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Boundary Conditions for Fluid Equations with Flux Sources and Sinks

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Abstract

I use a piece-wise linear approximation to the directed flux expressions for a flowing Maxwellian fluid to write down boundary conditions for the fluid description of a multicomponent plasma. These boundary conditions are sufficiently robust to treat particle reflection, surface reactions leading to secondary production, diffusion, and field-induced drift of charged species.

Introduction

The fluid equations of motion may be applied to plasma dynamics under certain conditions. Both ions and electrons as well as neutral species can each be described by the macroscopic fluid variables of density, velocity or flux, and internal energy. The charged multifluid equations are solved self-consistently with the Poisson equation in order to complete the description. The kinetics of the fluid description require temperature-dependent rates as well as details about the interaction of the fluid with the boundaries of the system. It is the latter that I analyze by an approximate method in this work to formulate general boundary condition methods that may prove useful in plasma simulations.

In general one may not know the temperature-dependent rates of the electronic processes. This requires that the rates be obtained by other means, typically from zero-D Boltzmann calculations using known cross sections or from measurements in discharges. The same might hold for the boundary conditions at the walls or electrodes which contact the plasma; namely that 1-D Boltzmann calculations might be used to compute the correct interaction with the wall, and the results transferred to the fluid description by some scaling argument.

In this note I am not going to argue for the validity of the fluid description. It is obvious that some problems simply should not be addressed by the fluid description. These include an electron distribution that is a mixture of a thermal part and a "beam" part. I will present a simple method for the imposition of boundary conditions to the fluid equations of motion that can be applied in very general circumstances of reactive surface processes producing secondary fluxes, surface reflections, diffusion, and field-induced mobility. I am assuming that the space and time numerical differencing is small enough to resolve all diffusion profiles and physical oscillations of the plasma.

Fluid Basics

All of the results in this note could be written in full 3-D form, but the analysis is much simpler if we assume that the plasma is 1-D with coordinate z as the space variable. In general, z would be the normal coordinate to a surface. The left boundary is taken to be at z = 0 and the right boundary at z = L. Consider a Maxwellian distribution function of a flowing fluid; the fluid velocity along z is specified as v and n, m, and T are the fluid number density, particle mass, and temperature:

$$\begin{aligned} f(\vec{v}|v) &= n \quad (\beta/\pi)^{3/2} \quad \exp(-\beta(v_x^2+v_y^2+(v_z-v)^2)) \\ \beta &= m/2kT \end{aligned} \qquad (1)$$

The fluid flux and the directed fluxes, here called ϕ and $S^{\rightarrow}$and $S^{\leftarrow}$, are calculated to be:

$$\begin{aligned} \phi &= \int d^3v\, v_z\, f(\vec{v}|v) \\ &= n\, v, \\ S^{\rightarrow} &= \int_{v_z>0} d^3v\, v_z\, f(\vec{v}|v) \\ &= n\, v_{th}/4, \quad if \quad v=0, \\ S^{\leftarrow} &= \int_{v_z<0} d^3v\, v_z\, f(\vec{v}|v) \\ &= -n\, v_{th}/4, \quad if \quad v=0, \end{aligned} \qquad (2)$$

with analytic evaluations of the directed fluxes expressible as error functions in the case of a Maxwellian distribution as given in Eq.(1). In these expressions, the "thermal velocity" v_{th} and "thermal flux" ϕ_{th} are defined as

$$\begin{aligned} v_{th} &= \sqrt{8kT/\pi m} \\ \phi_{th} &= n\, v_{th}/4. \end{aligned} \qquad (3)$$

Note that the directed fluxes are not vectors as defined above, they represent the number of particles per area per second crossing a plane normal to the z axis in the specified direction.

Surface Kinetic Relations

Consider the left, or z=0, real surface. At this surface we define the non-negative quantities S_e^{inc} and S_e^{out}, which are the fluxes of species e incident on, and outgoing from, the actual surface. A general kinetic relation is assumed to hold at this surface, namely,

$$S_e^{out} \;=\; \gamma_{ee}\, S_e^{inc} + \gamma_{ie}\, S_i^{inc} \;, \tag{4}$$

where I use γ_{ee} to denote the reflection probability of the incident species e, and γ_{ie} to denote the production of species e by incident species i. Typically, these will denote electrons and ions. These gamma coefficients are true secondary coefficients as measured by surface scattering experiments and contain no modifications due to bulk processes. The source term $\gamma_{ie}\, S_i^{inc}$ represents a secondary flux due to a single incident species; in general it is to be replaced by a sum over all incident species i (metastables, photons, etc.) that create secondary e.

What remains is to combine the surface kinetic relation, Eq.(4), with the directed flux expressions, Eq.(2). This immediately leads to, for the left boundary, for species e:

$$S^{\rightarrow} \;=\; \gamma_{ee}\,(-S^{\leftarrow}) + \gamma_{ie}\, S_i^{inc}. \tag{5}$$

This expression is somewhat impractical for numerical computation because the directed fluxes contain the fluid velocity buried under the integrals over the assumed Maxwellian distribution function for a flowing fluid. Moreover we have not enforced the fact that the directed fluxes must make physical sense when applied to a particular boundary. I will remedy this in the next section by introducing a simple, trivial approximation for these fluxes.

Simple Approximation for Directed Flux

Now let us consider $S^{\rightarrow}$. It is a function of the fluid velocity or of the fluid flux $\phi = nv$ as well as the thermal character of the fluid. We can approximate it in a simple piece-wise manner as

$$\begin{aligned} S^{\rightarrow} &\approx \frac{1}{2}[\,\phi + \phi_T\,] + \frac{1}{2}[\,\phi - \phi_T\,], \\ [x] &\equiv x\,\theta(x). \end{aligned} \tag{6}$$

In this equation $\theta(x)$ is the Heaviside function, zero for x < 0 and one for x > 0, and I have denoted $\phi_T = n\,v_{th}\,/\,2$, which is twice the thermal flux incident on a surface in a stationary fluid, ie. $\phi_{th} = \phi_T\,/\,2$. A plot of this approximation to $S^{\rightarrow}$ vs ϕ is shown in Fig. 1. Eq.(6) may also be expressed in terms of its piecewise linear parts:

$$\begin{aligned} S^{\rightarrow} &= 0, \quad \phi < -\phi_T, \\ S^{\rightarrow} &= \frac{1}{2}(\phi + \phi_T), \quad -\phi_T < \phi < \phi_T, \\ S^{\rightarrow} &= \phi, \quad \phi > \phi_T. \end{aligned} \tag{7}$$

The leftward-bound flux is approximated as

$$S^{\leftarrow} \approx -\frac{1}{2}[\,-\phi + \phi_T\,] - \frac{1}{2}[\,-\phi - \phi_T\,], \tag{8}$$

using the same notation for the "bracket" function. An examination of the approximations to $S^{\rightarrow}$ and $S^{\leftarrow}$ shows that

$$\begin{aligned} S^{\leftarrow}(\phi) &= -S^{\rightarrow}(-\phi), \\ S^{\rightarrow} + S^{\leftarrow} &= \phi, \\ S^{\rightarrow}(\phi=0) &= -S^{\leftarrow}(\phi=0) = \phi_{th} = v_{th}\,n\,/\,4, \\ \frac{\partial S^{\rightarrow}}{\partial\phi}(\phi=0) &= \frac{\partial S^{\leftarrow}}{\partial\phi}(\phi=0) = \frac{1}{2}, \end{aligned} \tag{9}$$

as required by the exact expression found by substituting Eq.(1) into (2). The function and slope values at $\phi=0$ were used in fixing the piece-wise linear approximation to the exact directed flux expression. Fig. 1 displays a plot of the directed fluxes as a function of the fluid flux.

Approximations for Boundary Conditions

Consider the left boundary, we combine Eq.(4) with approximations given in Eqs.(6) and (7) and have

$$
\begin{aligned}
S_e^{inc} &= -S^{\leftarrow} , \\
S_e^{out} &= \gamma_{ee} \, S^{inc} + \gamma_{ie} \, S_i^{inc} = S^{\rightarrow} , \\
\frac{1}{2}[\phi + \phi_T] + \frac{1}{2}[\phi - \phi_T] &= \gamma_{ee} \left(\frac{1}{2}[-\phi + \phi_T] + \frac{1}{2}[-\phi - \phi_T] \right) \\
&\quad + \gamma_{ie} \, S_i^{inc} \quad .
\end{aligned}
\tag{10}
$$

This equation will be greatly simplified for some specific cases in a few moments. Note that the non-negative nature of the surface fluxes is insured. At the right boundary the relation is identical except that $\phi \;\; \rightarrow \;\; -\phi$. In all the specific cases that follow I will be working with the left boundary which is subscripted o. In Fig. 2, I show a plot of the RHS and LHS of Eq.(10) for some typical values of the parameters. The intersection of the RHS and the LHS determines the roots, which are the boundary values for the fluid flux.

<u>Case 1:</u> Total reflection of species e with no sources, ie:

$$\gamma_{ee} = 1 \quad , \quad \gamma_{ie} = 0.$$

Eq.(10) has a unique root for the value of the fluid flux at the boundary, namely,

$$\phi \;=\; \phi_o \;=\; 0$$

which can be used in the continuity equation to evaluate the gradient of flux at the boundary, eg:

$$dn \,/\, dt \;=\; -\phi' \;\approx\; -(\phi_{\Delta z} - \phi_o) \,/\, \Delta z$$

where the prime denotes the space derivative. Alternatively, we can use the solution to introduce boundary conditions on the density gradients by means of the drift-diffusion equation:

$$
\begin{aligned}
\phi_o &= 0 = \mu \, E \, n_o - D \, n_o' , \\
n_o' / n_o &= \mu \, E / D
\end{aligned}
$$

which, if charge is zero or the field is zero, reduces to $n' = 0$. This log derivative condition on n indicates the slope of n at z=0 necessary to balance the mobility (if charged) and diffusion at a reflecting wall.

<u>Case 2:</u> Total absorption or reaction and no source, ie:

$$\gamma_{ee} = 0 \quad , \quad \gamma_{ie} = 0.$$

The solution of Eq.(10) tells us that the fluid boundary flux must satisfy:

$$\phi_o \quad \leq \quad -\phi_T \quad = \quad -\frac{1}{2} v_{th}\, n_o,$$

which requires that the fluid flux at the boundary be more negative than twice the diffusion flux associated with density n_o. In other words the fluid is allowed to flow into the wall at any velocity exceeding twice the negative of the thermal velocity. In FORTRAN this condition would be implemented at the left boundary by replacing

$$\phi_o \quad = \quad a\min 1(\phi_o, -n_o\, v_{th} / 2).$$

Invoking the drift-diffusion relation for the flux enables this to be restated as a bound on the log derivative:

$$\begin{aligned} \phi_o \quad &= \quad \mu E n_o - D n_o' \quad \leq \quad -\phi_T \quad = \quad -v_{th} n_o / 2 \\ n_o' / n_o \quad &\geq \quad (\mu E + v_{th} / 2) / D \end{aligned}$$

Note that if μE is zero, we have a bound on the log derivative that is approximately the reciprocal of the mean free path (reducing the quantities). This is the extrapolated length boundary condition used for neutral diffusion.

<u>Case 3:</u> Total absorption with secondary source:

$$\gamma_{ee} = 0 \quad , \quad \gamma_{ie} \neq 0.$$

The root of Eq.(10) must now be expressed conditional upon the density and secondary flux:

$$\begin{aligned}
\phi_o &\leq -\phi_T \;, && if \quad \gamma_{ie}\, S_i^{inc} = 0\,, \\
\phi_o &= -\phi_T + 2\,\gamma_{ie}\, S_i^{inc}\,, && if \quad \phi_T > \gamma_{ie}\, S_i^{inc}\,, \\
\phi_o &= \gamma_{ie}\, S_i^{inc}\,, && if \quad \phi_T < \gamma_{ie}\, S_i^{inc}\,.
\end{aligned}$$

These different conditions occur as the density n_o varies and causes the diffusion feedback to the wall to change. In Fig. 3, I show a plot of the solution versus thermal flux (proportional to density) at the wall. This solution may be directly used in the numerical evaluation of the flux gradient in the continuity equation. Note that the value of n_o which appears in the solution is an evolving quantity in both the conditions and values of the flux. Thus the actual amount of flux from the electrode is calculated dynamically from the evolving fluid solution and is not a prescribed fraction of the secondary flux.

An interesting result for Case 3 occurs when we require a positive net flux from the surface. Carrying out a simple steady state solution to the drift-diffusion equation gives the following:

$$dn / dt \;=\; -\phi' \;=\; 0$$

$$\phi \;=\; \phi_o \;=\; 2\gamma_{ie}\, S_i^{inc} - \phi_T \;=\; \mu E n - D n'$$

for $\phi_T \;\geq\; \gamma_{ie}\, S_i^{inc}$, or

$$\phi \;=\; \phi_o \;=\; \gamma_{ie}\, S_{ie}^{inc}$$

for $\phi_T \;\leq\; \gamma_{ie}\, S_i^{inc}$.

The solution for the space dependence in the first condition shows that the only bounded solution occurs for (an alternative argument is to neglect D in the bulk),

$$\begin{aligned}
n_o &= \phi_o / \mu E, \\
v_o &= \mu E,
\end{aligned} \quad ,$$

which may be reworked into

$$\phi_o = 2\gamma_{ie} S_i^{inc} \frac{\mu E}{\mu E + v_{th}/2}$$

$$\gamma_{ie}^{eff} = \gamma_{ie} \frac{2}{1 + v_{th}/2\mu E} = \gamma_{ie} \frac{2 v_o}{v_o + v_{th}/2}$$

One may show that γ_{ie}^{eff} rises from 0 at $v_o = 0$ to γ_{ie} at $v_o = v_{th}/2$. Expressions similar to this effective gamma, γ_{ie}^{eff}, have been previously used in the literature.[1-3] They were first discussed by J. J. Thomson in the third edition of *Conduction of Electricity Through Gases*. The previous expressions take the form, using the present notation,

$$\frac{j}{j_o} \equiv \frac{e\,n\,v}{e\,\gamma_{ie} S_i^{inc}} = \frac{v}{v + v_{th}/4},$$

where the current ratio[1] has been defined in terms of the fluid current in the plasma and the true secondary emission current. This can be interpreted as an effective secondary coefficient:

$$\gamma_{ie}^{eff} = \gamma_{ie} \frac{v}{v + v_{th}/4}.$$

The difference between this result and mine is a slower saturation with increasing v. The reason for the difference is that Thomson's derivation assumes that the fluxes at the electrode are additive:

$$\phi_o = -\phi_{th} + \gamma_{ie} S_i^{inc},$$

which makes no allowance for the thermal flux to be modified by the net fluid velocity in the surface region. In other words the kinetic particle distribution is centered about zero rather than the fluid velocity. The effect of a moving fluid on the directed flux is shown in Fig. 1.

One point of this Case 3 derivation is to demonstrate that the use of an effective secondary coefficient can be redundant in the presence of diffusion and mobility terms in the fluid equations of motion. Moreover, if the secondary electrons are released into an electron fluid whose temperature is not too different than the ejected energy, my formulae should be more accurate than the earlier results. If the electrons are of much higher energy the opposite may be true, although in this case the thermal effect is minimal.

Summary

To implement these boundary conditions, one does the following:

(1) For neutrals with complete absorption and no sources, the results are the usual extrapolated length imposed on the density in the diffusion equation. Alternatively, the flux may be specified on the boundary as in the Case 2 example.

(2) For electrons and ions, which potentially have reflections, and certainly have sources, one collects all the incident fluxes on the electrode and generates the source terms for the particular particle due to the impact of other species.

(3) One then calculates the thermal component ϕ_T, which depends on the temperature and density of the particular particle.

(4) These quantities are used in Eq.(10) to obtain a root ϕ_o, which is the value of the fluid flux to be used as a boundary condition in the gradient in the continuity equation.

(5) This completes the process for the left boundary. An analogous procedure must be done for the right boundary, with care given to the proper signs of certain terms.

The only complication in this whole procedure is the root of Eq.(10), which it appears to me has only to be done by comparing the size of ϕ_T to $\gamma_{ie} S_i^{inc}$ (plus other source terms such as metastables) and writing down the algebraic expression for the root in the appropriate interval as done in the Case 3 example.

Acknowledgements

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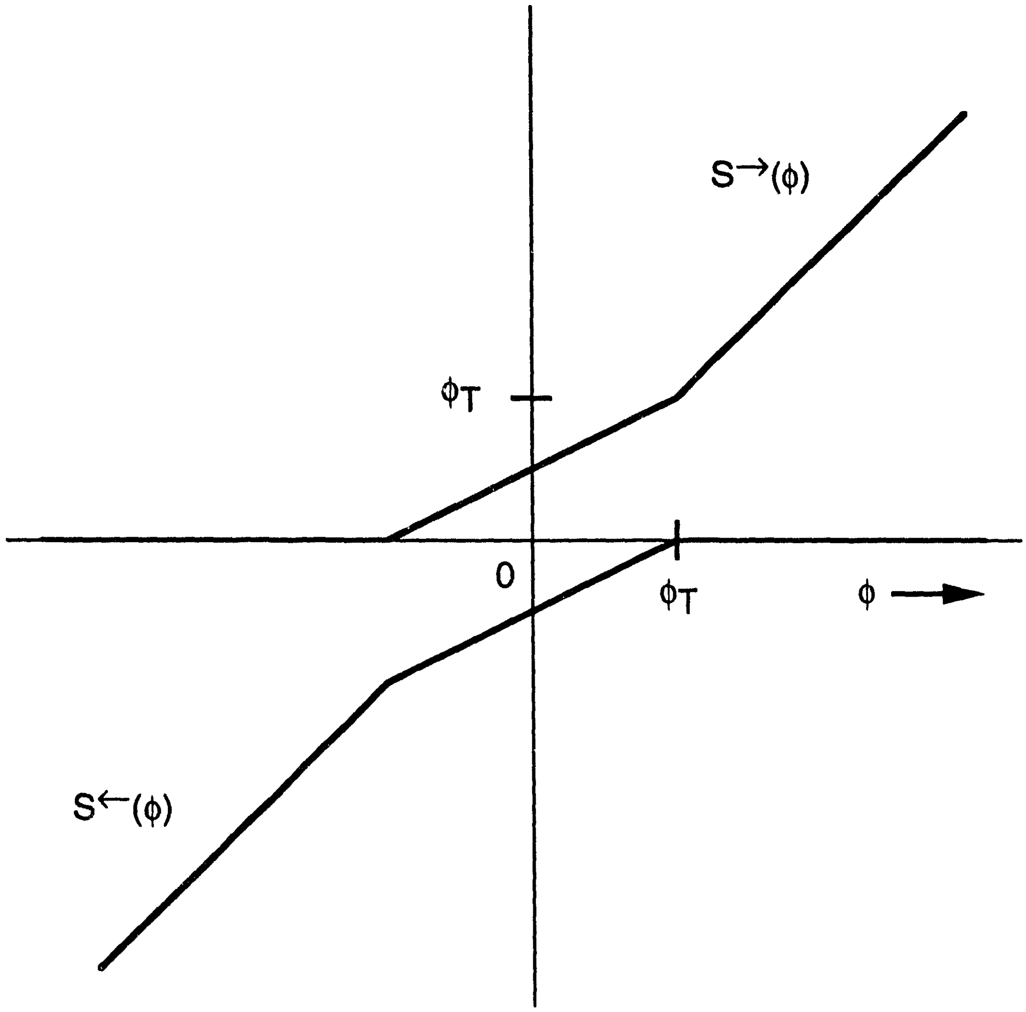

Figure 1. Approximations to the right-going and left-going fluxes which are used in this work. These quantities are defined in Eqs. (6), (7), and (8). ϕ_T is $2\phi_{th}$, which is defined in Eq.(3).

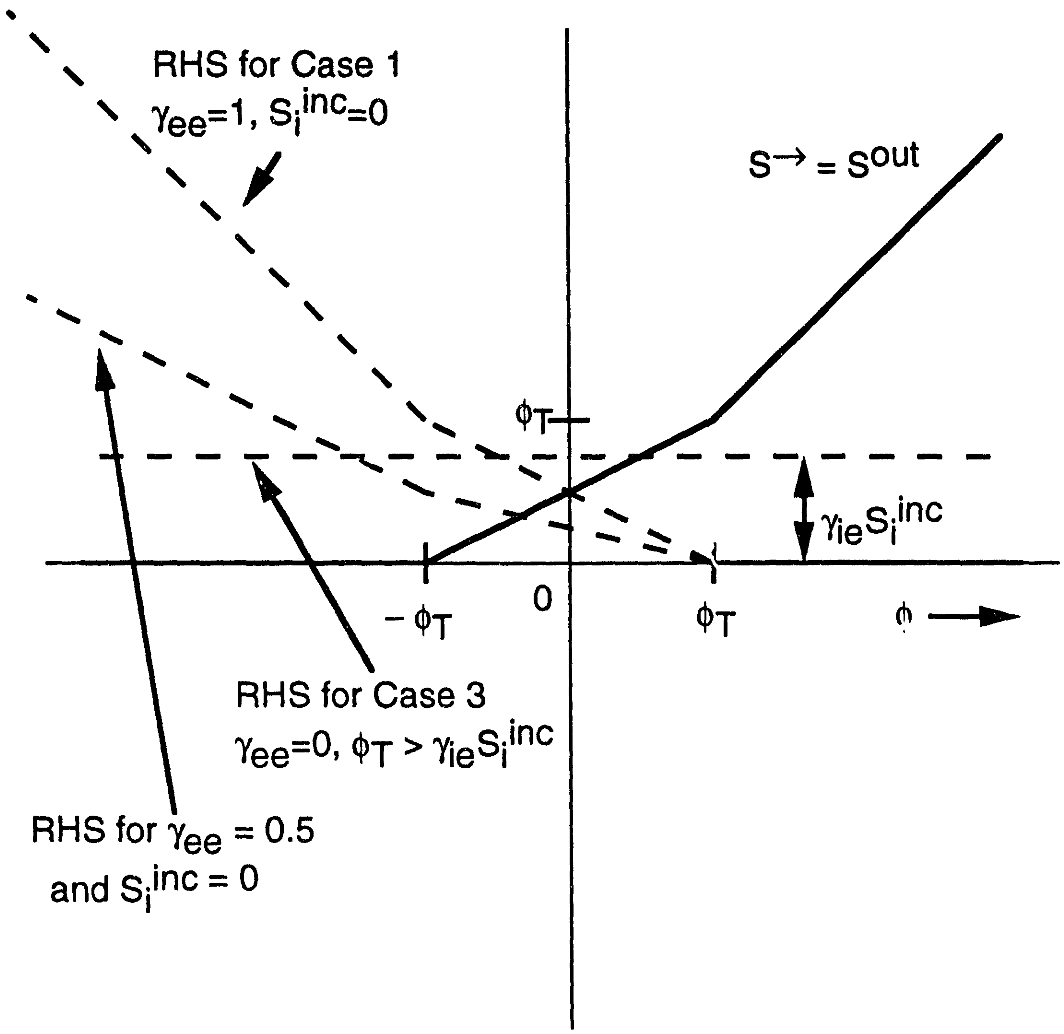

Figure 2. Plot of Eq.(10) for three special cases . ϕ_T is defined via ϕ_{th} from Eq. (3). RHS (dashed lines) denotes the right-hand side of Eq.(10). Case 1 and Case 3 are discussed in the text. The intersections of the RHS curves with the S^{out} curve (which is the LHS (solid line) of Eq.(10)) determines the roots for the boundary fluid flux.

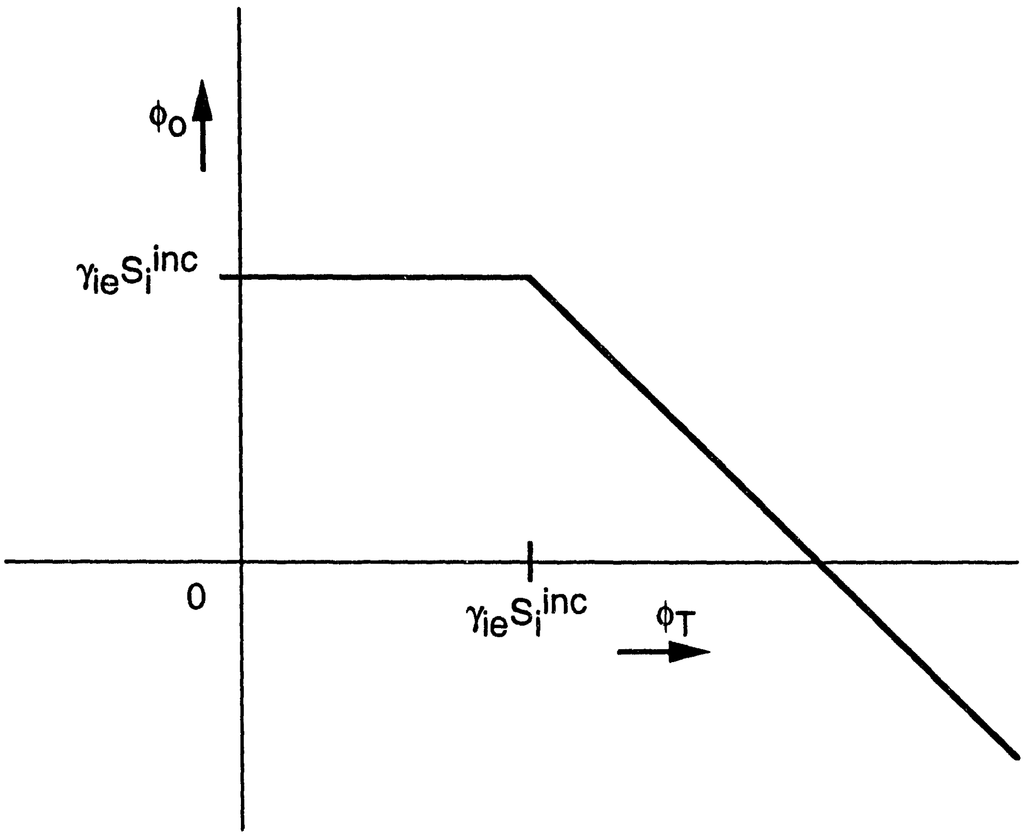

Figure 3. Plot of the root of Eq.(10) *vs* ϕ_T, which is $2\phi_{th}$ from Eq. (3) in the text. These are Case 3 conditions. Notice that the root ϕ_o vanishes when $\phi_T/2 = \phi_{th} = \gamma_{ie}S_i^{inc}$.

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