

## The effect of coating layers on diamond heat sinks

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Report WD 88-05

**The Effect of Coating Layers on  
Diamond Heat Sinks**

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June 1988

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## 1. Introduction

In references [1,2,3] we reported results of calculations on heat diffusion in diamond-copper heat sinks. There, we neglected the presence of coating layers between heat source and diamond. These layers usually consist of Au, Pt and Ti. The effects of heat diffusion in these thin layers is the subject of the present study.

First, we present the model used to describe the system and show how the temperature distributions in the layers can be expressed in terms of the system parameters. The resulting analytical expressions have been implemented numerically. We analyse both the general features of heat diffusion in thin layers and the temperature behaviour in a commonly used configuration. The software, developed to calculate the present results, has been integrated with the existing computer programmes for diamond-copper heat sinks.

## 2. The Modeling of Thin Coating Layers

Because the effect of the coating is expected to be most appreciable in case of a line source (cf. ref. [3]), we direct our investigations to this geometry. In this case, the heat diffusion has a 2-dimensional character as far as the coating is concerned. Therefore, we model the coating in two dimensions as drawn in figure 1 (page 3). The heat flux  $F_0$  enters layer 1 from above via an opening with length  $2R_0$  and leaves the system via the bottom of layer 4. Regions 1, 2 and 3 represent 3 coating layers with thicknesses in the order of  $10^{-6}$ m. Region 4 represents the diamond, which is considerably thicker. The thermal conductivities  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_4$  are taken constant. This is not correct for diamond (region 4). However, we are in this context mainly interested in the heat diffusion in regions 1, 2 and 3 and it has therefore no sense to take into account subtle effects within region 4. It is an essential feature of the system, that these thin layers are mounted on top of a medium, which conducts much better ( $k_4 \gg k_1, k_2$  and  $k_3$ ) and really acts as a 'heat sink'. That is also the reason to assume a homogeneous temperature at the bottom of region 4. Because the differential equations to be solved are linear, we may choose the origin of the temperature scale arbitrarily. For convenience, we choose  $T = 0$  everywhere at the bottom of region 4. An alternative choice for the condition at this boundary would be a homogeneous flux, but this makes hardly any difference in the eventual results.

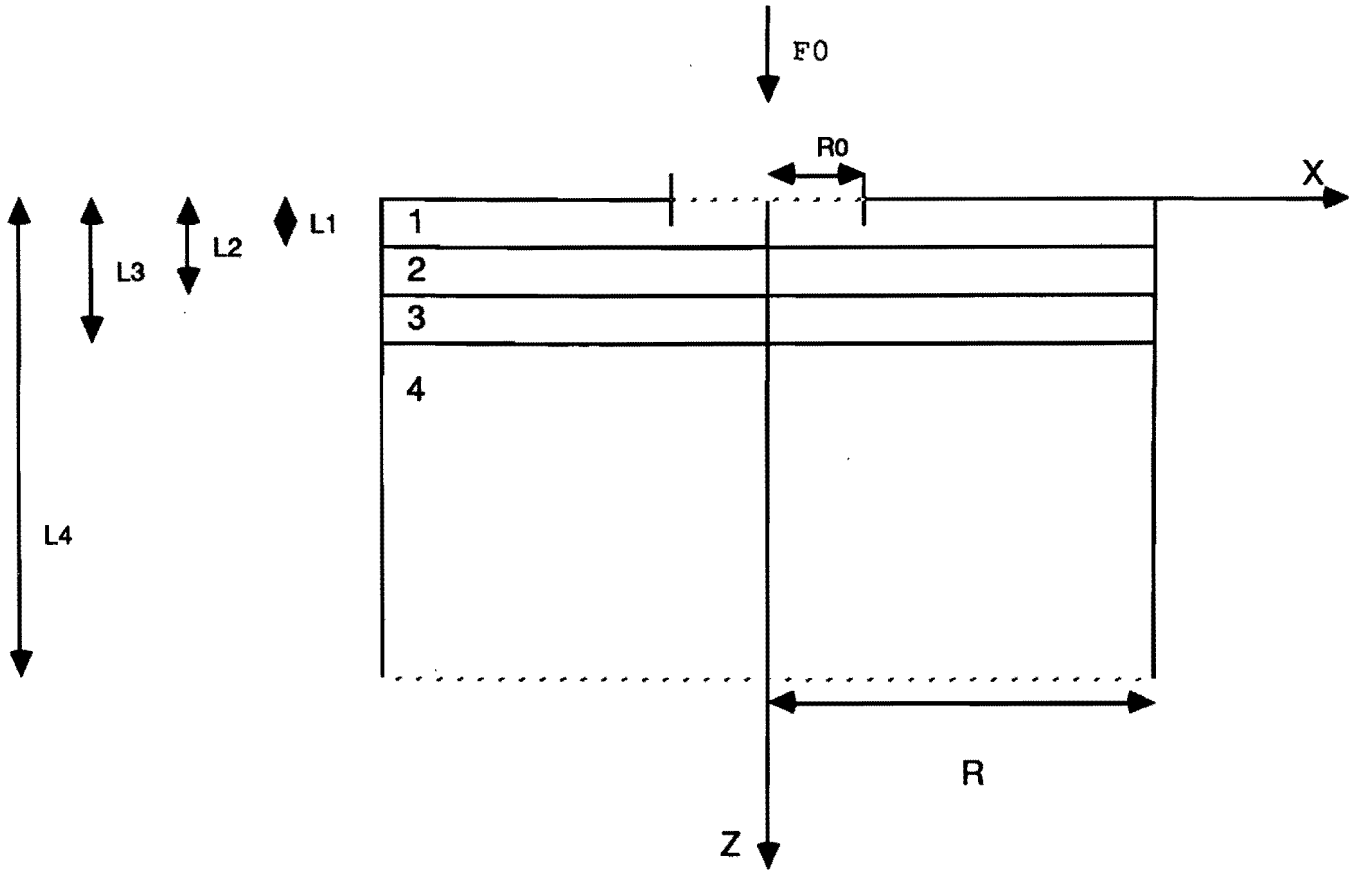


Figure 1. The geometry studied in this report. The geometrical parameters are  $R_0$ ,  $R$ ,  $L_1$ ,  $L_2$ ,  $L_3$  and  $L_4$ . The thermal conductivities of regions 1,2,3 and 4 are denoted by  $k_1$ ,  $k_2$ ,  $k_3$  and  $k_4$  respectively. The applied heat flux is denoted by  $F_0$ . For  $(z = 0, -R_0 \leq x \leq R_0)$  the flux density is uniform with value  $\frac{F_0}{2R_0}$ . The heat leaves the system through the boundary  $(-R \leq x \leq R, z = L_4)$ . The temperature is uniform at this boundary.

As shown in fig. 1, we choose our coordinates  $(x, z)$  such that the origin coincides with the centre of the flux input opening. The system has  $x = 0$  as an axis of symmetry. The temperature distribution to be calculated, is a function of the following system parameters:

- $F_0$  : total heat flux
- $R_0$  : half width of flux input opening
- $R$  : half width of all regions
- $L_1, L_2, L_3, L_4$  : bottom positions along the z-axis of regions 1,2,3,4 respectively
- $k_1, k_2, k_3, k_4$  : thermal conductivities of regions 1,2,3,4 respectively

### 3. Separation of Variables

We are looking for the stationary temperature distribution  $T(x, z)$ . This distribution has in all regions to satisfy the Laplace equation

$$T_{xx} + T_{zz} = 0 \quad (1)$$

The boundary and matching conditions, which have already partly been discussed in the preceding section, will be successively introduced hereafter. Because the differential equation is linear and homogeneous and the boundary and matching conditions are linear, it is convenient to solve this equation by separation of variables, i.e. to assume

$$T(x, z) = U(x)V(z) \quad (2)$$

If we substitute this into (1), we obtain two ordinary differential equations

$$U_{xx} = \mu U \quad (3a)$$

$$V_{zz} = -\mu V \quad (3b)$$

with  $\mu$  a constant, which is still to be determined. The boundary conditions on  $U$  are the same for all regions and given by

$$U_x(-R) = U_x(+R) = 0, \quad (4)$$

which implies, that no heat leaves the system across the boundaries at  $x = R$  and  $x = -R$ . Now, we have to consider the following three possibilities:

1.  $\mu = 0$ .

In this case,  $U$  and  $V$  are linear in  $x$  and  $z$  respectively. From the symmetry around  $x = 0$ , which implies that  $U(x) = U(-x)$ , it follows that  $U$  is constant.

2.  $\mu < 0$ .

For convenience, we introduce  $\lambda > 0$  such that  $\mu = -\lambda^2$ . The general solution for  $U$  has the form

$$U(x) \sim \cos \lambda x$$

We exclude the  $\sin \lambda x$  solution, in view of the symmetry around  $x = 0$ . From (4), we obtain a discrete spectrum for  $\lambda$  given by

$$\lambda_n = n\pi/R, \quad n = 1, 2, 3, \dots \quad (5)$$

The corresponding eigenfunctions of (3a) are denoted by  $U_n$ . The corresponding solutions of (3b) have the form

$$V_n(z) = ae^{\lambda_n z} + be^{-\lambda_n z} \quad (6)$$

with  $a, b$  constants.

Note that boundary value problem (3a) with (4) is of the Sturm-Liouville type [4]. That is why we need to consider real eigenvalues and real eigenfunctions only. The eigenvalues are  $\lambda_0 \equiv 0, \lambda_1, \lambda_2, \dots$  with eigenfunctions  $\cos \lambda_0 x (\equiv 1), \cos \lambda_1 x, \cos \lambda_2 x, \dots$  respectively. These eigenfunctions form a complete, orthogonal basis set in the space of continuous functions on the interval  $[R, -R]$ . The usual inner product for squared integrable elements  $f, g$  of this space is

$$(f, g) \equiv \int_{-R}^{+R} f(x)g(x)dx \quad (7)$$

For the basis functions  $U_n \equiv \cos \lambda_n x$  we have

$$\begin{aligned} (U_n, U_m) &= 2R \quad \text{if } n = m = 0 \\ &R \quad \text{if } n = m \neq 0 \\ &0 \quad \text{if } n \neq m \end{aligned} \quad (8)$$

### 3. $\mu > 0$

In this case no solutions, that satisfy conditions (4), exist.

The general solutions  $T^i$  of (1) with  $i$  indexing the regions 1,2,3 and 4 can be written in terms of the  $U_n$  and  $V_n$  obtained above:

$$T^i(x, z) = \sum_{n=0}^{\infty} U_n^i(x) V_n^i(z) = (a_0^i z + b_0^i) + \sum_{n=1}^{\infty} (a_n^i e^{\lambda_n z} + b_n^i e^{-\lambda_n z}) \cos \lambda_n x. \quad (9a)$$

For completeness, we also give the derivatives  $T_z^i$  in the  $z$ -direction:

$$T_z^i(x, z) = a_0^i + \sum_{n=1}^{\infty} \lambda_n (a_n^i e^{\lambda_n z} - b_n^i e^{-\lambda_n z}) \cos \lambda_n x \quad (9b)$$

#### 4. Boundary and Matching Conditions in the $z$ -direction

It remains to determine the coefficients  $a_n^i$  and  $b_n^i$  in expansions (9a,b). In the following, we deal with the boundary conditions at  $z = 0$  and  $z = L_4$ , and with the matching conditions at  $z = L_1, z = L_2$ , and  $z = L_3$  respectively.

1. At  $z = 0$ , the flux density  $F(x, 0)$  is given by

$$F(x, 0) \equiv k_1 T_z^1(x, 0) = \begin{cases} -F_0/(2R_0) & \text{if } |x| \leq R_0 \\ 0 & \text{if } |x| > R_0 \end{cases} \quad (10)$$

If we substitute expression (9b) into this equation, take at both sides the inner product (7) with some particular basis function  $U_n$ , and make use of (8b), we obtain the following relations:

$$a_0^1 = -F_0/(2k_1 R) \quad (11a)$$

and for  $n > 0$

$$b_n^1 = a_n^1 + \frac{F_0}{(k_1 \lambda_n R)} \frac{\sin(\lambda_n R_0)}{\lambda_n R_0} \quad (11b)$$

2. At  $z = L_4$  a vanishing temperature is assumed:

$$T(x, L_4) = 0 \quad |x| \leq R \quad (12)$$

Inserting expansion (9a) and taking inner products results in:

$$b_0^4 = -L_4 a_0^4 \quad (13a)$$

and for  $n > 0$

$$b_n^4 = -e^{2\lambda_n L_4} a_n^4 \quad (13b)$$

3. At  $z = L_1, L_2$  and  $L_3$  the matching conditions are

$$\begin{aligned} T^i(x, L_i) &= T^{i+1}(x, L_i) \\ k_i T_z^i(x, L_i) &= k_{i+1} T_z^{i+1}(x, L_i) \end{aligned} \quad (14)$$

with  $i = 1, 2, 3$  and  $|x| \leq R$ . If we take inner products, these conditions yield linear relations between the pairs  $(a_n^i, b_n^i)$  and  $(a_n^{i+1}, b_n^{i+1})$ , which are appropriately summarised by

$$\begin{pmatrix} a_n^{i+1} \\ b_n^{i+1} \end{pmatrix} = M^n(i+1, i) \begin{pmatrix} a_n^i \\ b_n^i \end{pmatrix} \quad (15)$$



If we introduce the parameters

$$\begin{aligned}\alpha_{i,j} &= k_j/k_i \\ \beta_{n,i} &= \exp(2\lambda_n L_i)\end{aligned}\tag{16}$$

the transition matrices  $M^n$  are given by

$$M^0(i+1, i) = \begin{pmatrix} \alpha_{i+1,i} & 0 \\ (1 - \alpha_{i+1,i})L_i & 1 \end{pmatrix}\tag{17a}$$

and for  $n > 0$

$$M^n(i+1, i) = \frac{1}{2} \begin{pmatrix} (1 + \alpha_{i+1,i}) & (1 - \alpha_{i+1,i})\beta_{n,i}^{-1} \\ (1 - \alpha_{i+1,i})\beta_{n,i} & (1 + \alpha_{i+1,i}) \end{pmatrix}\tag{17b}$$

## 5. General Solution

From (15), we conclude that the coefficients in regions 2,3 and 4 can be calculated from those in region 1. It remains to derive explicit expressions for  $(a_n^1, b_n^1)$ . If we apply transformation (15) three times, we obtain

$$\begin{pmatrix} a_n^4 \\ b_n^4 \end{pmatrix} = N^n \begin{pmatrix} a_n^1 \\ b_n^1 \end{pmatrix} \quad (18)$$

with

$$N^n \equiv M^n(4,3)M^n(3,2)M^n(2,1) \quad (19)$$

If we combine equations (11), (13) and (18), 4 linear equations with 4 unknowns are obtained, which have the following solutions:

1.  $n = 0$

Because the matrices  $M^0$  are lower triangular with simple diagonal elements, the matrix  $N^0$  has the form

$$N^0 = \begin{pmatrix} \alpha_{4,1} & 0 \\ N_{21}^0 & 1 \end{pmatrix} \quad (20)$$

with the element  $N_{21}^0$  a function of the parameters  $\alpha_{4,3}, \alpha_{3,2}, \alpha_{2,1}, L_1, L_2$  and  $L_3$ . Because the form of this function is lengthy and obvious we omit it here. The pair  $(a_0^1, b_0^1)$  is given by

$$\begin{aligned} a_0^1 &= -F_0/2k_1R \\ b_0^1 &= (\alpha_{4,1}L_4 + N_{21}^0)F_0/2k_1R \end{aligned} \quad (21)$$

2.  $n > 0$

We write (11b) and (13b) in the form

$$b_n^1 = a_n^1 + \gamma_n \quad (22a)$$

$$b_n^4 = -\beta_{n,4}a_n^4 \quad (22b)$$

with  $\beta$  defined by (16) and  $\gamma$  by

$$\gamma_n = \frac{F_0}{k_1\lambda_n R} \frac{\sin \lambda_n R_0}{\lambda_n R_0} \quad (23)$$

If we substitute relations (22) into equation (18), we obtain two linear equations in two unknowns :

$$a_n^4 \begin{pmatrix} 1 \\ -\beta_{n,4} \end{pmatrix} = a_n^1 N^n \begin{pmatrix} 1 \\ 1 \end{pmatrix} + N^n \begin{pmatrix} 0 \\ \gamma_n \end{pmatrix} \quad (24)$$

From (24), we find:

$$a_n^1 = -\gamma_n(\beta_{n,4}N_{12}^n + N_{22}^n)/[\beta_{n,4}(N_{11}^n + N_{12}^n) + (N_{21}^n + N_{22}^n)] \quad (25)$$

while  $b_n^1$  follows from (22a) with (23).

## 6. Results

To analyse heat diffusion in coating layers, we evaluated the formulae above numerically. The temperature profiles, obtained from (9a), are calculated along the straight lines  $z = 0, L_1, L_2$  and  $L_3$  and denoted by  $T(0), T(1), T(2)$  and  $T(3)$ . They are presented in the “a” figures. Evaluating equation (9b), we obtained the corresponding flux profiles  $F(0), F(1), F(2)$  and  $F(3)$ , which are presented in the “b” figures.

In the following, we vary the parameters such, that we deal with a one coating, a two coatings and a three coatings system. Only the latter case describes the situation in practice. The other cases are used to show general relationships.

### One Coating.

To simulate heat diffusion in one coating layer, we choose (see figure 1)  $k_1 = k_2 = k_3 = 1 \text{ W/cm/}^\circ\text{C}$  and  $k_4 = 20 \text{ W/cm/}^\circ\text{C}$ . Further, we use the values  $L_1 = .0001 \text{ cm}$ ,  $L_2 = 2L_1$ ,  $L_3 = 3L_1$ , so that the profiles are read out at equal distances. Results are given for the cases  $R_0 = L_1$  (fig. 2) and  $R_0 = 8L_1$  (fig. 3). These examples are representative for two quite different situations, namely  $R_0$  comparable to or smaller than  $L_1$  and  $R_0$  bigger than  $L_1$ . In the first geometry, the flux input opening is apparently seen as a point source at  $z = L_1, L_2, L_3$  and the lateral heat diffusion (i.e. in the  $x$ -direction) is appreciable. In the latter geometry, the lateral heat diffusion in the coating layer is nearly negligible.

### Two Coatings

We present results for two coating layers, which differ much in thermal conductivity. The parameters are as in the one coating system with  $R_0 = .0008$  and the  $k_3$  value varied over the rather extreme values  $k_3 = 1000$ . (fig. 4) and  $k_3 = .01$  (fig. 5). Fig. 4a shows that the temperature hardly varies in an extremely well conducting layer. The heat spreads so easily, that temperature differences tend to smooth out, as seen in fig. 4b. In fig. 5 it is demonstrated that a (relatively) badly conducting layer acts as a barrier, which forces the heat to spread in the layer on top of it.

### Three Coatings

We give results for a 'standard geometry' (SG), which has been inspired by coating specifications commonly used in practice. In this SG, the layers 1,2,3 and 4 in fig.1 consist of *Au*, *Pt*, *Ti* and diamond respectively. The thermal conductivities are  $k_1 = 3.19$ ,  $k_2 = 0.72$ ,  $k_3 = 0.22$  and  $k_4 = 20 \text{ W/cm/}^\circ\text{C}$ . The thicknesses of the layers follow from the values  $L_1 = .0001$ ,  $L_2 = .00011$  and  $L_3 = .00012 \text{ cm}$ . The exact values of  $R$  and  $L_4$  are not important, provided that they are much bigger than the  $L_i$  values. We use the values  $R = .01$  and  $L_4 = .001 \text{ cm}$ . For  $F_0$  the rather arbitrary value of  $F_0 = 100 \text{ W}$  is chosen.

#### *Dependence on $R_0$*

For the SG, we present results for  $R_0 = .001$  (fig. 6),  $R_0 = .0005$  (fig. 7),  $R_0 = .00025$  (fig. 8) and  $R_0 = .0001$  cm (fig. 9). The *Pt* and *Ti* layers are apparently such thin compared to the *Au* layer, that lateral heat diffusion takes appreciably place only in the *Au* layer. That is why  $F(1)$ ,  $F(2)$  and  $F(3)$  in the figures 6b, 7b, 8b, and 9b coincide. The temperature jumps in the *Pt* and *Ti* layers are inversely proportional to the corresponding thermal conductivities, as seen in figures 6a, 7a, 8a, and 9a.

#### *Dependence on $k_4$*

We investigate the dependence of the results on  $k_4$  by choosing two extreme values, namely  $k_4 = 1$  (fig. 10) and  $k_4 = 1000$ . (fig. 11). The other parameters are as in the SG with  $R_0 = .00025$ . If we compare fig. 9 and 10, we notice that decreasing  $k_4$  by a factor of 20 leads to enhancement of the lateral heat diffusion in all coating layers. The temperatures (with respect to the temperature at the bottom of region 4) are enhanced by a factor of about 4. If we compare fig. 9 and 11, little difference is found. The value of  $k_4 = 20$ , as used in fig. 9, is apparently such high compared to the values of  $k_1$ ,  $k_2$  and  $k_3$ , that further enhancement of that value hardly affects the temperature and flux profiles in the coating layers.

## References

1. Molenaar, J., Staarink, G.W.M., Temperature Distributions in Diamond Heat Sinks, Report WD 85-01, University of Nijmegen, 1985, Part I.
2. Molenaar, J., Staarink, G.W.M., Temperature Distributions in Diamond Heat Sinks, Report WD 85-01, University of Nijmegen, 1985, Part II.
3. Molenaar, J., Diamond Heat Sinks, The Line Geometry, Report WD 86-04, University of Nijmegen, 1986.
4. Courant, R. and Hilbert, D., Methods of Mathematical Physics, Vol. 1, Interscience Publishers Inc., New York, 1953.

## Figure Captions

In figures 2-11 temperature ('a') and flux ('b') profiles are given. The temperature profiles at  $z = 0, L_1, L_2$  and  $L_3$  are denoted by  $T(0), T(1), T(2)$  and  $T(3)$  respectively. The corresponding flux profiles are denoted by  $F(0), F(1), F(2)$  and  $F(3)$ . The units are Watt, cm and °C with respect to the temperature at  $z = L_4$ , which is fixed at 0 °C for convenience.

Fig.2. Results for the parameter set:

$$k_1 = k_2 = k_3 = 1, k_4 = 20, L_1 = .0001, L_2 = .0002, L_3 = .0003, R = .01, L_4 = .001, R_0 = .0001, F_0 = 100.$$

Fig.3. As fig. 2 with  $R_0 = .0008$ .

Fig.4. As fig. 2 with  $R_0 = .0008$  and  $k_3 = 1000$ .

Fig 5. As fig. 2 with  $R_0 = .0008$  and  $k_3 = .01$ .

Fig.6. Results for the 'standard geometry' with parameter set:  $k_1 = 3.1(Au)$ ,  $k_2 = 0.72(Pt)$ ,  $k_3 = 0.22(Ti)$ ,  $k_4 = 20$ . (diamond),  $L_1 = .0001$ ,  $L_2 = .00011$ ,  $L_3 = .00012$ ,  $L_4 = .001$ ,  $R = .01$ ,  $F_0 = 100.$ ,  $R_0 = .001$ .

Fig.7. As fig. 6 with  $R_0 = .0005$ .

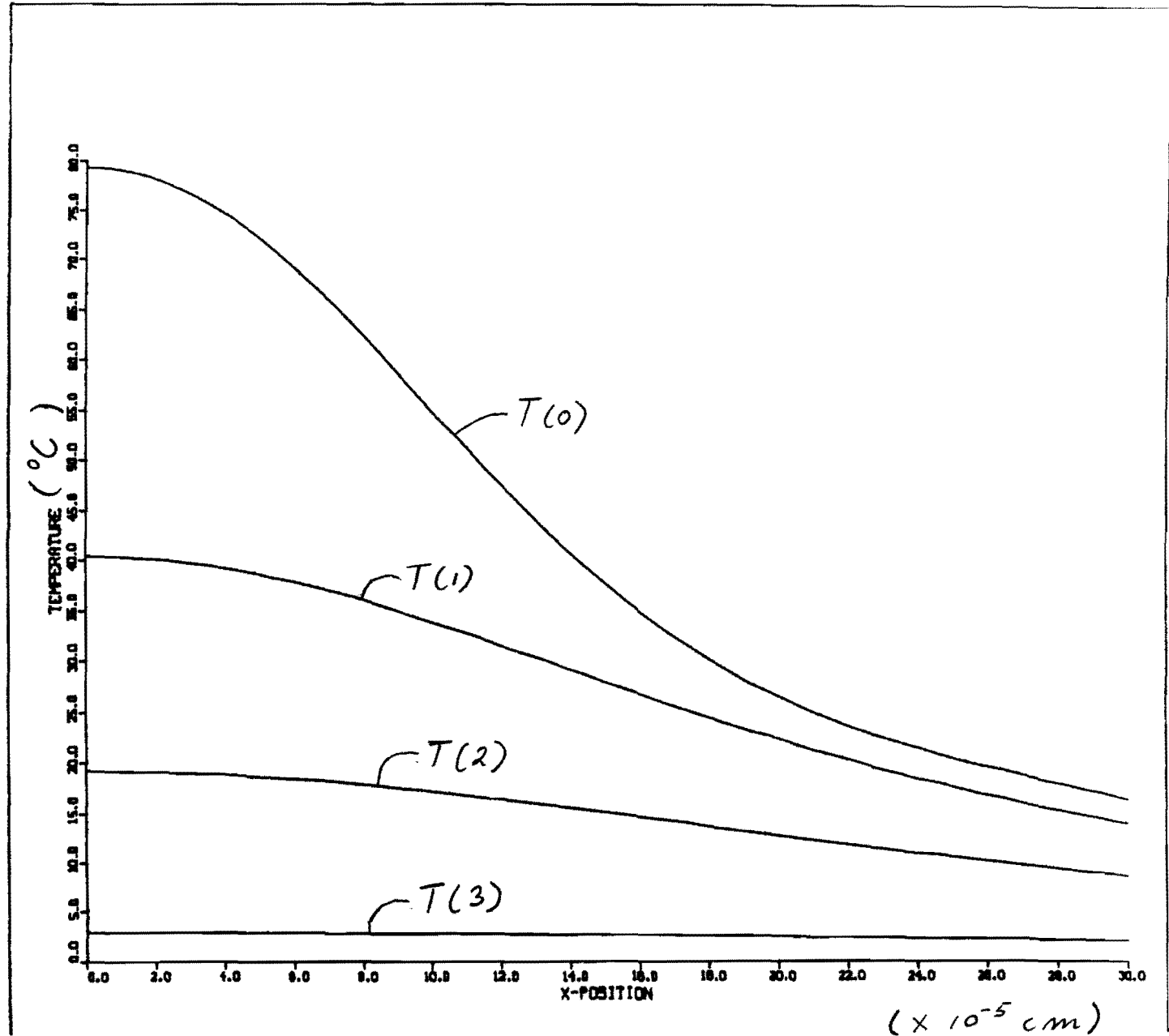
Fig.8. As fig. 6 with  $R_0 = .00025$ .

Fig.9. As fig. 6 with  $R_0 = .0001$ .

Fig.10. As fig. 6 with  $R_0 = .00025$  and  $k_4 = 1$ .

Fig.11. As fig.6 with  $R_0 = .00025$  and  $k_4 = 1000$ .

Fig. 2.a



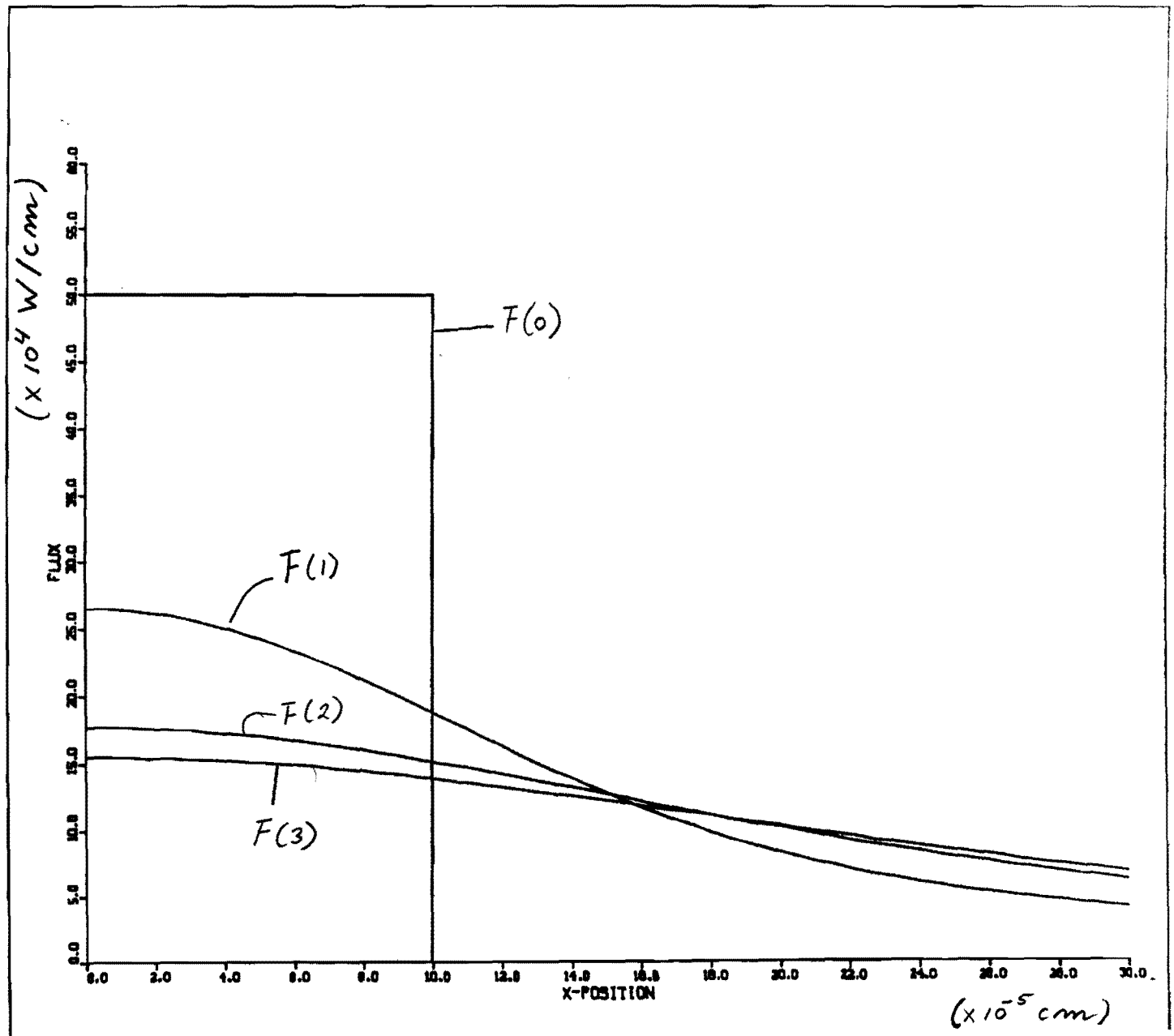
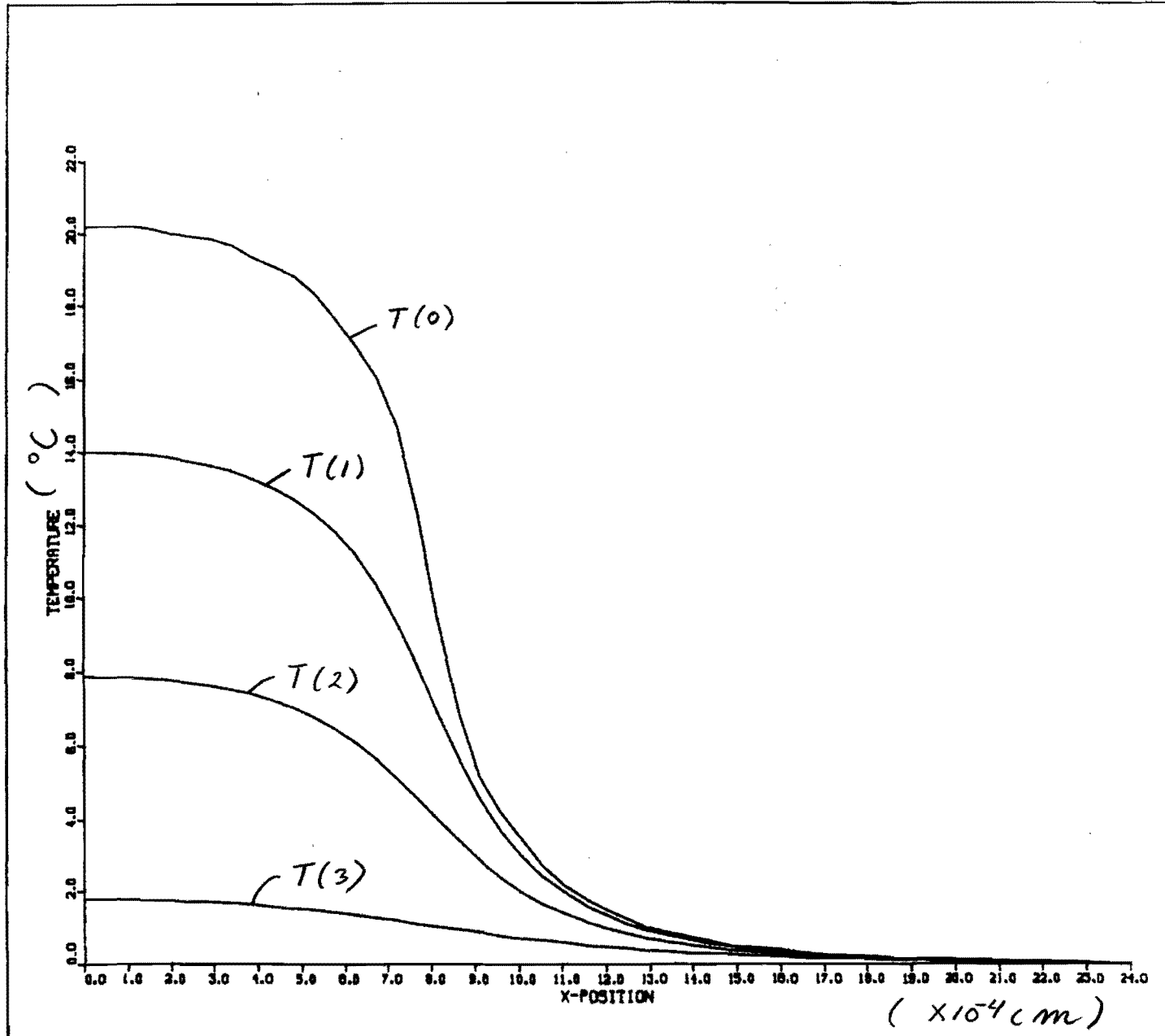


Fig. 2.b

Fig. 3.a





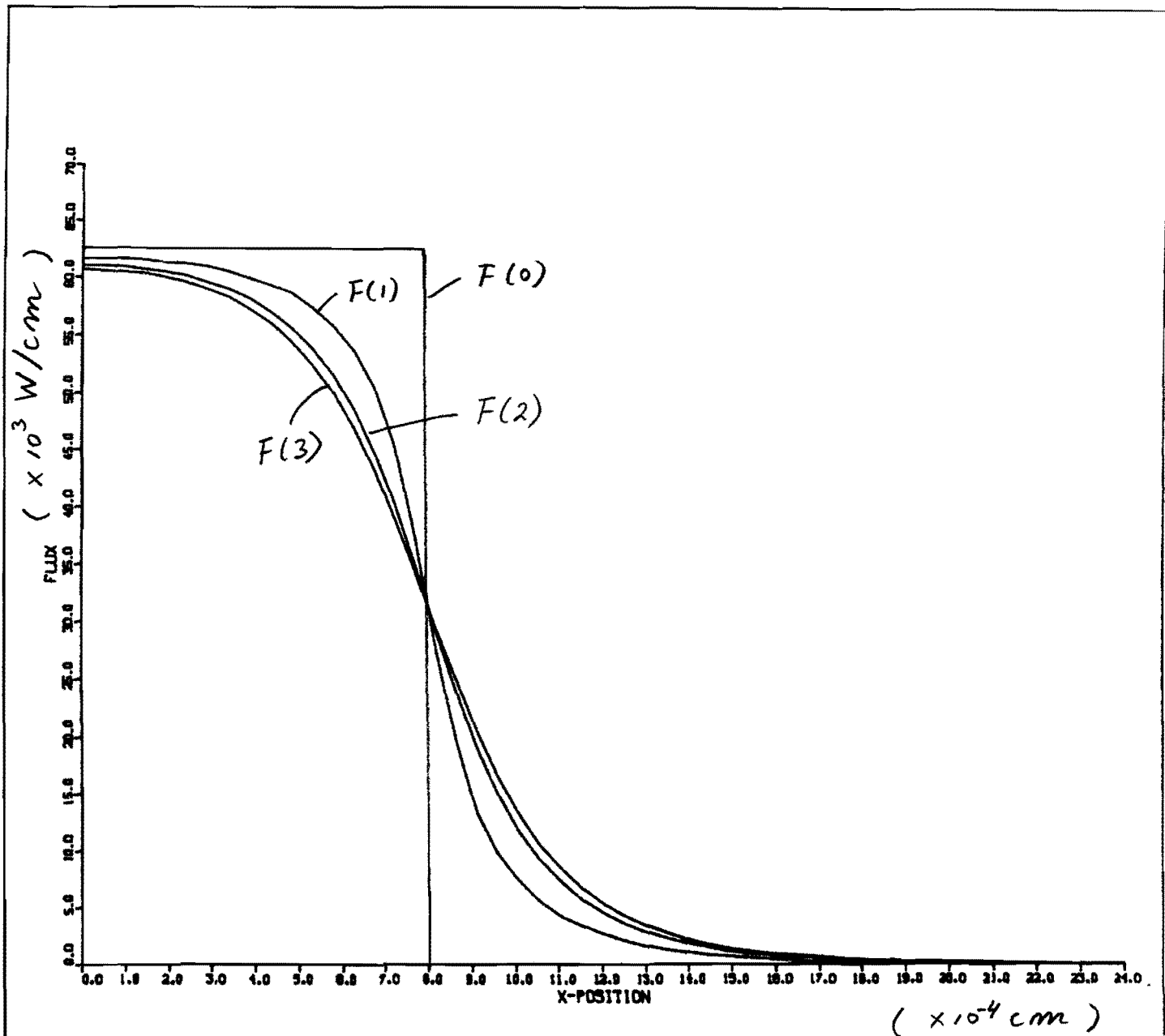
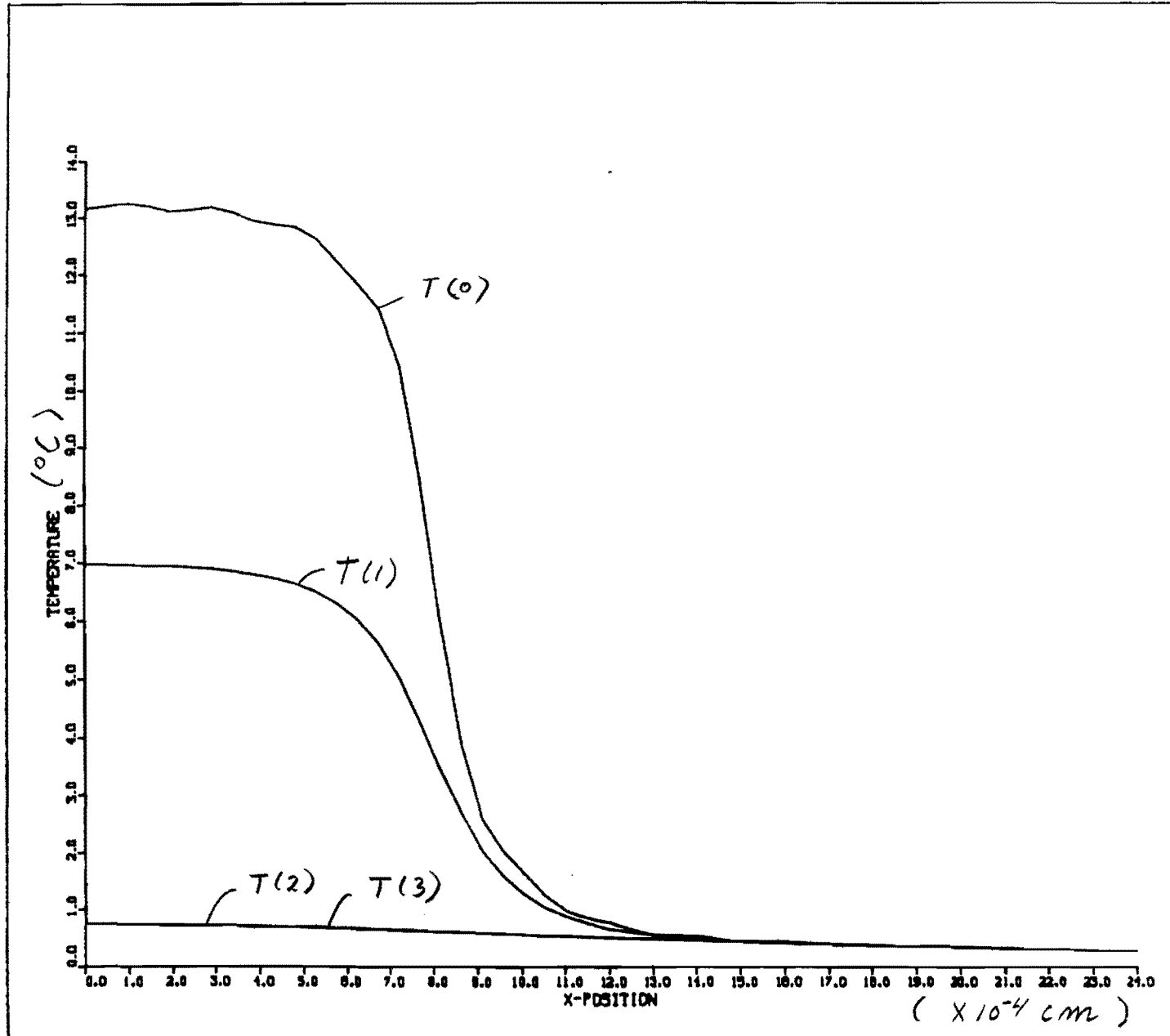


Fig. 3.b

Fig. 4.a



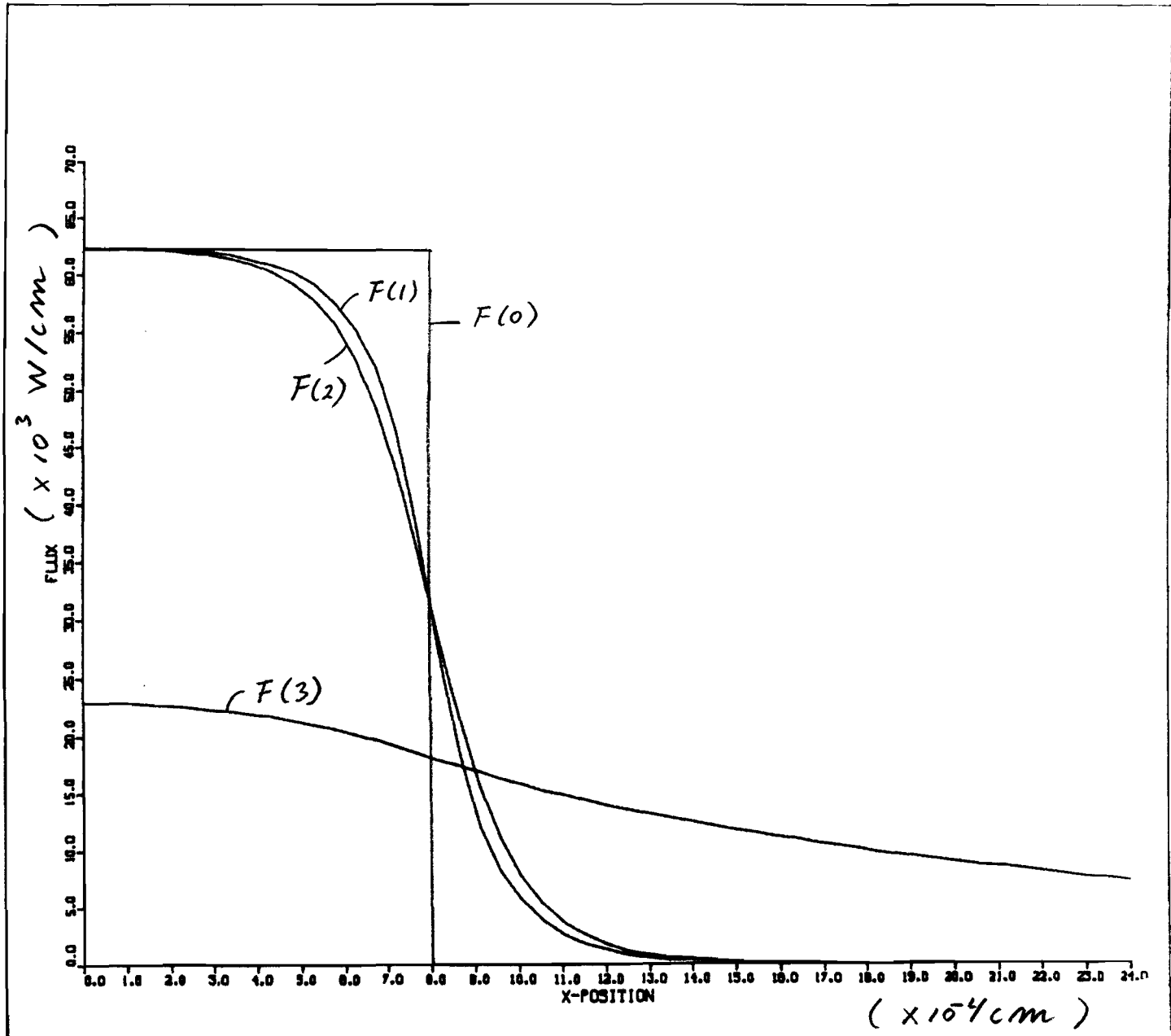
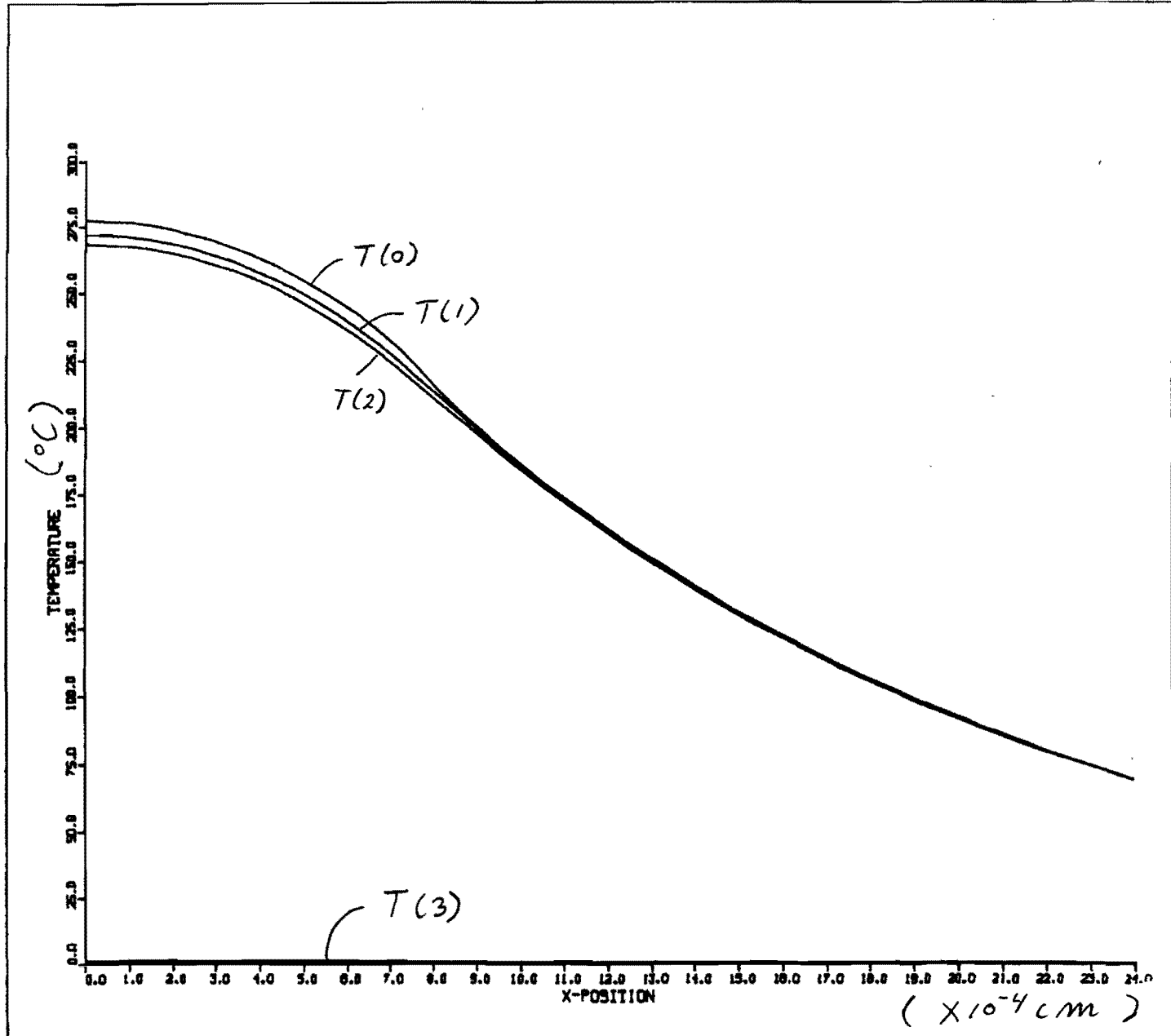


Fig. 4.6

Fig. 5.a



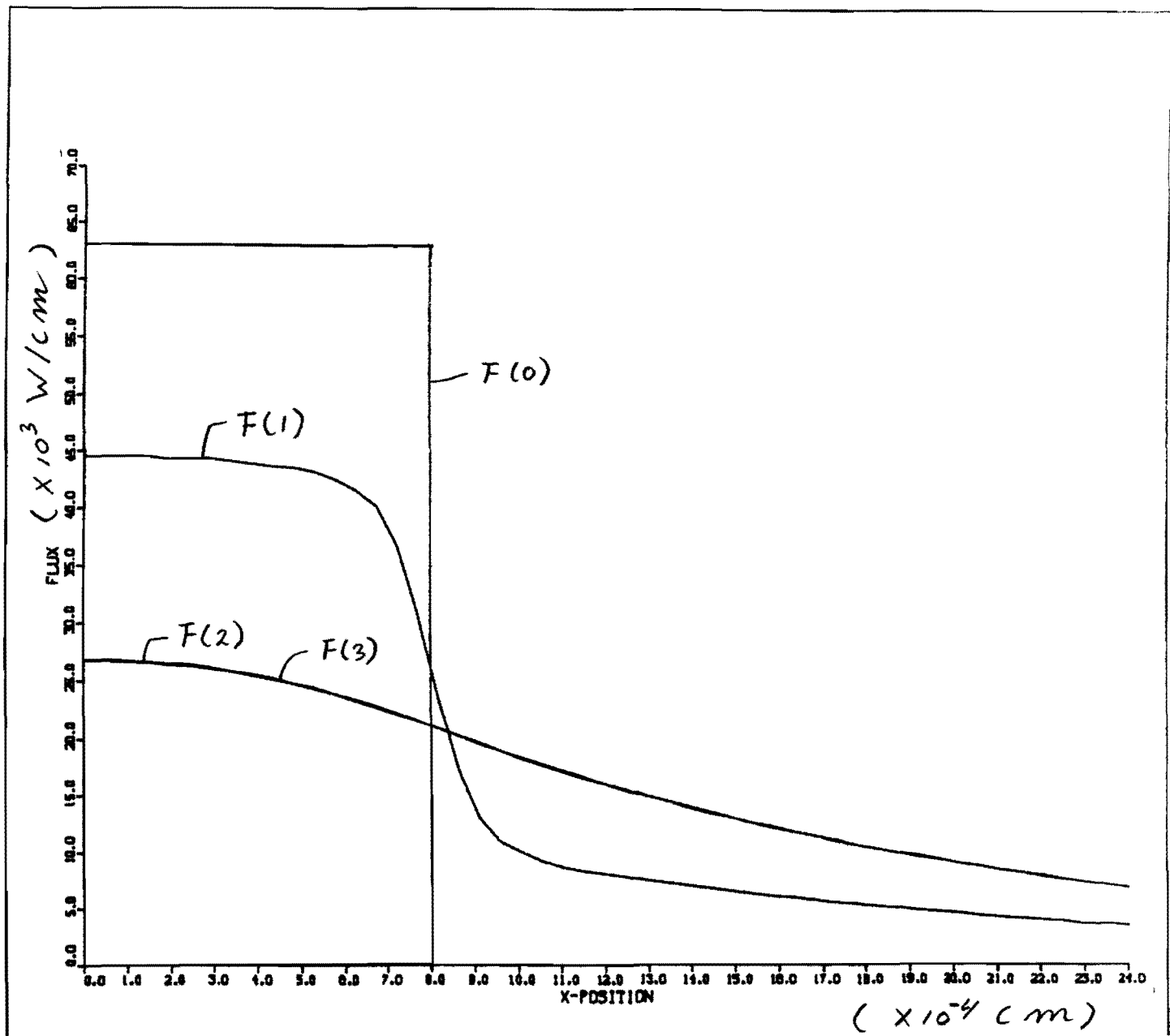
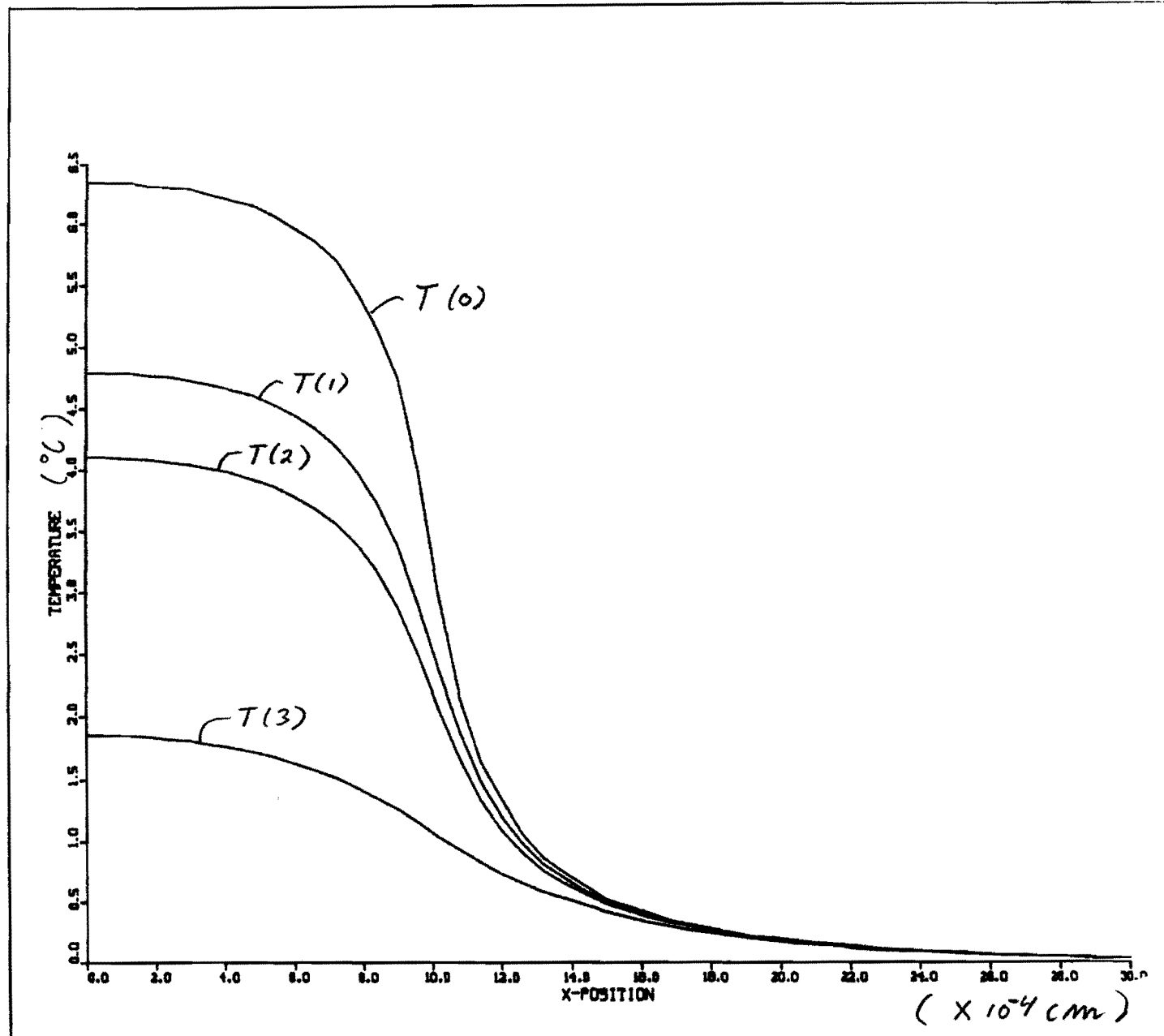


Fig. 5.6

Fig. 6.a



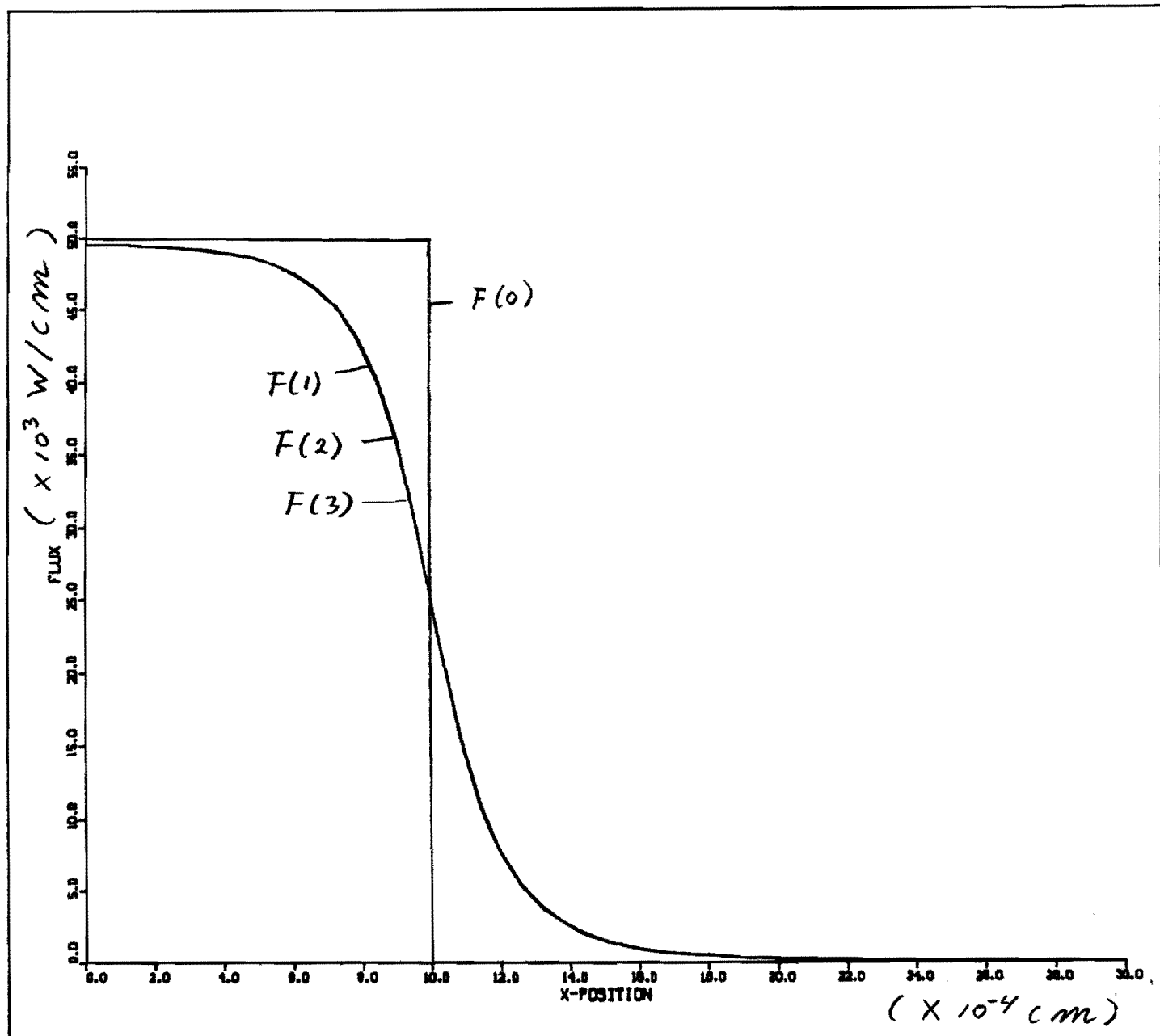
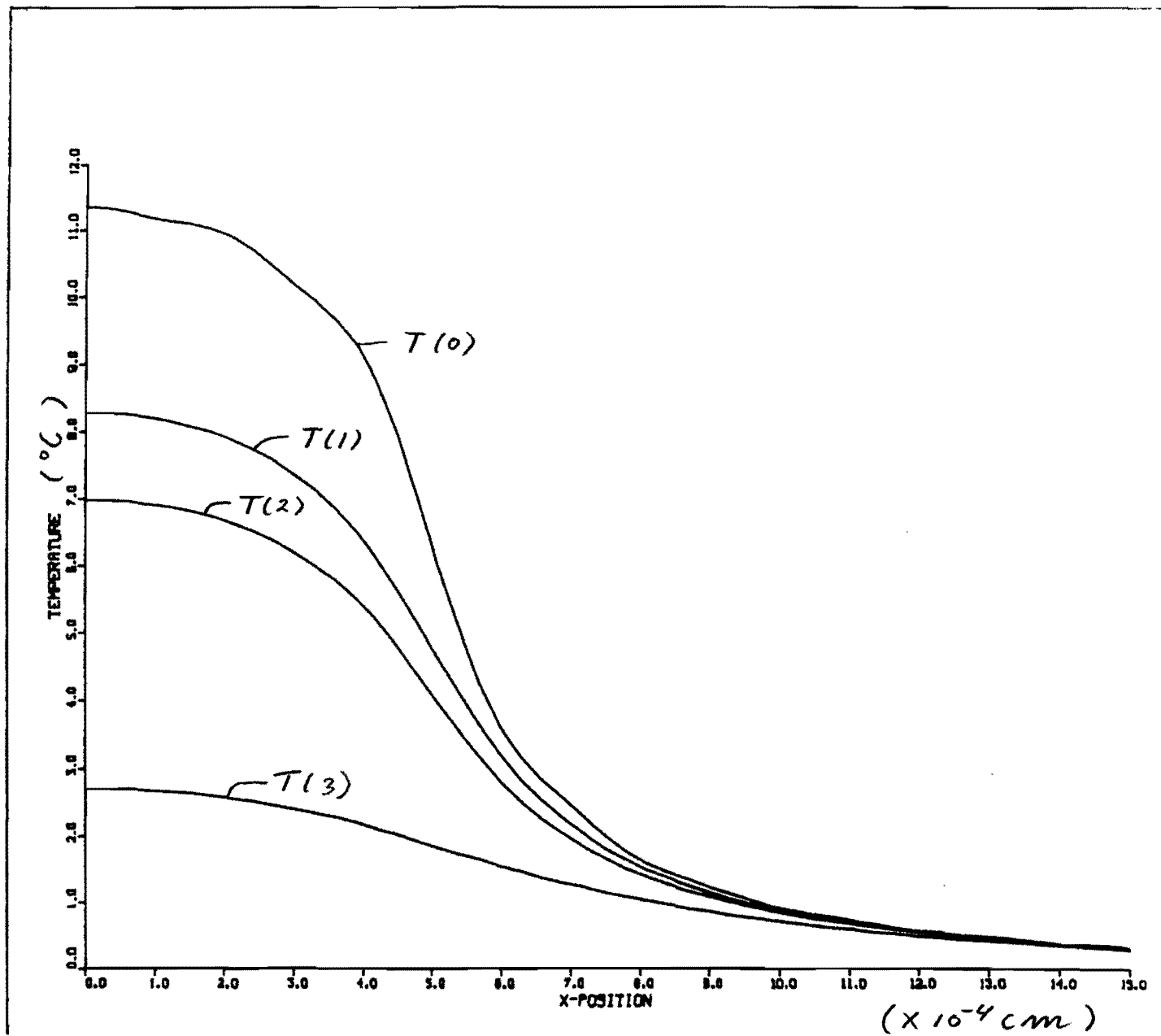


Fig. 6.6

Fig. 7.a





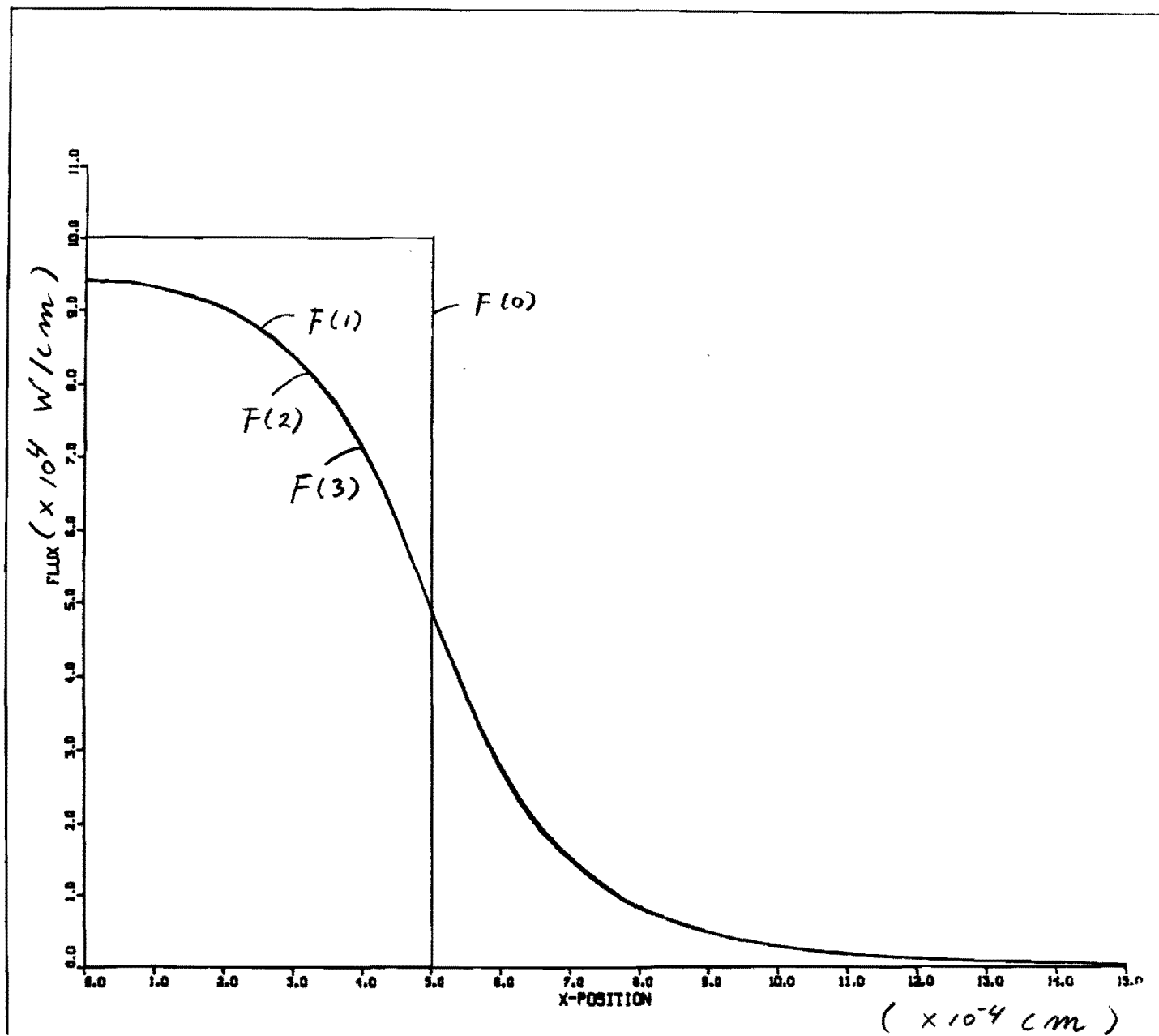
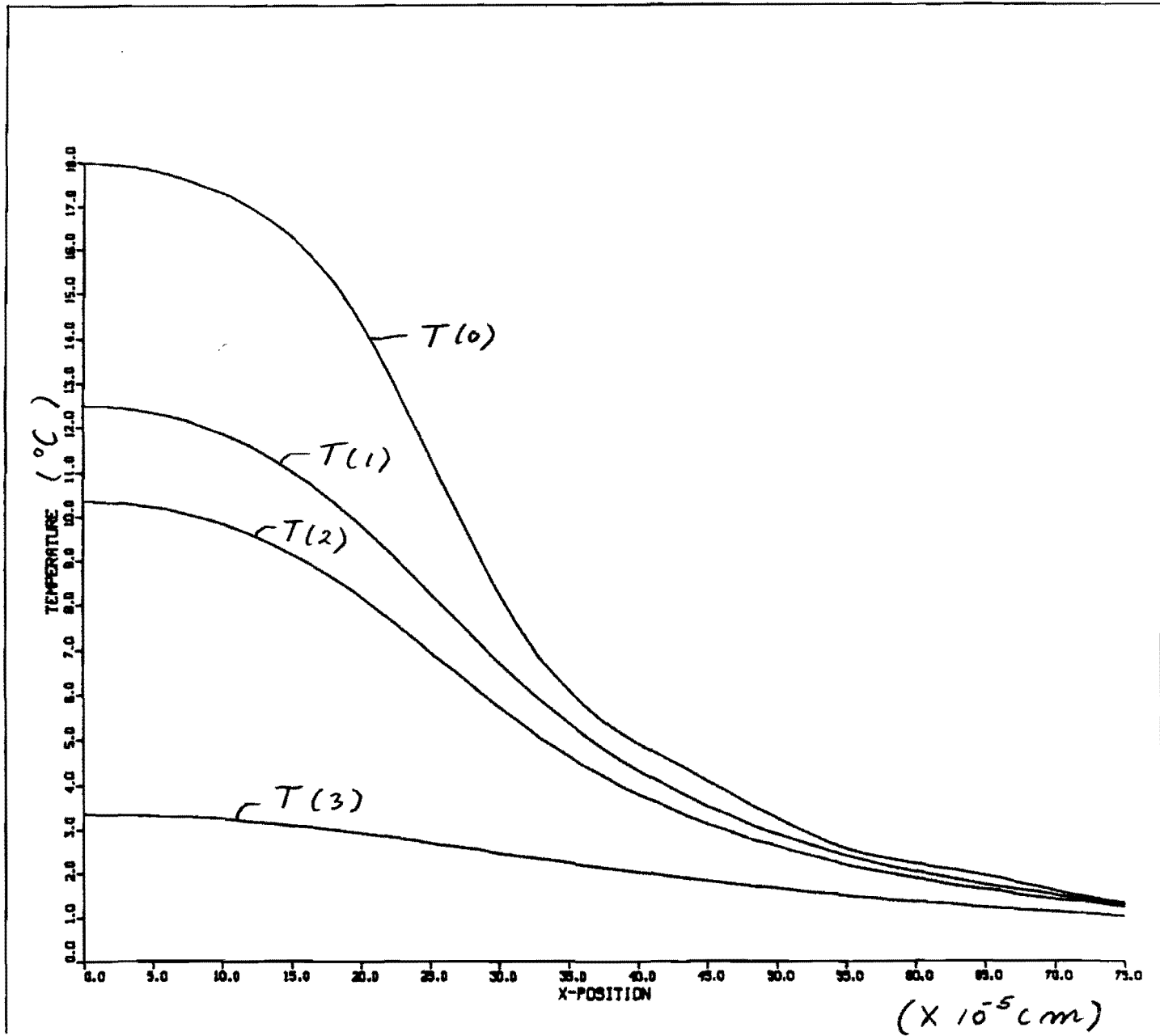


Fig. 7.6

Fig. 8.a



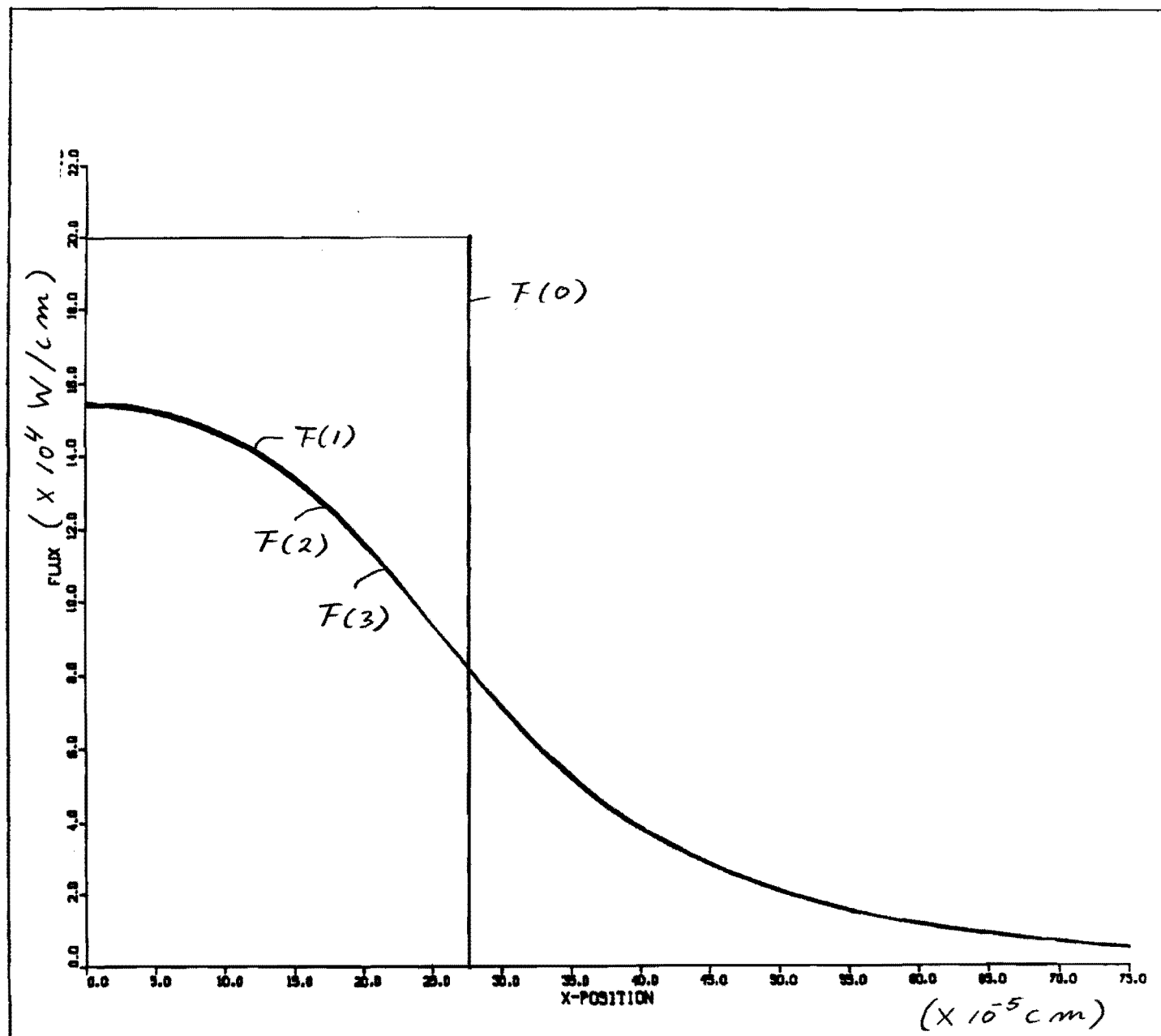
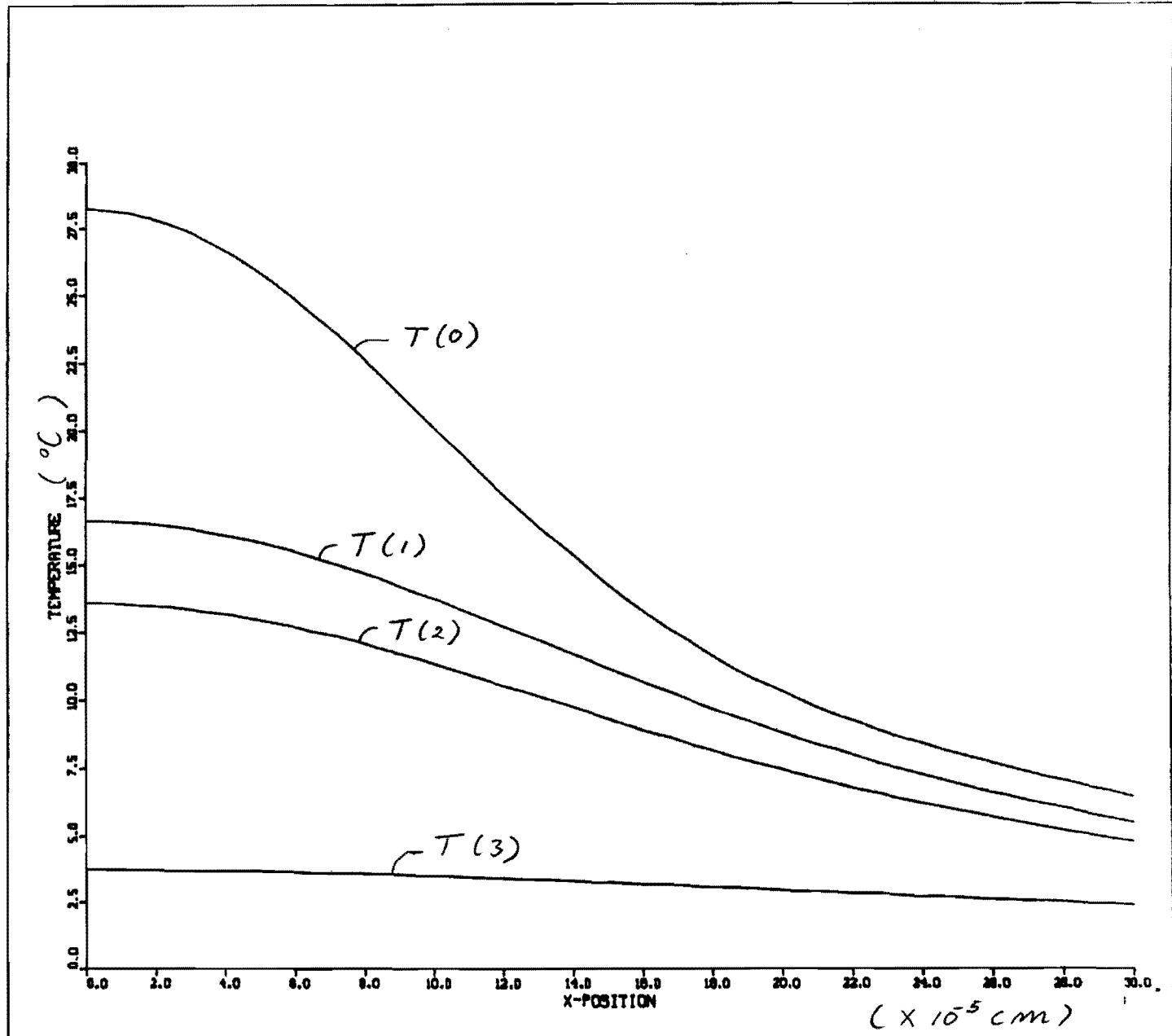


Fig. 8.6

Fig. 9.a



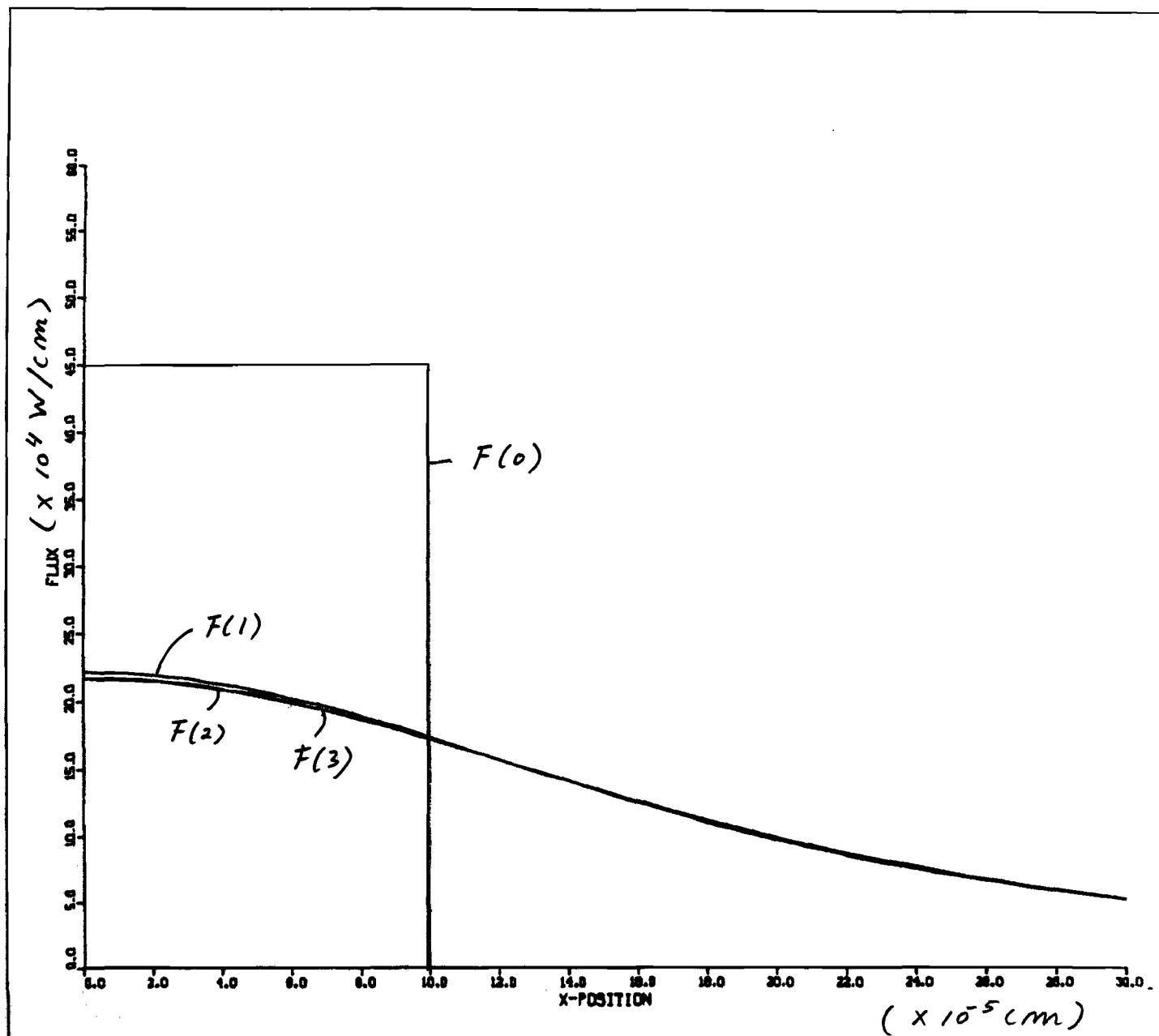
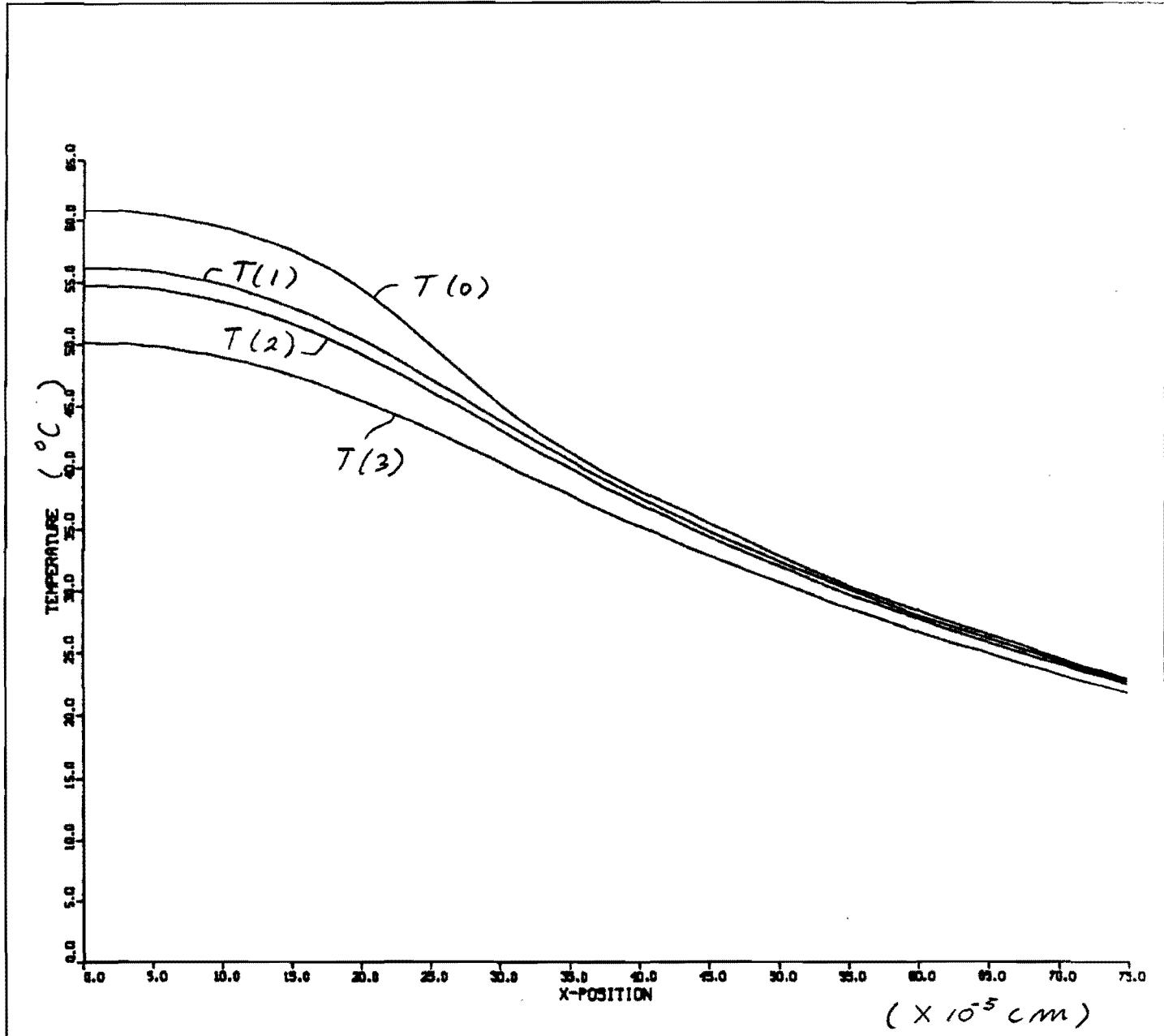


Fig. 9.6

Fig. 10.a



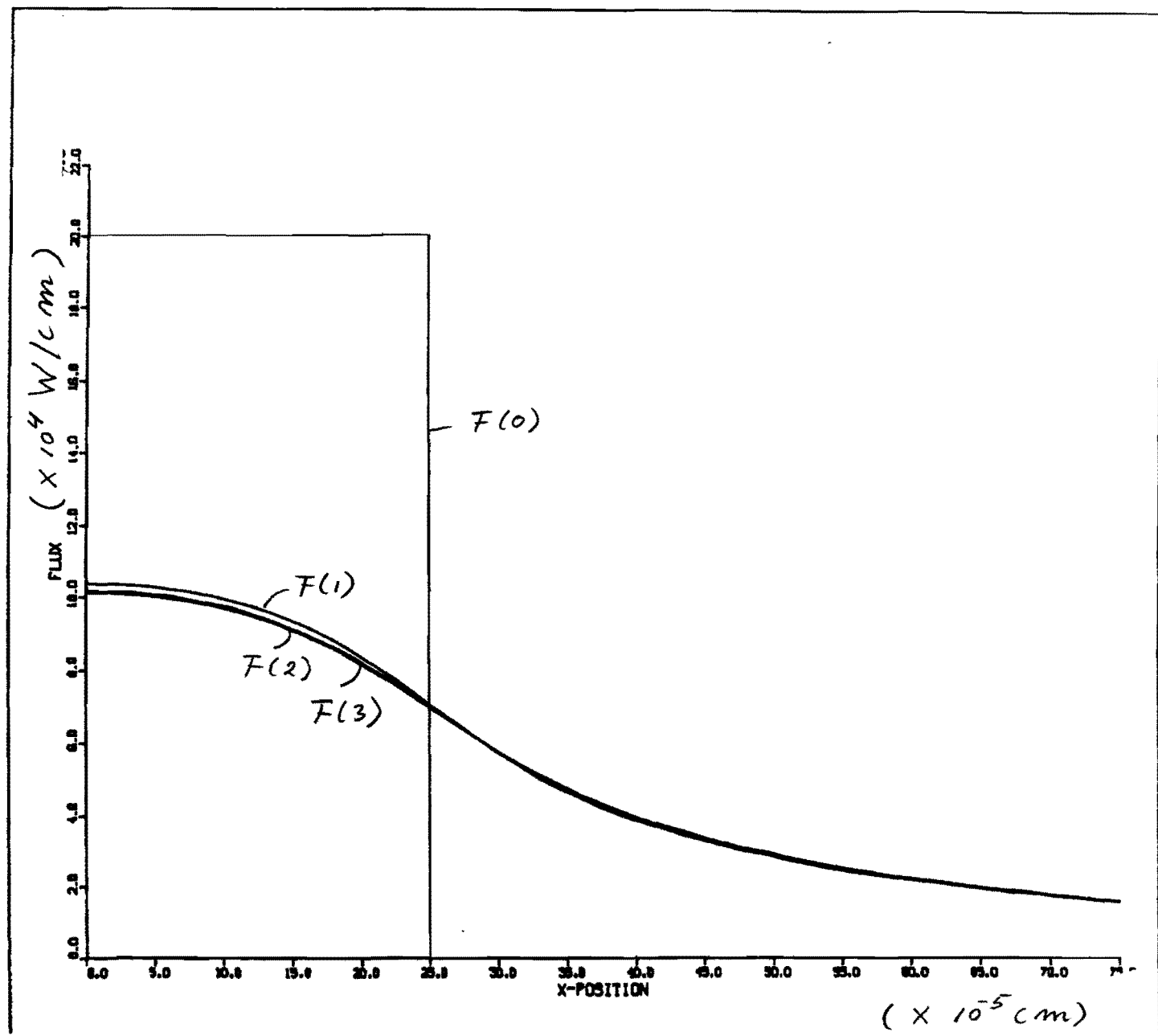
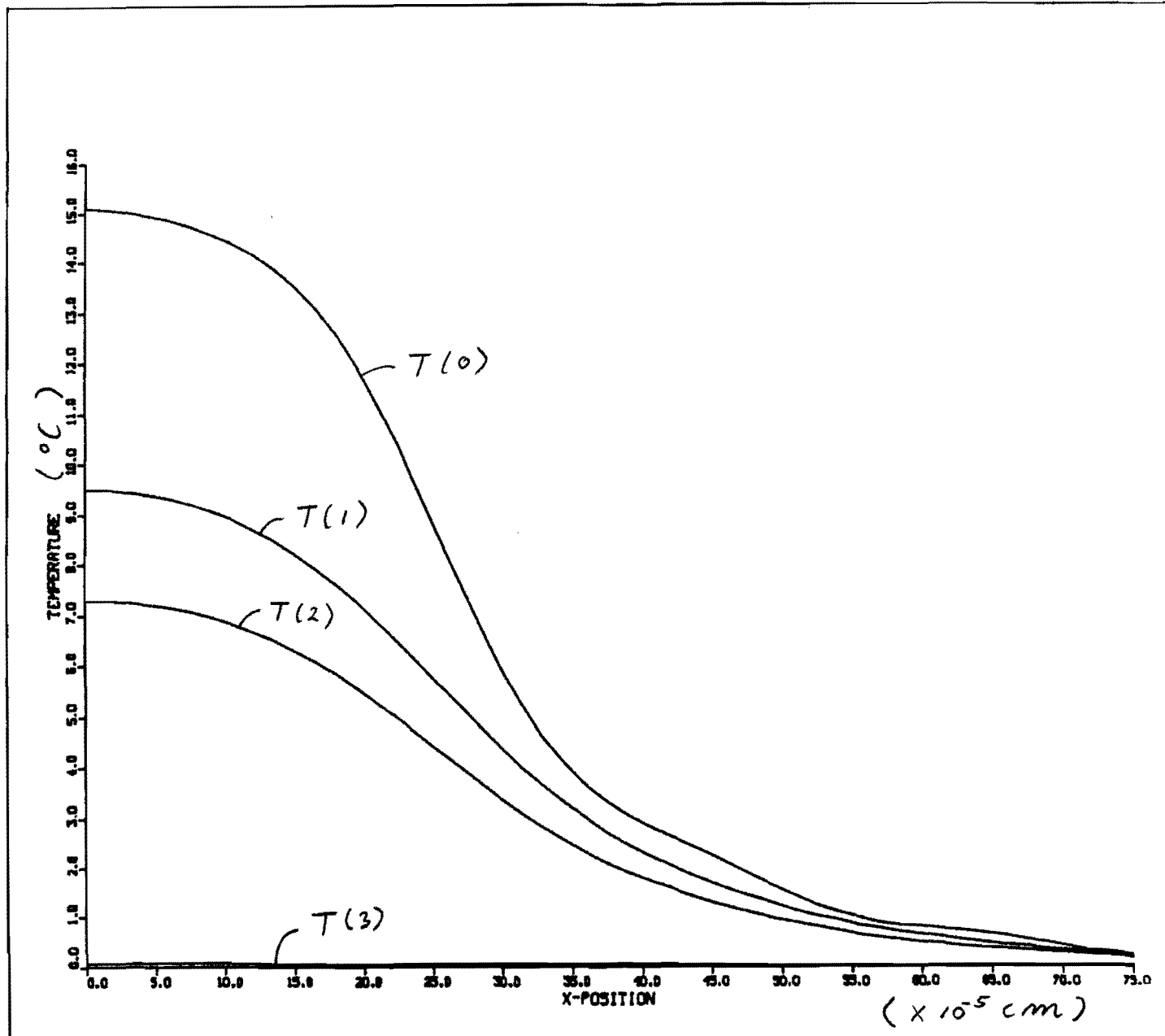


Fig. 10.6

Fig. 11.a





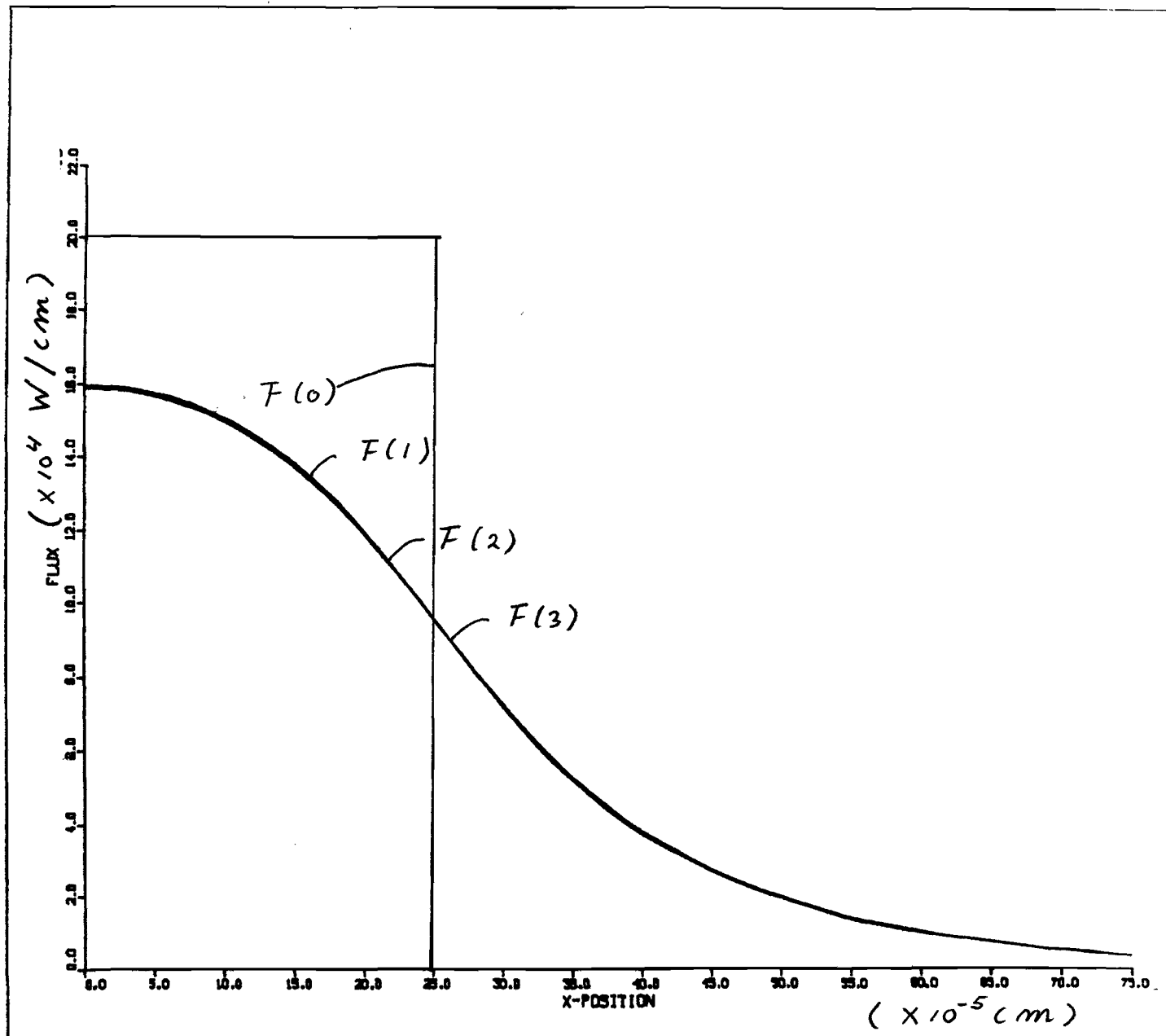


Fig. 11.6