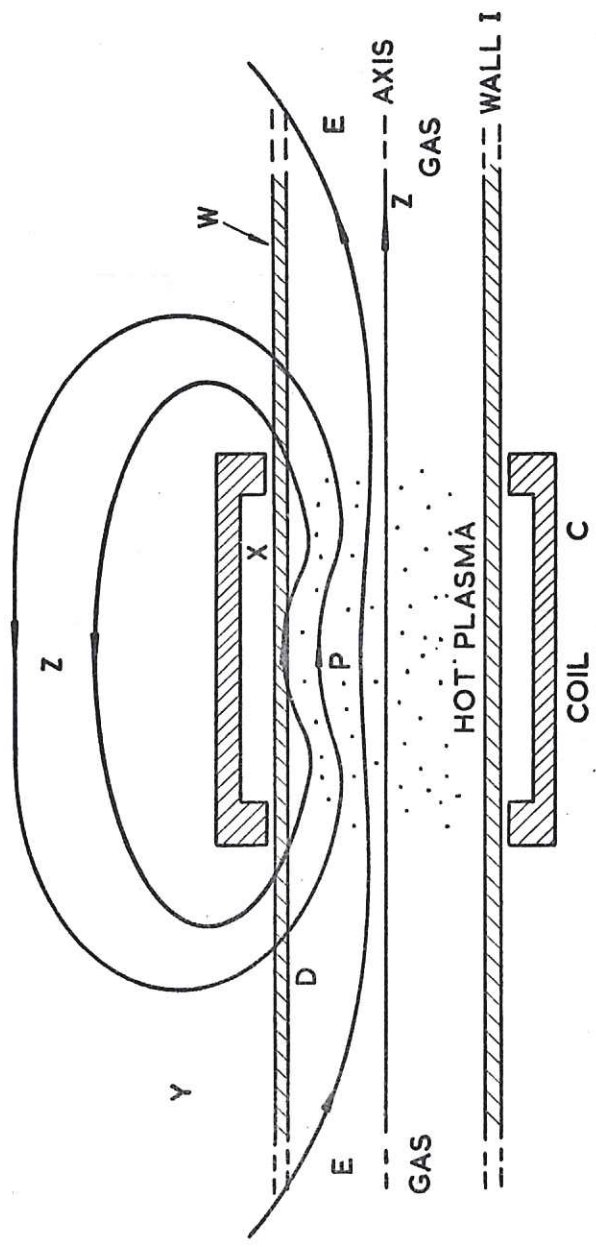
Since \underline{B} is tangential to the wall of each conductor, the flux Φ_i through each cross-section of a conductor C_i must be the same, (although different in general from any other flux C_j).

COMPUTATIONAL DIFFICULTIES

Two difficulties now arise in a numerical calculation, the first being physical and the second mathematical:



CLM-R-29 Fig. 1. Ideal azimuthally-symmetric apparatus.



CLM-R 29 Fig. 2 Practical θ -pinch.

- (i) The interaction between plasma and wall, and also with any neutral gas which may be present in the tube, e.g. at the two ends, is not known.
- (ii) In order to determine the magnetic field, it is necessary to solve field equations everywhere outside the conductors C_i , and not only within the plasma, (i.e. within the tube I).

for example

- W. Within the walls of the insulating tube I.
- X. Between tube and coil, (if the coil radius varies, as when mirrors are used at the ends).
- Y. Beyond the ends of the coil.
- Z. At the back of the coil.

The field lines evidently behave like elastic strings which can transmit forces from regions W - Z into P, and therefore a full numerical calculation requires the solution of the 'vacuum' equations

$$\text{div } \underline{B} = 0, \quad \text{Curl } \underline{B} = 0 \quad (3.2)$$

throughout W - Z, in addition to the magnetohydrodynamic equations in P.

This combined insulating region W - Z is of infinite extent and complicated geometry, which makes it awkward and inefficient to introduce an external space mesh for solving equations (3.2). In addition to this the equations are elliptic, which means that physical influences can propagate from point to point with unlimited speed*, so that some implicit method of solution is needed. But implicit methods are time-consuming and difficult to programme in two dimensions, and it seems unreasonable to have to use them for the physically-unimportant insulating regions, whilst one can at the same time use a much simpler explicit method for the plasma itself, (because of the finite Alfvén and magnetosonic speeds - see section 5).

It is probable that this purely mathematical difficulty could largely be avoided by solving (3.2) with the aid of Green's functions for the insulating region⁽³⁾, instead of using a space mesh. But there still remains the physical problem of the end regions E, which are also traversed by field lines emerging from the plasma, and which presumably contain gas which is only partially ionised, the degree of ionisation depending on the distance from

* Because the displacement current has been dropped from the second equation (3.2). But the velocity of light is virtually infinite for our purposes.

the main plasma P. An accurate numerical solution in these regions E would seem to require a partially ionised programme, but again it seems unreasonable to use this degree of complication in the unimportant regions beyond the ends of the tube, if the main body of the plasma P can be treated with the much simpler full-ionised equations.

Finally, it is evident that some of the plasma which escapes from region P along the magnetic field lines will hit the wall I beyond the ends of the coil at a point such as D (Fig.2), and it is not clear what boundary conditions apply here.

In all three cases, the difficulty is that the physically-interesting region P is coupled, though rather weakly, with other regions such as W - Z, E or the wall at D where it is either technically awkward to solve the equations numerically, or even hard to see physically what is happening at all. To avoid this problem we have set up a model of the θ -pinch in which the boundary conditions are much simpler, but the behaviour of the plasma in P should remain essentially the same.

MODEL USED IN THETATRON

To avoid any insulating region, the θ -pinch conductor is assumed to be periodic and of infinite length, as shown in Fig.3. $O_1A_1A_2O_2$ corresponds to the region inside the coil of the real apparatus. (This might for example have a mirror at either end, as indicated.) The conductor is assumed to be symmetric about the midplane OA, and so only the half-region P need be calculated. Q represents a region of weaker field beyond the end of the coil, which is also included in the calculation.

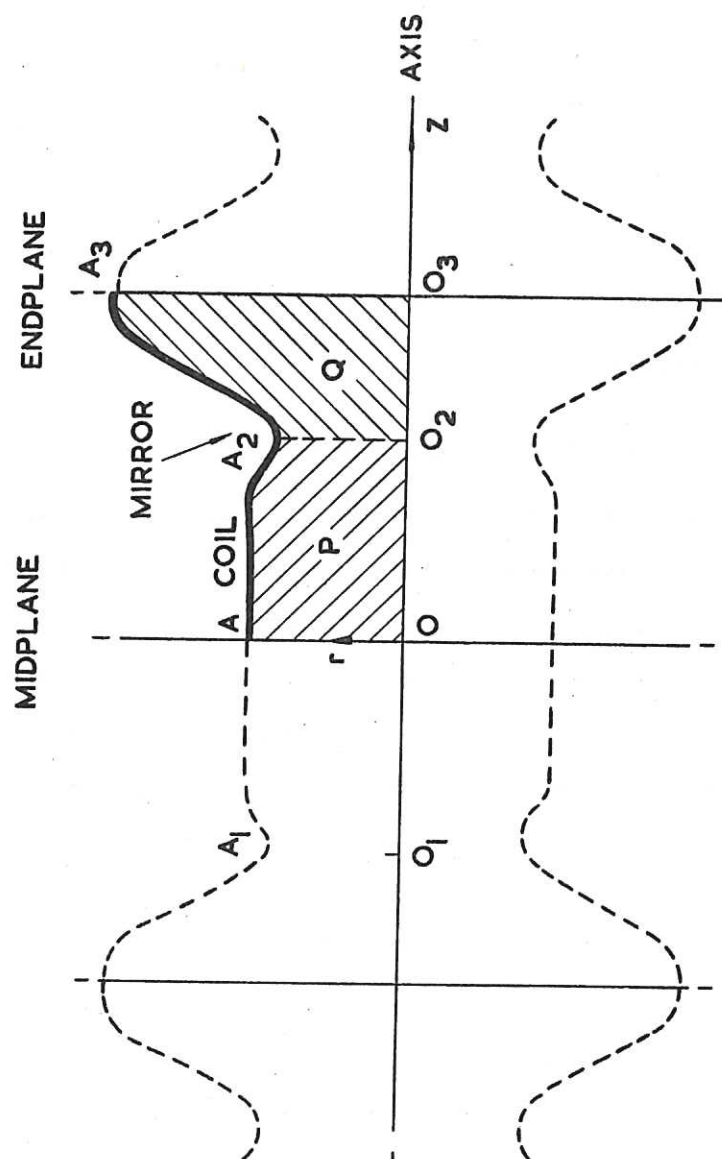
This arrangement excludes Y and Z of Fig.2. To remove X we assume that the insulating wall I is shaped to fit the conductor, and W is avoided by supposing that I is only infinitesimally thick.

If $r_c(z)$ is the conductor radius, symmetry requires

$$\frac{dr_c}{dz} = 0$$

At A and A_3 . Boundary conditions on the magnetic field are

$$\begin{aligned} B_z &= 0 && \text{on conductor } AA_3 \\ B_r &= 0 && \text{on axis } OO_3, \\ B_r = B_\theta &= 0 && \text{on midplane } OA, \\ B_r = B_\theta &= 0 && \text{on endplane } O_3A_3. \end{aligned}$$



CLM-R 29 Fig. 3 Region of calculation used in θ - pinch programme.

Since $\text{div } \underline{B} = 0$ the total flux Φ is independent of z , and it satisfies

$$\frac{d\Phi}{dt} = -V \quad (3.3)$$

where V is the voltage applied to the coil from some external circuit.

The magnetic field will on average have a magnitude

$$B_z(z) \sim (r_c(z))^{-2},$$

and since the magnetic pressure varies as B_z^2 , and forces perhaps as B_z^2/r_c , the dynamical effect of the magnetic field in region Q on the plasma in P should be comparatively small, if the radius of the conductor is made sufficiently large at the endplane O_3A_3 . Therefore the misrepresentation of this field need not matter too much.

The endplane corresponds to the rather indefinite boundary between plasma and neutral gas in the real θ -pinch. Boundary conditions on ρ and p will be discussed in section 4.

4. BOUNDARY CONDITIONS ON DENSITY AND TEMPERATURE

It is assumed that the region $P + Q$ of Fig.3 initially contains plasma which is fully ionised, and has some density and pressure distribution

$$\rho_0(r, z), p_0(r, z) = \rho_0(r, z)T_0(r, z)$$

which may or may not be uniform. We normally assume also that the initial magnetic field has a z -component which is independent of r , and proportional to $(r_c(z))^{-2}$, although this field is not exactly in equilibrium. (B_r is determined from B_z by the condition $\text{div } \underline{B} = 0$).

When the magnetic field at the conducting wall rises, due to the discharge of a current through the coil, the plasma is pushed inwards by the excess magnetic pressure, and the density in the outer region near the wall will then become almost zero unless some new plasma is created. Since it is observed in practice that the region outside the discharge is usually a good electrical conductor⁽⁴⁾, we shall suppose that new plasma is continually created very close to the wall in such a way that the wall density is maintained approximately at or above some minimum value ρ_{\min} . This newly-created plasma continually moves inwards as the implosion proceeds, forming the region outside the main pinch. For inward motion we assume in fact that

$$(\rho_W(t + \Delta t) - \rho_{\min}) = e^{-|v_\perp|\Delta t/\lambda} (\rho_W(t) - \rho_{\min}) \quad (4.1)$$

where λ is a suitable characteristic length which determines the scale of the plasma boundary, v is the normal velocity at the wall, Δt is the time-step and ρ_W is the wall density. This technique, which is based on an idea of Colgate, Ferguson and Furth⁽⁵⁾, has previously been used in the one-dimensional programme⁽¹⁾. It has the advantage that the Alfvén and magnetosonic speeds never become too high, (which would have the effect of increasing the maximum permissible timestep - see section 5).

For outward motion, the coil wall is allowed to absorb the plasma, and we set

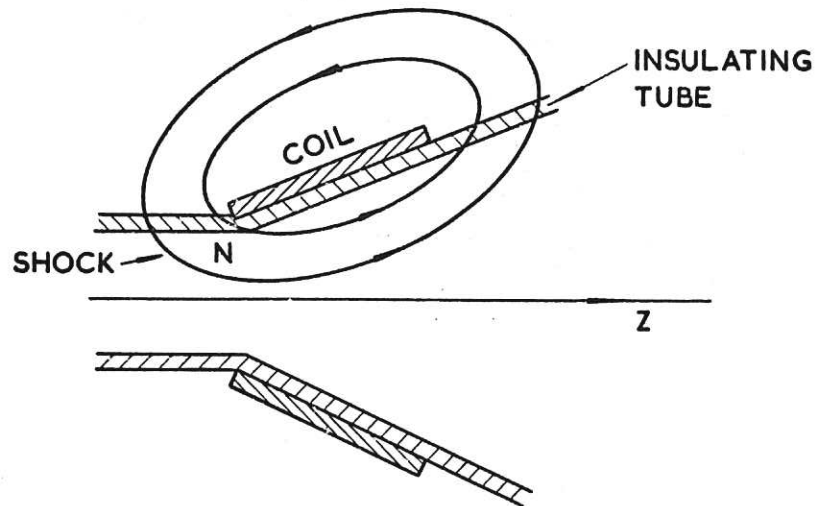
$$\frac{\partial \rho_W}{\partial t} = - \underline{v} \cdot \underline{\nabla} \rho - \rho_W (\underline{\nabla} \cdot \underline{v}), \quad (4.2)$$

where $(\underline{\nabla} \cdot \underline{v})$ is assigned the value belonging to the point one mesh interval inside the plasma, and $\underline{\nabla} \rho$ is evaluated by using a one-sided difference formula.

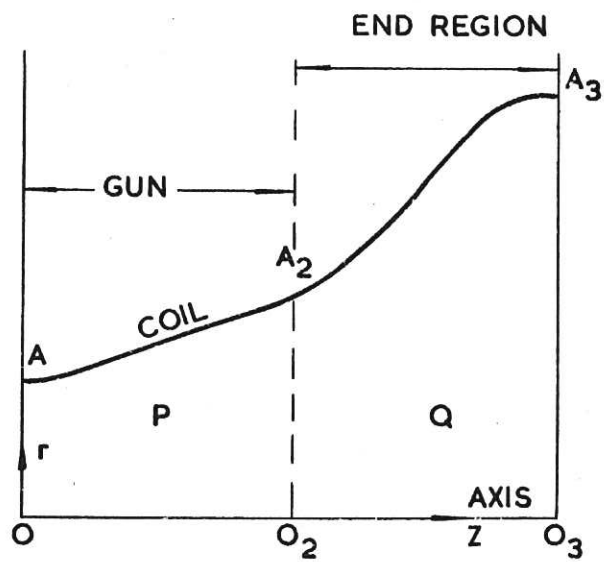
Various boundary conditions have been tried for the temperature, but it has been found most successful in the two-dimensional programme simply to fix the wall temperature T_W at its initial value, e.g. $T_0 = 2\text{eV}$.

The same boundary conditions on ρ and T are used for the endplane O_3A_3 of Fig.3; i.e. the escape of plasma is treated as absorption by a fictitious wall. Since the temperature on this plane is maintained at T_0 the plasma pressure will be very small, and therefore the plasma will escape freely almost as if into a vacuum. This is not quite correct because in a real θ -pinch the gas would pile up and resist the outward motion by its inertia; however if O_3A_3 is some distance from O_2A_2 the error is not likely to be serious. The boundary conditions at OA are determined by the symmetry, in the case of a standard θ -pinch.

In the conical θ -pinch both ends are treated alike, i.e. plasma is allowed to escape. It is clear that in a real device of this kind conditions at the narrow end must be very complicated. Fig.4 illustrates how the magnetic field lines will be most compressed near the narrow end of the coil N , while just behind they bend back rapidly so that the field is greatly reduced, and the shock is directed mainly in the negative Z -direction. (We assume that the insulating tube is open; if it is closed at N conditions will be even more obscure.) N is initially the region of maximum plasma



CLM-R 29 Fig. 4 Conical θ -pinch gun.



CLM-R 29 Fig. 5 Region of calculation used in conical gun programme.

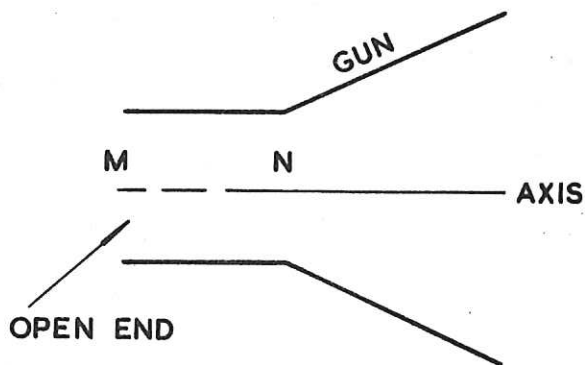
pressure, but the plasma will rapidly shoot out backwards, since there is little to prevent this, and either move into weakly ionised gas or hit the wall.

In using the THETATRON programme to describe a conical θ -pinch we again make OA a symmetry plane, as shown in Fig.5, so that

$$\frac{dr_c(z)}{dz} = 0, \quad B_r = 0.$$

This is not unreasonable since in the real device there must be a point near N where $B_r = 0$. However the plasma pressure will now be always small on the plane OA, which unlike O_3A_3 is not very far from the physically interesting region P. Plasma will therefore shoot backwards at this end as it should, but one cannot hope to calculate the details correctly.

It would be easier to understand the operation of a conical θ -pinch if it were constructed as in Fig.6, with a short cylindrical section MN separating the actual gun region from the open end. Then the boundary conditions at M would not be so important.



CLM-R 29 Fig. 6 Gun with cylindrical stub.

5. NUMERICAL METHODS

EXPLICIT CALCULATIONS

A time-dependent calculation may be made explicitly or implicitly. Suppose that we are given functions $f_{i,j}$ on a space mesh at time t , and require to find new functions $f_{i,j}^*$ at $t + \Delta t$. In the explicit method, space derivatives occurring in the differential equations are expressed in terms of differences at t only, and df/dt as

$$\frac{df}{dt} \approx \frac{f_{i,j}^* - f_{i,j}}{\Delta t} \quad (5.1)$$

so that we get a relation

$$f_{i,j}^* = \sum_{k,l} A_{ijkl} f_{k,l}^* \quad (5.2)$$

which enables $f_{i,j}^*$ to be found at once. In the implicit method space derivatives are expressed in terms of differences at both t and $t + \Delta t$ in general, and we get a relation

$$\sum_{k,l} (A_{ijk} f_{k,l} + A_{ijkl}^* f_{k,l}^*) \quad (5.3)$$

which has to be solved for $f_{i,j}^*$.

The explicit method only allows a numerical influence to propagate a distance Δ (space mesh) in time Δt , and hence the calculation permits a maximum propagation speed $C_p = \Delta/\Delta t$. Physically it is clear that the solution cannot be correct if this C_p is less than the actual Alfvén speed,

$$C_a = (B^2/4\pi\rho)^{\frac{1}{2}},$$

or the magnetosonic speed

$$C_m = \left(\frac{B^2}{4\pi\rho} + \frac{\gamma p}{\rho} \right)^{\frac{1}{2}},$$

because the interaction of different regions of the plasma cannot then be treated adequately. Therefore we get restrictions on Δt of the kind

$$\Delta t \leq \Delta/C_a, \quad \Delta/C_m, \quad (5.4)$$

and the timestep will be reduced by strong magnetic fields such as are commonly used in the θ -pinch, or by low densities (e.g. outside the main discharge). Mathematically it is found that the solution goes unstable if (5.4) is not satisfied.

Other stability conditions on Δt can be given a physical interpretation in terms of the propagation of influences by diffusion (resistive,

viscous), and particle velocity.

The implicit method imposes no restriction on the speed at which influences can propagate, and correspondingly there is no stability condition on Δt . However it now becomes necessary to solve (5.3). In one dimension (5.3) leads to a simple 3-term recurrence relation which can readily be solved explicitly by a form of Gaussian elimination^(6,8). This technique has been used by Hain et al (loc. cit) to solve the equation of motion, field equations and heat conduction equations in the one-dimensional pinch collapse programme. In two dimensions (5.3) can no longer be solved explicitly, but it is possible to use an alternating direction method⁽⁹⁾ in which (say) the r-direction is first treated implicitly by the Gaussian elimination process just as in one dimension, while the z-direction is treated explicitly, and then the two treatments are interchanged. The Gaussian process strictly applies only to linear equations; in our problem the equations are non-linear and therefore the solution would have to be iterated.

Despite this possibility, we decided to use a fully explicit method for all equations because it greatly simplifies the difference formulae. Unless the alternating direction technique allows a much larger timestep, it is not necessarily worthwhile in practice because of the greater complexity and hence longer computation time for each step. There is a range of problems involving rapid flow velocities and short timescales for which the explicit THETATRON programme will be efficient, but eventually it will be necessary to use an implicit version.

LAGRANGIAN OR EULERIAN FORMULATION

If a fixed or Eulerian space mesh is used, there is a difficulty in the treatment of the convective term $\underline{v} \cdot \nabla f$ which appears in all equations. It is not possible to centre this term in the obvious way in an explicit calculation, i.e. to express $\frac{df}{dx}$ as

$$\frac{df}{dx} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} \quad (5.5)$$

because this formula is unstable⁽⁷⁾. Richtmyer quotes a one-sided method by Lelevier, which uses

$$\frac{df}{dx} \approx \frac{f_{i+1} - f_i}{\Delta x}, \quad (v < 0) \quad (5.6)$$

$$\frac{df}{dx} \approx \frac{f_i - f_{i-1}}{\Delta x}, \quad (v > 0)$$

This is stable, but evidently df/dx is being evaluated a distance $\pm \Delta x/2$ from the required position. Therefore an error term is introduced, so that an equation

$$\frac{df}{dt} = -v \frac{\partial f}{\partial x} \quad (5.7)$$

becomes

$$\frac{\partial f}{\partial t} = -v \frac{\partial f}{\partial x} + \frac{|v|\Delta x}{2} \frac{\partial^2 f}{\partial x^2} \quad (5.8)$$

Unfortunately this leads to a fictitious diffusion in each equation, which is often much larger than the true diffusion due to heat conduction or resistivity. The effect could be reduced by using a smaller Δx , but this is impracticable in two or three dimensions.

One method of avoiding fictitious diffusion is to use a Lagrangian mesh, which moves with the fluid, since the term $\underline{v} \cdot \nabla f$ then disappears from the equations. However this is quite awkward in two dimensions, especially for problems in which considerable distortion of the fluid takes place, and so we decided to retain the Eulerian mesh for simplicity.

It is in fact not difficult to avoid the error term in (5.8), while still using an explicit calculation. We do this by representing df/dx as

$$\frac{df}{dx} \approx \frac{f_{i+1} - f_{i-1}^*}{2\Delta x} + \frac{\Delta t}{2\Delta x} \frac{\partial f}{\partial t}, \quad (5.9)$$

where the star as before denotes the value at $t + \Delta t$. (5.9) can be evaluated because f_{i-1}^* is already known when f_i^* is being calculated, (and the same applies for any number of dimensions). This technique, which may be termed the angled-derivative method, is quite convenient because at each stage f_i^* can simply be written into the store location previously used for f_i .

The angled-derivative method is stable, and the amplification factor for each mode has modulus unity as it should, since (5.7) simply corresponds to a wave moving with velocity v with no change in amplitude or shape. But it is now found that in practice the third-order error terms are serious. In fact for each mode e^{ikx} , equation (5.7) is solved approximately in this

difference scheme as

$$\frac{\partial f}{\partial t} = -v \left(\frac{\sin \xi}{\xi} \right) \frac{\partial f}{\partial x} \quad (5.10)$$

where $\xi = k\Delta x$. For the shortest possible mode $\xi = \pi$ (or $\lambda = 2\Delta x$), the factor $(\sin \xi / \xi)$ is zero and the mode cannot propagate at all. Other modes have their velocities reduced.

Another failing of the second-order-accurate angled-derivative method is that there is now no guarantee that an everywhere-positive function remains positive, and ρ , T can in fact become negative unless precautions are taken. This is not particularly surprising, since equation (5.7) is linear and so the condition $\rho(x) = 0$ has no absolute significance. But the one-sided method does guarantee $\rho > 0$, since it corresponds to linear interpolation,

$$f_i^* = \left(1 - \frac{v\Delta t}{\Delta x}\right) f_i + \frac{v\Delta t}{\Delta x} f_{i-1}, \quad (v > 0, \frac{v\Delta t}{\Delta x} < 1)$$

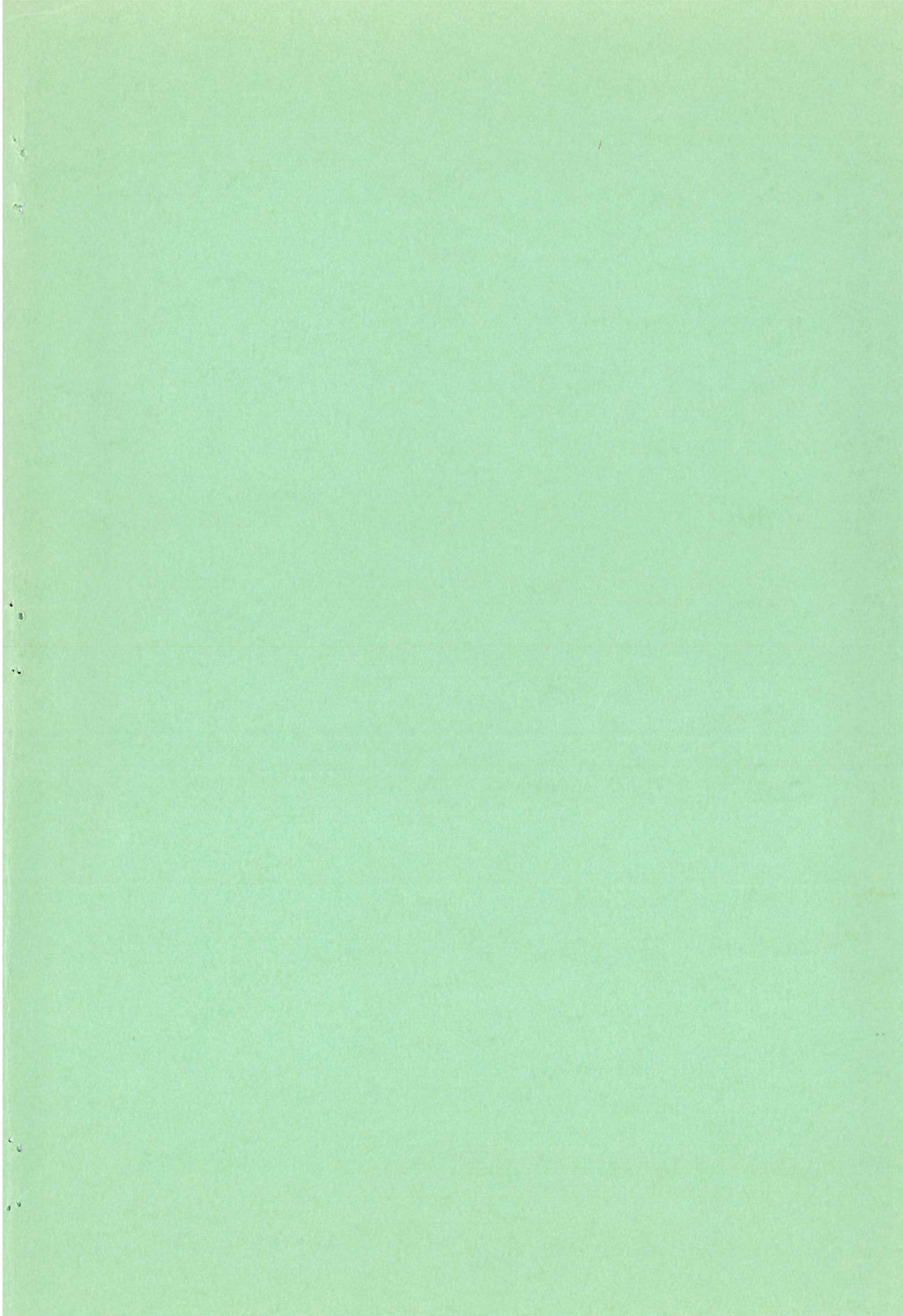
Ad hoc precautions have been taken in THETATRON to keep ρ , T positive, but it is not yet clear what is the best thing to do.

A fundamental problem is the following. In magnetohydrodynamics narrow regions develop where the functions vary quite rapidly; e.g. shock fronts, current sheaths, plasma boundaries, layers where the magnetic field changes sign, neutral points where cutting and rejoining of magnetic lines takes place. In two dimensions it is just not possible to use a uniform mesh with spacing Δ fine enough to accommodate these phenomena, since the amount of computation time varies as Δ^{-3} or Δ^{-4} . Therefore short-wavelength Fourier components with $\lambda \approx \Delta$ have substantial amplitudes, and such components can never be treated accurately with any difference scheme.

In the case of a shock, the region can be widened artificially by increasing the viscosity, with negligible effect on the rest of the calculation. (Von Neumann method, Richtmyer 1957, p.208). It would be desirable to do something similar for the other phenomena, but it is not yet clear how. An alternative would be to crowd mesh points into regions of rapid variation. This is done in the one-dimensional programme, but has not yet been attempted in THETATRON.

6. REFERENCES

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