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NATIONAL BUREAU OF STANDARDS REPORT

9646

A REVIEW OF THE STATUS OF

FIRE PREFORMANCE PREDICTIVE METHODS

by

Stanley P Rodak; Physicist, Heat

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

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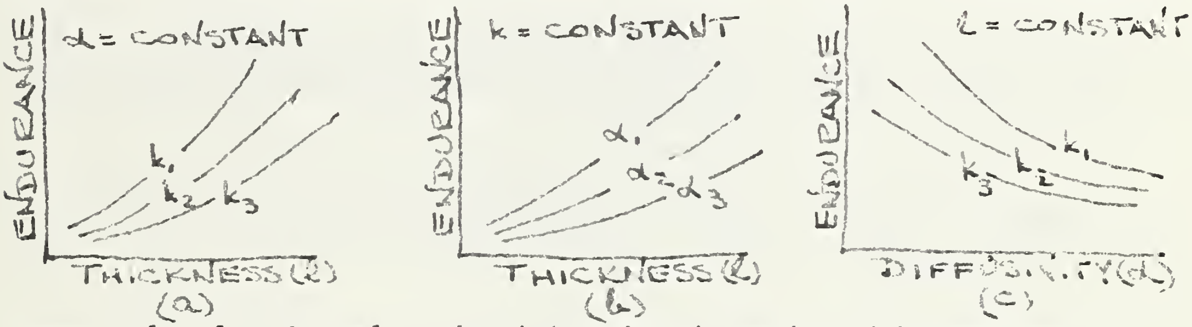
The problems of fire-resistance have attracted the attention of various workers. This project is concerned with the theoretical aspects of fire resistance. From a knowledge of the thermal propertities of a building material shaped into a particular geometry, we wish to be able to predict the thermal fire rating** of scaled constructions of the same material. Ideally, we would like the calculations techniques to include variable thermal properties and endothermic and exothermic processes.

In order to circumvent certain numerical difficulties in using variable thermal properties, it was felt that sufficient information would be had if the calculations are made in a manner that will allow the information to be displayed in the following fashion. Giedt (1) has suggested



a mean value for thermal conductivity when it varies with temperature.

Endothermic and Exothermic processes are to be disregarded until the numerical techniques are sufficiently developed.

The mathematical equations to be used are as follows:

parabolic equation of heat flow* $$\left(\nabla^2 - \alpha\frac{\partial}{\partial t}\right) T = 0 \qquad (1)$$

boundary condition $$k\frac{\partial T}{\partial n} = -hT \qquad (2)$$

(n is the normal surface component)

* Nomenclature is at end of text.

** The thermal fire rating will be taken as the time before the temperature in a region in the specimen under consideration reaches a value predetermined to be unsafe for fire-resistance purposes.

The mathematical model which we will work with is a homogeneous solid bounded by two parallel planes. The problem will be two-dimensional.

Over one surface, the exposed surface, we define a temperature rise by

$$T(o,y,t) = f_o\ (t) \tag{3}$$

where $f_o\ (t)$ is the ASTM time-temperature curve.

On the other surface, the unexposed surface, the heat flux is that for a horizontal surface (2,3)

$$h = h_n + h_c \tag{4}$$

$$h_n = (.174\epsilon/(T_s-T_o)) \cdot ((T_s/100)^4 - (T_o/100)^4) \tag{5}$$

$$h_c = .275\ T_s^{\ 1/3} \tag{6}$$

For a high, vertical surface, h_c would still be proportional to $T^{1/3}$, but the coefficient changed (3,4). The mechanism of transpiration cooling was not considered (5).

The numerical technique we choose should be accurate enough to calculate temperatures for our test example (6, pg 126).

TEST CASE:

The region $o<x<\ell$ has zero initial temperature. The end $x=o$ is kept at temperature T_o for $t>o$. At $x=\ell$ there is radiation into a medium at zero temperature; then, temperatures for $o<x<\ell$ are given by

$$T(x,\ell) = T_o \quad \frac{1+\ell h(i-x/\ell)}{1+\ell h} - \sum_{n=1}^{\infty} \frac{2(\beta_n^2 + (\ell h)^2 \sin(\beta_n x/\ell}{\beta n\ (\ell h+(\ell h)^2+\beta_n^2)}\ e^{-\beta_n^2}\ \left(\frac{\alpha t}{\ell^2}\right) \tag{7}$$

where β_n are the positive roots of $\beta_n \cot \beta_n + \ell h = 0$.

The exponential term causes the series to converge rapidly.

Three finite-difference methods of approximating the partial differential equations have been studied.

The first studied was the forward-difference explicit algorithm (8):

$$\rho c \Delta x^2 \left(T_{i,j}^{k+1} - T_{i,j}^{k}\right) = k\,\Delta t \left(T_{i-1,j}^{k} + T_{i+1,j}^{k} + T_{i,j-1}^{k} + T_{i,j+1}^{k} - 4T_{i,j}^{k}\right) \quad (8)$$

Here, $\Delta Y = \Delta X$

For a slab $N\Delta X$ thick and $M\Delta Y$ tall,

$$T_{i,j}^{k} = f_o(k\Delta t) \qquad j = 1,\ 2,\ \ldots,\ m \quad (9)$$

is the temperature on the exposed surface at the k^{th} interval of time*.

The requirement that $\Delta t/\Delta x^2$ be chosen such that

$$\frac{k\Delta t}{\rho c \Delta x^2} < \frac{1}{4} \quad (10)$$

in order to have stability, that is, the finite-difference algorithm is immune to the accumulation of round-off errors (7), caused a survey of other methods (metal rods were to be imbedded in the test example interior).

The backward difference implicit algorithm (8) is defined by

$$\rho c \Delta x^2 \left(T_{i,j}^{k+1} - T_{i,j}^{k}\right) = k\,\Delta t \left(T_{i-1,j}^{k+1} + T_{i+1,j}^{k+1} + T_{i,j-1}^{k+1} + T_{i,j+1}^{k+1} - 4T_{i,j}^{k+1}\right) \quad (11)$$

This method is stable for all values of $\Delta t/\Delta x^2$. Iterative and matrix reduction techniques are available to solve the resulting unknown equations (9,10,11,12). For a solid of N interior points in each direction, N^2 equations result for the two-dimensional problem.

The backward-difference implicit algorithm was applied to a particular problem: finite thick slab exposed on one surface to temperature

* To meet the boundary condition (2), we replace $(T_{i+1,j}^{k} - T_{i,j}^{k})$ by $-\frac{h}{k}\Delta x T_{i,j}^{k}$ and multiply $(T_{i,j+1}^{k} - T_{i,j}^{k})$, $(T_{i,j-1}^{k} - T_{i,j}^{k})$ & $(T_{i,j}^{k+1} - T_{i,j}^{k})$ by 1/2 in equation 8. The unexposed surface is at $i = \frac{\ell}{\Delta x} + 1$; $i = 1$ is the exposed surface, we make a similar replacements in (11) and (12) to meet boundary conditions of (2).

$f_o(t)$, unexposed surface has constant "cooling" coefficient h_o, metal rods were placed 1" from exposed face. The equations were solved for each successive time increment (Δt = 1 min., $\Delta x = \Delta y$ = .2") by Gauss Siedel Iteration*. Figs. 1 & 2 are graphs of the computer solved problem.

Fig. 2 contains two different profiles of the distance from exposed slab surface versus temperature. One profile is taken along a line ($\overline{AA'}$) normal to the slab surface and passing through one of the steel rods. The other is along a line ($\overline{BB'}$), parallel to $\overline{AA'}$, but about 3" from the steel rod (the steel rods imbedded in the concrete slab were on 6" centers). Temperatures at 30 min., 50 min., and 210 min., intervals along the line AA' from 0 to .8" have negative curvature (13). This is not the correct slope (14).

The Crank-Nicolson algorithm (15) is reported to be unconditionally stable (16). It is obviously based on sounder physical arguments than the two previous methods. The algorithm is

$$\rho c \Delta x^2 \; (T^{k+1}_{i,j} - T^{k}_{i,j}) = (k\Delta t/2) \cdot (T^{k+1}_{i-1,j} + T^{k+1}_{i+1,j} + T^{k+1}_{i,j-1} + T^{k+1}_{i,j+1} +$$

$$T^{k}_{i-1,j} + T^{k}_{i+1,j} + T^{k}_{i,j-1} + T^{k}_{i,j+1} - 4T^{k+1}_{i,j} - 4T^{k}_{i,j}) \qquad (12)$$

The same test case (metal rods imbedded in a slab as used for the backward difference implicit algorithm was used to test this algorithm. Graphs of the computer solved problem are displayed in Fig. 3 & 4. The distance-temperature curves in Fig. 4 have the proper curvature.

As a precursory check of the Crank-Nicolson algorithm, it was used to calculate surface temperatures of the test example (homogeneous solid bounded by parallel planes). The resulting surface temperature calculations, as well as those predicted by theory, are displayed in Fig. 5. The surface temperatures differ by 30% at 100 minutes.

In order to make the Crank-Nicolson difference approximation more closely approximate the differencials, equations were derived that allow the Δx spacing to vary in an unequal manner through the slab; the spacing Δy is equal. This would allow a fine grid near the unexposed surface, where the temperatures vary more slowly with time. Note 2 discusses how a grid spacing was chosen for .1% "accuracy."

Another problem was encountered, for the above example used as a check in the variable Δx computer program, interior temperatures were higher than surface temperatures ($T^{k}_{i,j} = 100\ ^{o}F$, $k = 1, \ldots; j = 1, 2, \ldots M_o$)

* The equation showed diagnol-dominance, hence the choice of Gauss-Siedel Iteration techniques. See Note 1 for termination procedures.

The algorithm values had definitely converged($T^1_{1,j} < T^2_{2,j} \cong 139.9\ ^oF$ after 60 iterations). The conditions under which this algorithm will converge to values greater than the exposure surface temperatures (and hence apparently violate the first law of thermodynamics) are discussed in Note 3. This discussion is for $T^2_{i,j} < T^2_{2,j}$ where the "initial iteration quess" of $T^2_{i,j} = 0 \quad i = 2, \ldots, x_oj \quad j = 1, 2 \ldots, Y_o$. We also found that similar unstable conditions (i.e. $T^2_{i,j} < T^2_{2,j}$) occurred even if the initial iteration quess was $T^2_{i,j} = T^2_{i,j}$ or even if $T^2_{i,j}$ were assigned their exact values as predicted from theory (the convergence of $T^2_{2,j}$ was still 140 ^oF).

The present status of the project is to circumvent this problem. It may be that the constraints involved in keeping the Crank-Nicolson algorithm from violating the first law, a Δt several orders of magnitude smaller will have to be used.

NOMENCLATURE*

h	surface film coefficient
h_c	convection heat-transfer film coefficient
h_n	radiation heat transfer film coefficient
k	conductivity
l	thickness
T	temperature
T_o	unexposed surface temperature
T_s	exposed surface temperature
$T^k_{o,i}$	finite-difference notation for temperature at K^{th} time increment, x coordinate of $i\Delta x = \Delta x$ and y coordinate $j\Delta y = j\Delta x$.
t	time
x, y	space coordinates
∂	differsivity
ϵ	surface emissivity
ρ	density
$\Delta x, \Delta y$	finite division of x or y coordinate
Δt	finite division of time

* Units are English

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Note 1

A DISCUSSION OF WHEN TO TERMINATE CALCULATIONS OF $T^{k+1}_{i,j}$ BY GAUSS-SIEDEL ITERATION*

Consider the equations

$$(4 + \frac{2\Delta x^2 \rho c}{k \Delta t}) T^{k+1}_{i,j} = T^{k+1}_{i-1,j} + T^{k+1}_{i+1,j} + T^{k+1}_{i,j+1} + T^{k+1}_{i,j-1} + a^o{}_{i,j} \qquad (1)$$

$$(\frac{\Delta x^2 \rho c}{k \Delta t} + \Delta x \frac{h}{k} + 2) T^{k+1}_{i,j} = T^{k+1}_{i-1,j} + \frac{1}{2} (T^{k+1}_{i,j-1} + T^{k+1}_{i,j+1}) + a^1{}_{i,j} \qquad (2)$$

where

$$a^o{}_{i,j} = T^k_{i-1,j} + T^k_{i+1,j} + T^k_{i,j+1} + T^k_{i,j-1} - 4T^k_{i,j}$$

$$a^1{}_{i,j} = T^k_{i-1,j} + \frac{1}{2} (T^k_{i,j-1} + T^k_{i,j+1}) + (\frac{\Delta x^2 \rho c}{k \Delta t} - \Delta x \frac{h}{k} - 2) T^k_{i,j}$$

Equation 1 is the Crank-Nicolson (CN) algorithm for finding interior temperatures of a solid bounded by two infinite parallel planes. Equation 2 is the CN algorithm for the unexposed surface temperatures. (The solid is $N\Delta x$ thick and $M\Delta y$ tall ($\Delta x = \Delta y$)). Since the equations are diagonally dominate, Gauss-Siedel Iteration techniques are used to solve the $N \cdot M$ unknown $T^{k+1}_{i,j}$ ($i = 2,3, \ldots, N+1$; $j = 1,2,3, \ldots, M$; $i = 1$ is the unexposed surface).

All $T^k_{i,j}$ and $T^{k+1}_{i,j}$ are known.

As an initial start to the iteration, all $T^{k+1}_{i,j}$ are set equal to zero. Equation 1 is used to calculate $T^2_{2,1}$. This new value of $T^2_{2,1}$ is used now in the calculation of $T^2_{2,2}$. The iteration process of replacing the old values of $T^{k+1}_{i,j}$ by the newly calculated values of $T^{k+1}_{i,j}$ continues methodically by working through the $j = 1,2, \ldots M$ for

---

* The method of determining the termination of the calculations is mainly from (21). See also (9).

each i index until a new set of $T_{i,j}^{k+1}$ have been iterated.

Let

$$\Delta T_{i,j}^{n} = (T_{i,j}^{k+1} \text{ (nth iteration)} - T_{i,j}^{k+1} \text{ (n-1 iteration)}$$

(In the following discussion, it is convenient to consider only values of $n > 3$.)

For our diagonally dominate matrix, $\Delta T_{i,j}^{n}$ should become small after a finite number of iterations. That is, we assume

$$\lim_{n \to \infty} \Delta T_{i,j}^{n} = 0 \qquad \begin{array}{l} i = 2,3,\ldots,N \\ j = 1,2,\ldots,M \end{array}$$

In practice, this process must be terminated after a finite number of iterations (i_o). This is called truncating. Let $S_{i,j}$ be the "exact" temperature value at $[(i+1)\Delta x, j\Delta y]$. The radius of convergence is given by ($T_{i,j}^{k+1}$ in this formula assumes the value of the i_o iteration):

$$\left| T_{i,j}^{k+1} - S_{ij} \right| < \frac{L^{i_o}}{1-L} \Delta T_{i,j}^{3}$$

where*

$$L = \sup_{n=3}^{\infty} \left| \sup_{\substack{i = 2,3\ldots,N \\ j = 1,2\ldots,M}} \left| \frac{\Delta T_{i,j}^{n+1}}{\Delta T_{i,j}^{n}} \right| \right|$$

That is, for the (i+1) iteration, we find the maximum value $\lambda\tau$ of the ratio $\left| \frac{\Delta T_{i,j}^{\tau+1}}{\Delta T_{i,j}^{\tau}} \right|$.

$$\lambda_{\tau} = \sup_{\substack{i = 2,3,\ldots,N \\ j = 1,2,\ldots,M}} \left| \frac{\Delta T_{i,j}^{\tau+1}}{\Delta T_{i,j}^{\tau}} \right|$$

* reference 13, pg 9

From the set of λ_τ $(3 < \tau < \infty)$, we again find the maximum value L.

$$L = \sup_{\tau=3}^{\infty} \lambda$$

In practice, an approximate value of L is obtained from the set of λ_τ of the first ten iterations.

Note 2

GRID SIZE DETERMINATION

The following houristic method of arriving at an equation to determine the proper grid size to use in one-dimensional finite difference equations was described by Dr. Arms (21). We can extend the results to two-dimensional problems. Let $f_{\Delta x}$ $((i+1)\ \Delta x)$ be the iterative temperature value for grid size Δx. Call $f((i+1)\ \Delta x)$ the "exact" value. Then, in an approximate manner,

$$f_{\Delta x}\ ((i+1)\Delta x) = f((i+1)\ \Delta x) + \Delta x^2 . \bar{A}$$

$\bar{A}$ can be thought of as an operator. (The series expansion was terminated on the first term). Taking a grid size of $\Delta x/2$

$$f_{\Delta x/2} = f + \frac{\Delta x^2 .}{4} \bar{A}$$

or

$$\frac{f_{\Delta x} - f\ \Delta x/2}{\frac{3}{4}\ \Delta x^2} = \bar{A} \ + \text{2nd order terms.}$$

By doing the same problem for two different grid sizes, $\bar{A}$ can be determined (we neglect the 2^{nd} order terms), and hence the proper variable grid spacing for the desired degree of accuracy.

Note 3

A DISCUSSION OF THE CONSTRAINTS IMPOSED ON CRANK-NICOLSON FINITE-DIFFERENCE ALGORITHM BY GAUSS-SIEDEL ITERATION

Consider a solid (ℓ thick) bounded by two parallel planes. On one surface, there is a sudden temperature rise T_s for $t>0$. The initial temperature of the solid is zero. Using Crank-Nicolson difference equations, we wish to find the interior temperatures at time Δt. Gauss-Siedel Iteration will be used to solve for $T^2_{i,j}$. As a first quess set all $T^2_{i,j}$ equal to zero. The equations for a variable Δx and Δy are:

$$\sum_{i=1}^{N} \Delta x_i = \ell$$

i=1

exposed
surface
($T^k_{i,j} = T_s$
for $t>o$)

inside solid:

$$\left(\frac{\rho c \Delta y^2}{k \Delta t} + \frac{\Delta y^2}{\Delta x_1(\Delta x_1+\Delta x_2)} + \frac{\Delta y^2}{\Delta x_2(\Delta x_1+\Delta x_2)} + 1\right) T^{k+1}_{i,j}$$

$$= \frac{\Delta y^2}{\Delta x_1(\Delta x_1 + \Delta x_2)} T^{k+1}_{i-1,j} + \frac{\Delta y^2}{\Delta x_2(\Delta x_1 + \Delta x_2)} T^{k+1}_{i+1,j} + \frac{1}{2} \left(T^{k+1}_{i,j-1} + T^{k+1}_{i,j+1}\right) + a_{i,j} \qquad (1)$$

$$a_{i,j} = \frac{\Delta y^2}{\Delta x_1(\Delta y_1 + \Delta x_2)} T^{k}_{i-1,j} + \frac{\Delta y^2}{\Delta x_2(\Delta x_1 + \Delta x_2)} T^{k+1}_{i+1,j} + \frac{1}{2} \left(T^{k+1}_{i,j-1} + T^{k}_{i,j+2}\right) + \left(\frac{\rho c \Delta y^2}{k \Delta t} - \frac{\Delta y^2}{\Delta x_1(\Delta x_1 + \Delta x_2)} - \frac{\Delta y^2}{\Delta x_2(\Delta x_1 + \Delta x_2)} - 1\right) T^{k}_{i,j}$$

at surface $k = \ell$

$$T^{k}_{i+1,j}$$

$$(1 + \frac{\Delta y^2}{\Delta x_1} \frac{h}{k} + (\frac{\Delta y}{\Delta x_1})^2 + \frac{\rho x \Delta y^2}{k \Delta t}) T^{k+1}_{i,j} =$$

$$(\frac{\Delta y}{\Delta x_1})^2 T^{k+1}_{i-1,j} + \frac{1}{2} (T^{k+1}_{i,j-1} + T^{k+1}_{i,j+1}) + a_{i,j} \qquad (2)$$

$$a_{i,j} = (\frac{\Delta y}{\Delta x_1})^2 T^{k}_{i-1,j} + \frac{1}{2} (T^{k}_{i,j-1} + T^{k}_{i,j+1}) + (\frac{\rho c}{k \Delta t} \Delta y^2 - (\frac{\Delta y}{\Delta x_1})^2 -$$

$$\frac{\Delta y^2}{\Delta x} \frac{h}{k} - 1) T^{k}_{i,j}$$

let $\Delta x_1 = \Delta x_i \neq \Delta y \qquad i = 2, \cdot\cdot, m.$

Equation (1) then becomes (noting for our case $a_{ij} = 0$):

$$T^{k+1}_{i,j} = \beta [\omega (T^{k+1}_{i-1,j} + T^{k+1}_{i+1}) + (T^{k+1}_{i,j-1} + T^{k+1}_{i,j+1})] \qquad (3)$$

Where $\beta = (\frac{2\rho c \Delta y^2}{k \Delta t} + 2(\frac{\Delta y}{\Delta x})^2 + 2)^{-1} < 1$

$$\omega = (\frac{\Delta y}{\Delta x})^2$$

Let us introduce some symmetry into the boundry condition:

$$T^{k}_{i,1} \equiv T^{k}_{i,3}$$

Then the first iteration is:

$$T^{2}_{2,2} = \omega\beta T_s$$

$$T^2_{2,3} = \beta\omega T_s \ (1 + \beta) = T^2_{2,1}$$

$$T^2_{2,4} = \beta\omega T_s \ (1 + \beta + \beta^2)$$

$\cdot$
$\cdot$
$\cdot$

$$T^2_{2,m} = \beta\omega T_s \ (1 + \beta + \beta^2 + \ldots + \beta^{m-2}) = \beta\omega T_s \ (\frac{1-\beta^{m-1}}{1-\beta})$$

$$T^2_{3,2} = \beta^2\omega^2 T_s$$

$$T^2_{3,3} = \beta^2\omega^2 T_s \ (1 + 2\ \beta)$$

$$T^2_{3,3} = \beta^2\omega^2 T_s \ (1 + 2\beta + 3\beta^2)$$

$\cdot$
$\cdot$
$\cdot$

$$T^2_{3,m} = \beta^2\omega^2 T_s \ [1 + 2\beta + 3\beta^2 + \ldots + (m-1)\ \beta^{m-2}] = \frac{1-\beta^{m-1}-(m-1)\beta^m}{(1 - \beta)^2}$$

etc.

second iteration:

$$T^2_{2,2} = \beta\ [\omega T_s + \beta^2\omega^3 T_s + 2\beta\omega T_s (1 + \beta)]$$

$$= \beta\omega T_s \quad (+ 2\beta + 2\beta^2 + \beta^2\omega^2) < 1$$

For the various heat-conclusion problems under study, this type of analysis was used to understand the constraints imposed on the iteration techniques. It was found that when the constraints were violated, there was convergence of the $T^{k+1}_{i,j}$ (all equations had diagonal dominance), but the $T^{k+1}_{i,j}$ were larger than T_s for several Δx_i from the exposed surface $(T^k_{i,j})$.

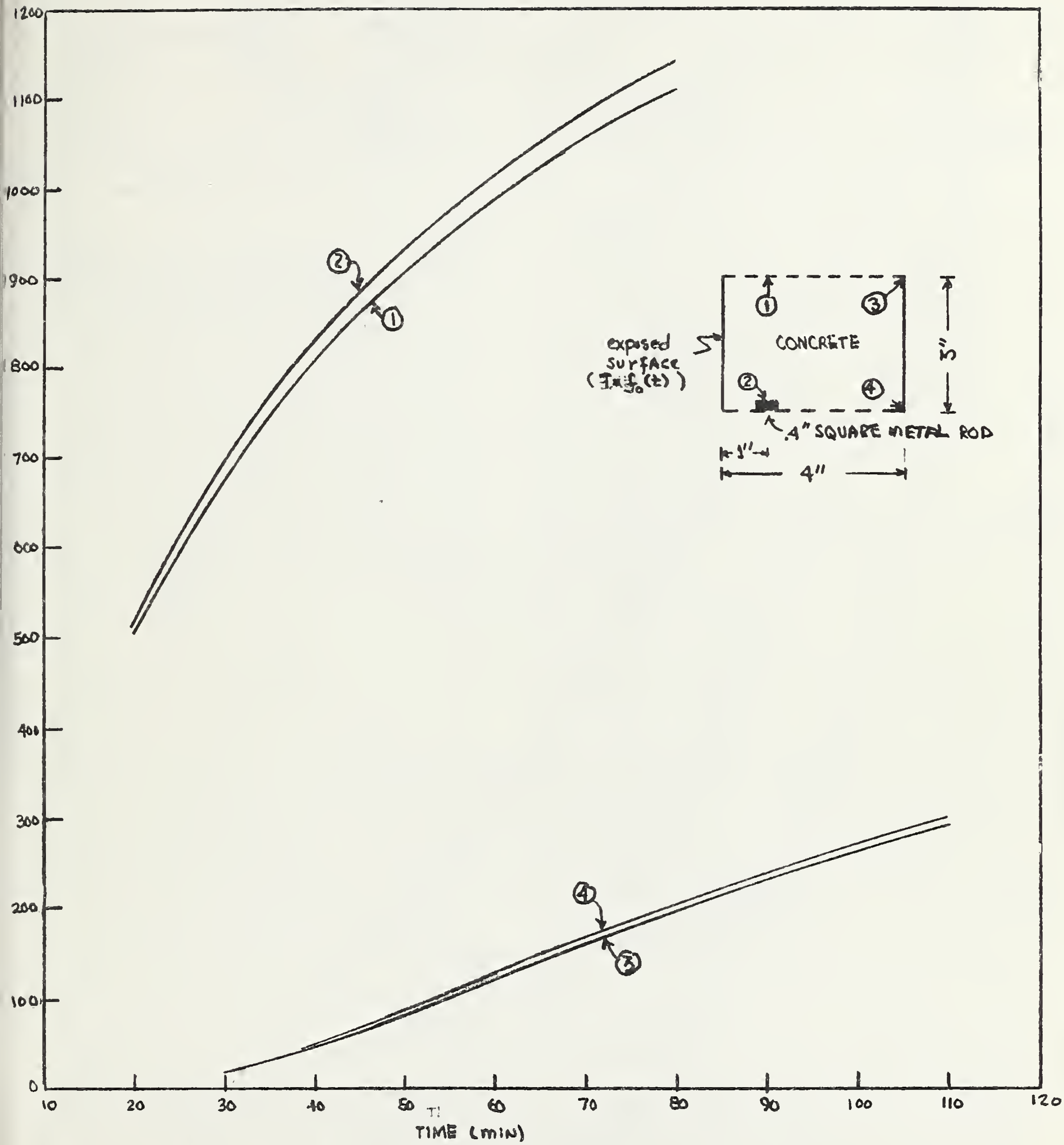

FIG. 1 — BACKWARD DIFFERENCE IMPLICIT CALCULATIONS

NOTE: CONCRETE: $K = .5327$; $\rho = 143.6$, $C = .23$
Steel: $K = 26.6$, $\rho = 490$, $C = .113$
$\Delta x = .2''$, $\Delta t = 1$ min, $\epsilon = .94$

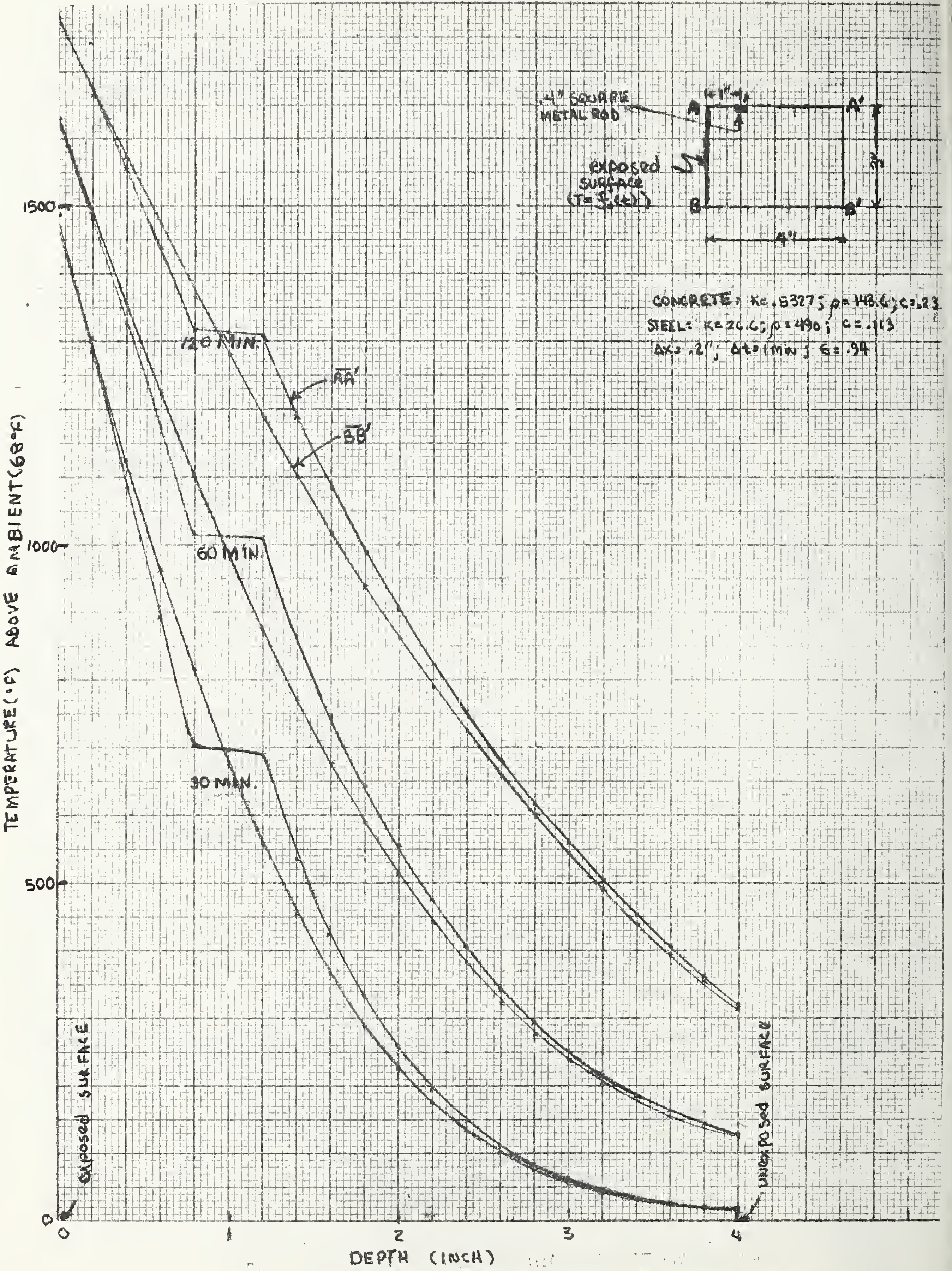

FIG. 2 - BACKWARD DIFFERENCE IMPLICIT CALCULATIONS

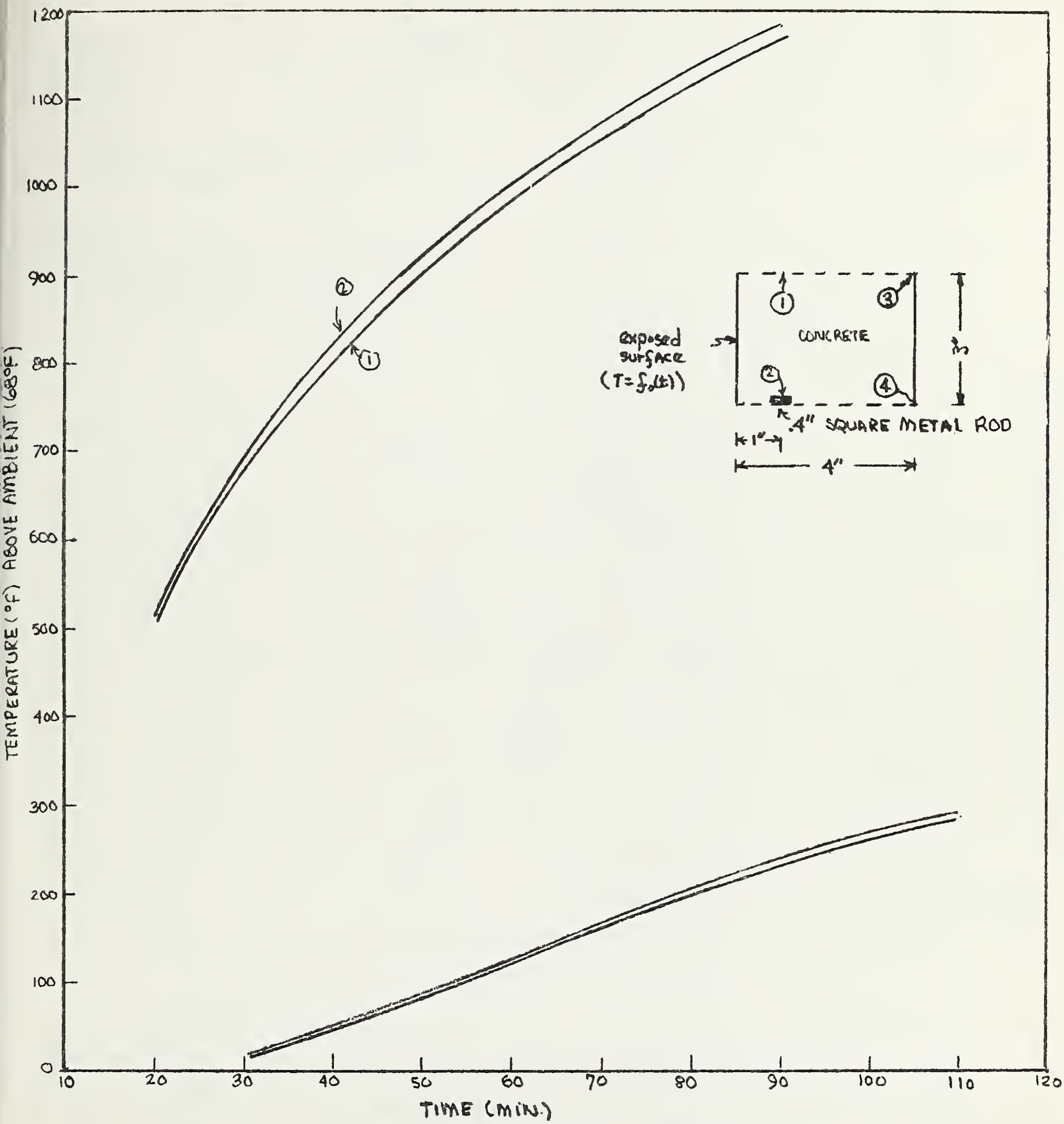

FIG. 3 - CRANK-NICOLSON DIFFERENCE CALCULATIONS

NOTE: CONCRETE: $K = .5327$; $\rho = 143.6$, $C = .23$
STEEL: $K = 26.6$, $\rho = 490$, $C = .113$
$\Delta x = .2''$, $\Delta t = 1$ min, $\epsilon = .94$

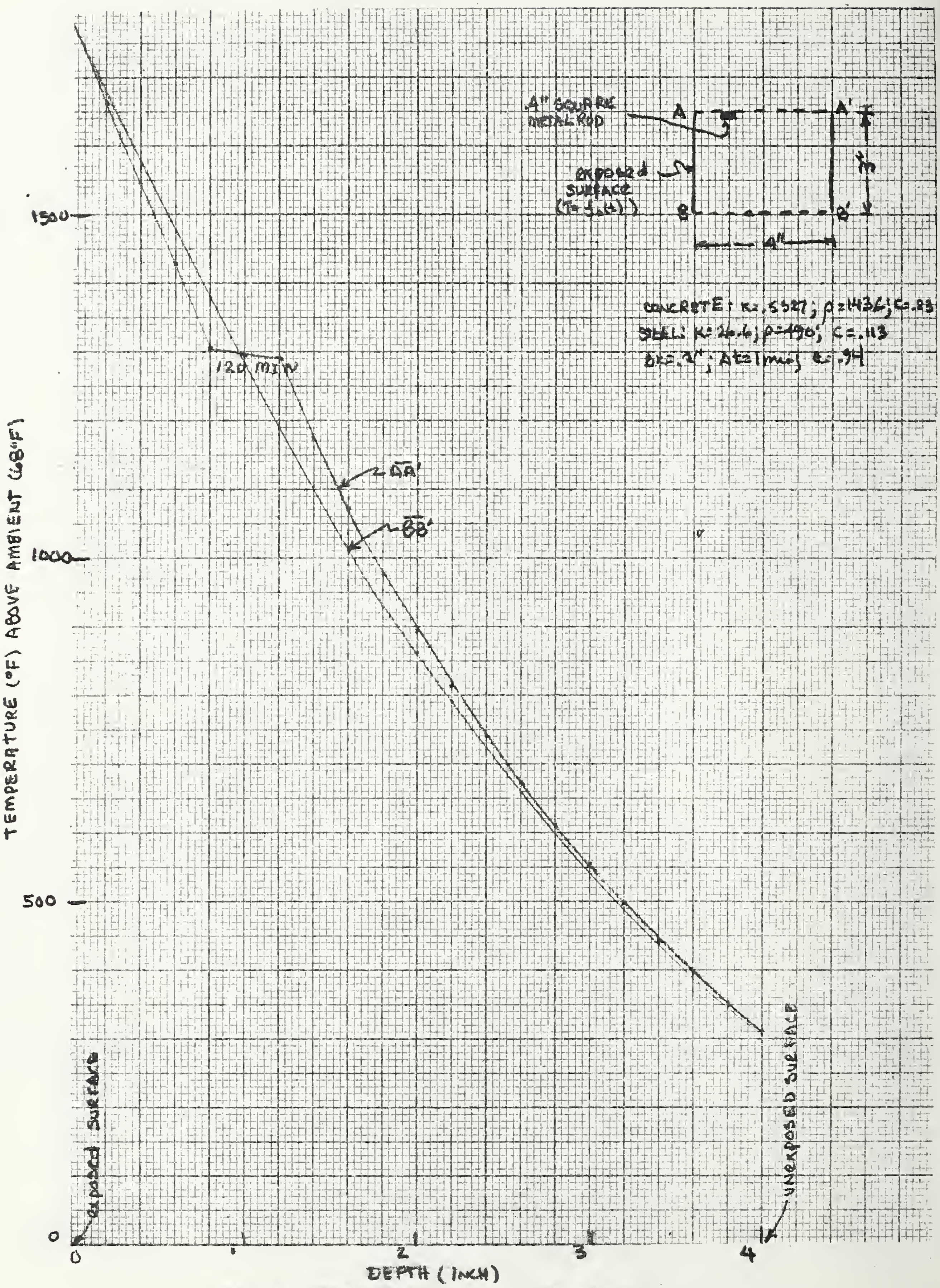

FIG. 4 - CRANK-NICOLSON DIFFERENCE CALCULATIONS

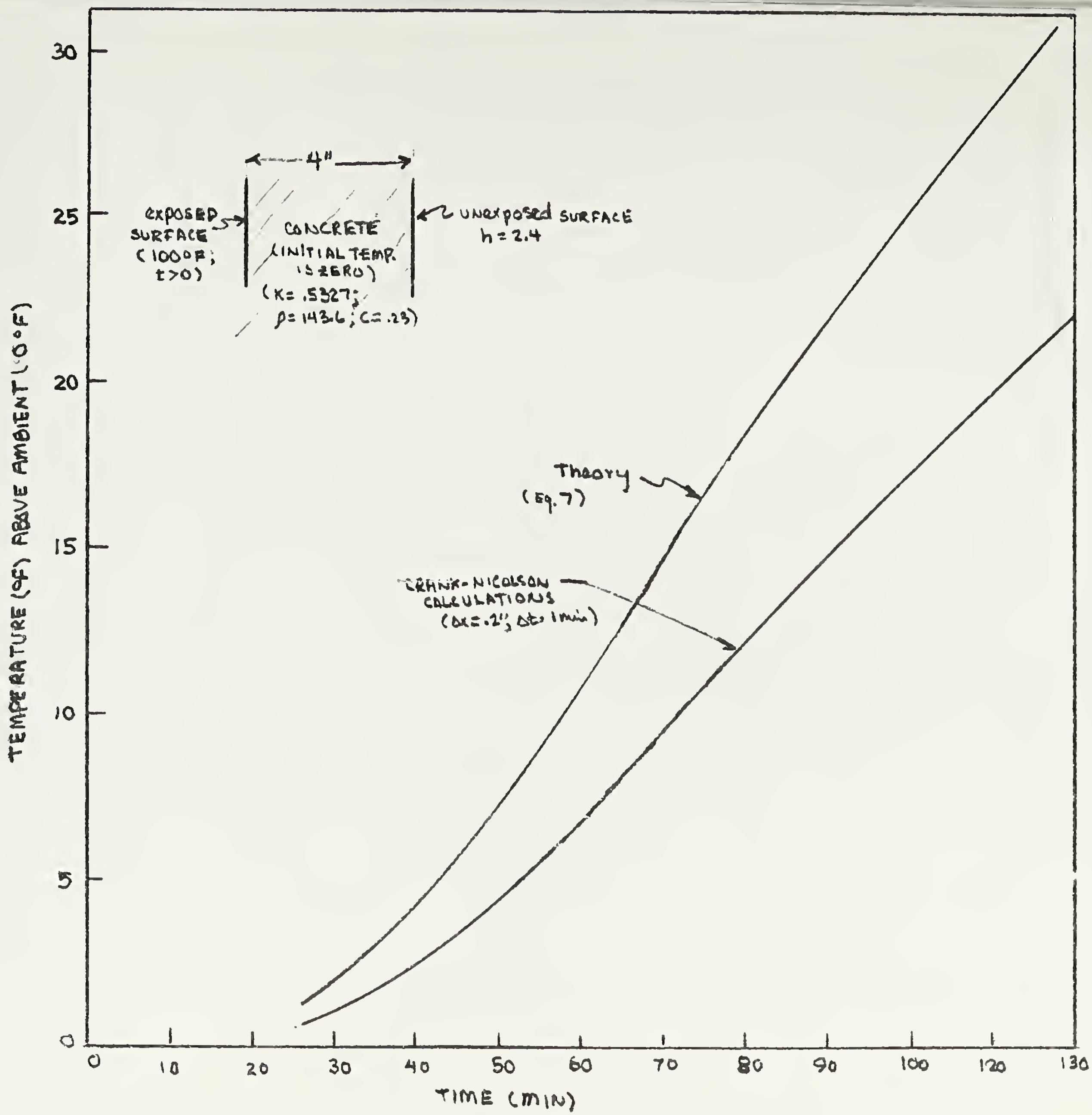

FIG.5 - SURFACE (unexposed) TEMPERATURES of 4-INCH THICK SLAB

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