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COMPARISON OF APPROXIMATE METHODS FOR THE DETERMINATION OF THERMAL COEFFICIENTS THROUGH A PHASE-CHANGE PROBLEM

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ABSTRACT

We study the determination of one or two unknown coefficients in the Lamé-Clapeyron Problem using three different approximate methods: the quasi stationary method, the Heat Balance Integral Method and Biot's variational method. We compare the results obtained in one example with the exact solutions already known.

Nomenclature

- x : space coordinate
- t : time
- $s(t)$: position of the solid-liquid interphase (free boundary) at time $t > 0$
- $\theta(x,t)$: temperature defined for $0 < x < s(t)$, $t > 0$
- k : thermal conductivity
- $a^2 = \frac{k}{\rho c}$: thermal diffusivity
- c : specific heat
- ℓ : latent heat of fusion
- ρ : mass density
- θ_o : constant temperature on the fixed face ($x = 0$)
- h_o : constant coefficient which characterizes the heat flux

on the fixed face (x = 0) defined by equation (6)

$Ste = \frac{c\,\theta_0}{\ell}$:Stefan number

$\gamma = \sqrt{1+2Ste}$

$$\mu = \frac{147\,Ste^2 + 630\,Ste}{52\,Ste^2 + 420\,Ste + 1260}$$

1. Introduction

The determination of unknown coefficients in the Lamé-Clapeyron problem was considered in [4] and [5].

In both cases, the problem was stated as follows:

(1) $\theta_t = a^2\theta_{xx}$ $\quad 0< x < s(t),\ t > 0$

(2) $\theta(s(t),t) = 0$ $\quad t > 0$

(3) $-k\theta_x(s(t),t) = \rho\ell\,\dot{s}(t)$ $\quad t > 0$

(4) $s(0) = 0$

(5) $\theta(0,t) = \theta_0$ $\quad t > 0$

(6) $k\theta_x(0,t) = -\frac{h_0}{\sqrt{t}}$ $\quad t > 0,\ h_0 > 0$

In [4], the case concerned with finding θ,s and one unknown coefficient (k,ρ,ℓ or c) was solved while in [5], s was supposedly known and two unknown coefficients were found.

In this paper we consider the determination of unknown coefficients using three different approximate methods: the quasi stationary method, the Heat Balance Integral Method and Biot's variational method.

In sections 2 and 3 respectively we study the problems with one and two unknown coefficients.

We compare the results obtained in an example with the Lamé-Clapeyron solution.

2. Determination of one unknown thermal coefficient

2.1. Quasi stationary method

In this method, equation (1) is replaced by

(7) $\theta_{xx}(x,t) = 0 \qquad 0 < x < s(t) \qquad t > 0$

The unique solution of problem (2)-(5),(7) is given by

$$(8)\quad \begin{cases} \theta(x,t) = \dfrac{\alpha_o}{\sqrt{t}}(x-s(t)) \quad , \quad \alpha_o = -\sqrt{\dfrac{\rho\ell\theta_o}{2k}} \\ s(t) = 2\sigma\sqrt{t} \quad , \quad \sigma = \sqrt{\dfrac{k\theta_o}{2\rho\ell}} \end{cases}$$

We use equation (6) to determine one of the unknown coefficients k, ℓ or ρ.

We find for the three cases that problem (2)-(7) has the unique solution (8), for any positive data. We obtain, in each case, an expresion for the unknown coefficient which is summarized in table 1.

2.2. Heat Balance Integral Method (H.B.I.M.)

In this method, following [3], we replace equation (1) by

$$(12)\quad \frac{d}{dt}\int_0^{s(t)} \theta(x,t)dx = -a^2\left[\frac{\rho\ell}{k}\dot{s}(t) + \theta_x(0,t)\right] , \ t > 0$$

and equation (3) by

$$(13)\quad \theta_x^2(s(t),t) = \frac{\ell}{c}\,\theta_{xx}(s(t),t)$$

If we choose a parabolic temperature profile:

$$(14)\quad \theta(x,t) = \alpha(t)(x-s(t)) + \beta(t)(x-s(t))^2$$

the solution of problem (2),(4),(5),(12) and (13) is given by

$$(15)\quad \begin{cases} \theta(x,t) = \dfrac{\alpha_o}{\sqrt{t}}(x-s(t)) + \dfrac{c}{2\ell}\dfrac{\alpha_o^2}{t}(x-s(t))^2 \\ \alpha_o = \dfrac{\ell(1-\gamma)}{2\sigma c} \\ s(t) = 2\sigma\sqrt{t} \end{cases}$$

(16) with $\sigma = \dfrac{a\sqrt{3}\sqrt{\gamma(\gamma-1)}}{\sqrt{4+\gamma+\gamma^2}} \quad , \quad \gamma = \sqrt{1+2\,Ste}$

We suppose k,ρ,ℓ or c are unknown and we consider the additional equation (6). We obtain from (6) and (16), in each of the four cases, that problem (2),(4)-(6),(12) and (13) has the solution (15) if and only if the data satisfy a complementary condition. The expressions for σ and the unknown coefficient are summarized in table 2.

2.3. Biot's Variational Method

In this method, following [1], we replace equation (1) by

$$(17) \qquad \frac{\partial}{\partial s}\int_0^{s(t)} c\theta^2 dx + \frac{\partial}{\partial \dot{s}}\int_0^{s(t)} \frac{1}{k}\dot{H}^2 dx = -2\theta\frac{\partial H}{\partial s}\Bigg|_{x=0}^{x=s(t)}$$

where $\frac{\partial H}{\partial x}(x,t,s) = -\rho c\theta$

and equation (3) by

$$(18) \qquad \dot{H}(s(t),t) = \rho\ell\dot{s}(t)$$

If we choose a parabolic temperature profile

$$(19) \qquad \theta = \theta_0\left(1-\frac{x}{s}\right)^2$$

the solution of problem (2),(4),(5),(17) and (18) is given by (19) and

$$(20) \qquad s(t) = 2\sigma\sqrt{t} \qquad \text{with}$$

$$(21) \qquad \sigma = a\sqrt{\mu} \quad , \quad \mu = \frac{147\,Ste^2 + 630\,Ste}{52\,Ste^2 + 420\,Ste + 1260}$$

We assume k,ρ,ℓ or c are unknown and we consider the additional equation (6). We obtain from (6) and (21), in each of the four cases, that problem (2),(4)-(6),(17) and (18) has the solution (19),(20) if and only if the data satisfy a complementary condition. The expressions for σ and the unknown coefficient are summarized in table 3.

2.4. Remark and Examples

A consequence of the stationary equation (7) is that we can not obtain the coefficient c in the quasi stationary method, while the others are easily given for any positive data.

The coefficients k and ρ (cases (1) and (2)) are also obtained in the other methods for any data as in the exact problem. Following [4], we must solve a trascendental equation por each case while in these methods k and ρ are given in an explicit form.

In cases (3) and (4), ℓ and c are given as solutions for equations of second or third order whereas in [4] they are obtained as solutions of trascendental equations.

There is not always a solution in these cases: moreover, for the coefficiant ℓ, the data must satisfy

$$\frac{\theta_o}{h_o}\sqrt{\frac{k\rho c}{3}} < 1 \qquad \text{or} \qquad \frac{\theta_o}{h_o}\sqrt{\frac{52}{147}\,k\rho c} < 1$$

while in the exact problem the condition is

$$\frac{\theta_o}{h_o}\sqrt{\frac{k\rho c}{\pi}} < 1$$

Then we cannot obtain results using H.B.I.M. or Biot's method if there isn't any solution for the exact problem.

For the coefficient c, the data must satisfy the same condition

$$\frac{k\rho\ \ell\theta_o}{2h_o^{2}} < 1$$

in H.B.I.M. and in the exact problem, while in Biot's method they must satisfy

$$\frac{2k\rho\ell\theta_o}{h_o^{2}} < 1$$

and we reach the same conclusion as before.

We apply these methods in one example we consider θ_o=15°C ; ρ=1gr/cm³ ; c=1 cal/gr°C ; ℓ=79.7 cal/gr ; k=0.00144 cal/seg cm°C .

We give, in each case, four of the five data in order to obtain the other one; and a range of variation for h_o (which depends on the complementary condition). The results obtained for the case 1 are shown in Fig.1 where we have considered

——— exact solution

----- quasi-stationary solution

..... H.B.I.M. solution

-.-.- variational method solution

For case 2, we obtained the same plot of Fig.1 if we change k by ρ.

Case 3 and 4 are shown respectively in Fig.2 and Fig.3.

We can see that the quasi-stationary method and the H.B.I.M. solutions stay quite near the exact solution while the variational method solution differs substancially from the others.

Moreover, for $h_o \cong 1$ we obtain approximately the thermal coefficients of water [2], except with the variational method.

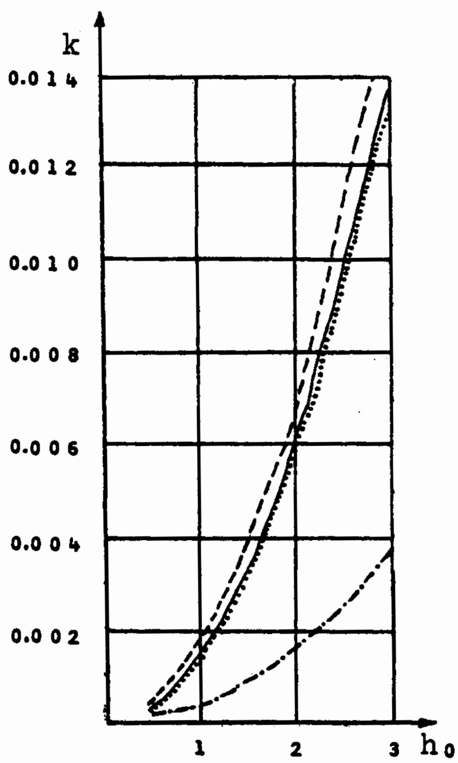

FIG.1
k(cal/seg cm°c)
vs. h_0(°C seg$^{1/2}$/cm)

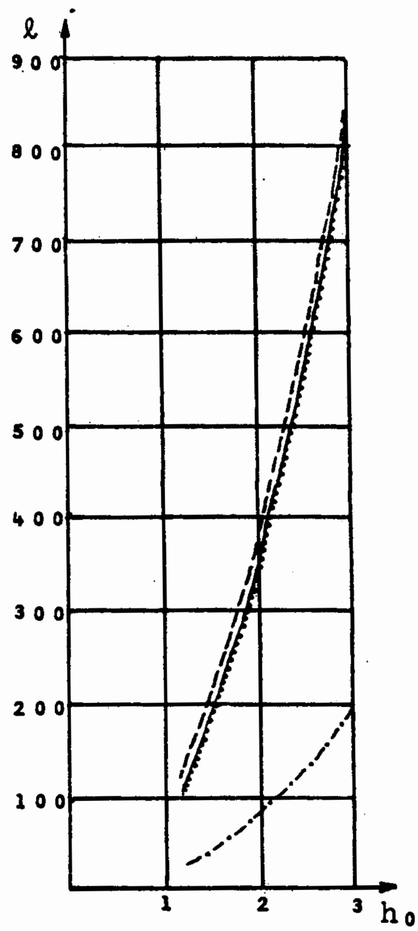

FIG.2
ℓ(cal/gr)
vs. h_0(°C seg$^{1/2}$/cm)

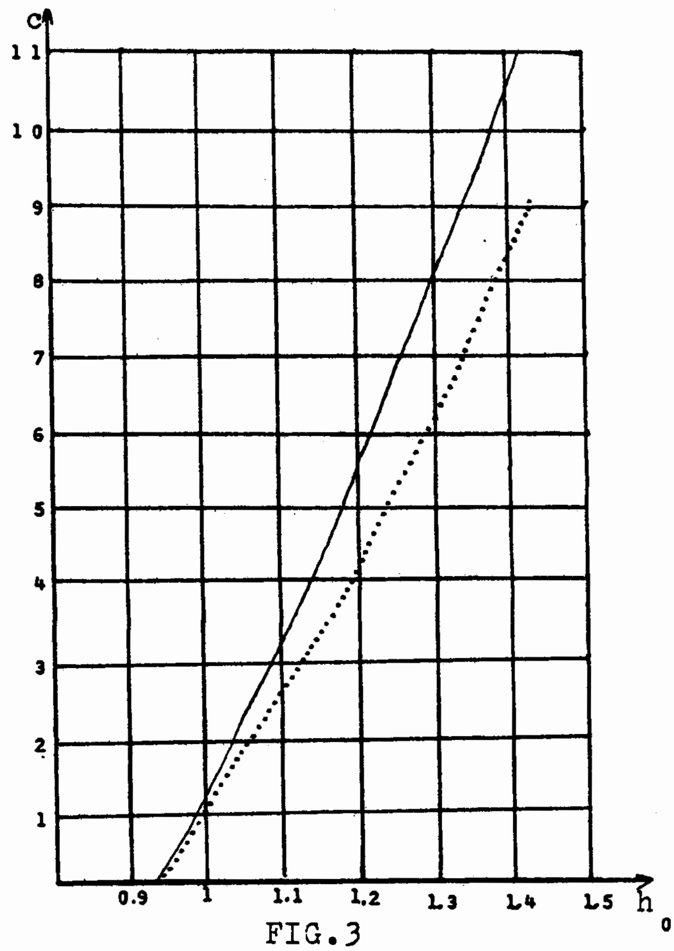

FIG.3
$c(cal/gr\,^0C)$ vs. $h_0(^0C\ seg^{1/2}/cm)$

TABLE 1

Determination of one coefficient using Quasi Stationary Method

Case	Unknown Coefficient	Solution
1.	k	$k = \frac{2h_0^2}{\rho \ell \theta_0}$
2.	ρ	$\rho = \frac{2h_0^2}{k \ell \theta_0}$
3.	ℓ	$\ell = \frac{2h_0^2}{\rho k \theta_0}$

TABLE 2

Determination of one coefficient using H.B.I.M.

Case	Unknown Coeffic.	Complementary condition for the existence and unicity of solution	Solution
1	k	——	$\sigma = \frac{6h_o}{\rho\ell(4+\gamma+\gamma^2)}$ $\quad k = \frac{12ch_o^2}{\rho\ell^2\gamma(\gamma-1)(4+\gamma+\gamma^2)}$
2	ρ	——	$\sigma = \frac{k\ell\gamma(\gamma-1)}{2ch_o}$ $\quad \rho = \frac{12ch_o^2}{k\ell^2\gamma(\gamma-1)(4+\gamma+\gamma^2)}$
3	ℓ	$\frac{\theta_o}{h_o}\sqrt{\frac{k\rho c}{3}} < 1$	$\sigma = \frac{\theta_o k\xi}{h_o(\xi+1)}$ $\quad \ell = \frac{2\theta_o c}{\xi^2-1}$ where ξ is the unique solution of $\begin{cases}(k\rho c\theta_o^2-3h_o^2)(\xi^3+\xi^2)+(4k\rho c\theta_o^2+3h_o^2)\xi+3h_o^2 = 0\\ \xi>1\end{cases}$
4	c	$\frac{k\rho\ell\theta_o}{2h_o^2} < 1$	$\sigma = \frac{\theta_o k\xi}{h_o(\xi+1)}$ $\quad c = \frac{\ell(\xi^2-1)}{2\theta_o}$ where ξ is the unique solution of $\begin{cases}k\theta_o\rho\ell(\xi^3+\xi^2)+(4k\theta_o\rho\ell-6h_o^2)\xi-6h_o^2 = 0\\ \xi>1\end{cases}$

TABLE 3

Determination of one coefficient using Biot's Variational Method

Case	unknown coeffic.	Compl.Condition for the existence and unicity of solution	Solution
1	k	——	$\sigma = \frac{h_o\mu}{\rho c}$ $\quad k = \frac{h_o^2\mu}{\theta_o^2\rho c}$
2	ρ	——	$\sigma = \frac{\theta_o k}{h_o}$ $\quad \rho = \frac{h_o^2\mu}{\theta_o^2 kc}$
3	ℓ	$\frac{\theta_o}{h_o}\sqrt{\frac{52}{147}k\rho c}<1$	$\sigma = \frac{\theta_o k}{h_o}$ ℓ is the unique solution of $\begin{cases}1260\theta_o\rho k\ell^2+(420k\rho c\theta_o^2-630h_o^2)\ell+(52\rho k\theta_o^3c^2-147c\theta_o h_o^2)=0\\ \ell > o\end{cases}$
4	c	$\frac{2k\rho\ell\theta_o}{h_o^2} < 1$	$\sigma = \frac{\theta_o k}{h_o}$ c is the unique solution of $\begin{cases}52\rho k\theta_o^3c^2+(420\rho k\theta_o^2\ell-147\theta_o h_o^2)c+(1260\rho k\ell^2\theta_o-630\ell h_o^2)=0\\ \ell > o\end{cases}$

3. Simultaneous determination of two unknown thermal coefficients.

3.1. Quasi-stationary method

We consider problem (2)-(7): In it coefficient c does not appear while coefficients ρ and ℓ appear always together, that is as $L=\rho\ell$

Then, if we assume that $s(t)=2\sigma\sqrt{t}$ is known, we want to find coefficients k and L.

From (8) we have $\sigma^2 = \frac{k\theta_o}{2L}$ and from (6) $kL\theta_o=2\ h_o^2$, then it follows that:

"For any data ($h_o>0$, $\theta_o>0$, $\sigma>0$) problem (2)-(7) has the unique solution

$$\theta(x,t)=-\sqrt{\frac{L\theta_o}{2kt}}\ (x - s(t)) \tag{22}$$

where k and L are given by

$$k = \frac{2h_o\sigma}{\theta_o} \tag{23}$$

$$L = \frac{h_o}{\sigma} \quad " \tag{24}$$

3.2. Heat Balance Integral Method (H.B.I.M.)

We consider problem (2),(4)-(6),(12) and (13). If we assume that $s(t) = 2\sigma\sqrt{t}$ and two of the thermal coefficients are known we now want to find the others.

There are six possible cases. We obtain, in each case, from (6) and (16) that problem (2),(4)-(6),(12) and (13) has the solution (15) if and only if the data satisfy a complementary condition. The expressions for the two unknowns are summarized in table 4.

3.3. Biot's Variational Method

We consider problems (2),(4)-(6),(17) and (18). If we assume that $s(t) = 2\sigma\sqrt{t}$ is known, from (6) it follows

$$k = \frac{h_o \sigma}{\theta_o} \tag{25}$$

That is, k is determinated even if all the other thermal coefficients are unknown.

Then, if two of the thermal coefficients ρ, c, ℓ are given we can obtain the third one from (21), and we can study only three possible cases by this method. In each case, we obtain that problem (2),(4)-(6),(17) and (18) has the solution (19),(20) if and only if the data satisfy a complementary condition and the expression for k is given by (25) while for the other unknown coefficient it is summarized in table 5.

3.4. Remarks and examples

We have seen that in the quasi stationary method there is only one case of simultaneous determination of thermal coefficients because c does not appear and ρ and ℓ are always together as $L=\rho\ell$. In this case we obtain a solution for any data as in the exact problem [3], while in the H.B.I.M. and in Biot's variational method the solution is obtained in case 1 (k,ρ) for any data and in case 3 (k,ℓ) if and only if the data verify conditions

$\frac{h_o}{\rho c \theta_o \sigma} > \frac{1}{3}$ and $\frac{h_o}{\rho c \theta_o} > \frac{52}{147}$ respectively.

In case 2 (k,c) the H.B.I.M. gives a solution if the data verify the same condition $\frac{h_o}{\rho \ell \sigma} > 1$ of the exact problem while in Biot's method, the condition $\frac{h_o}{\rho \ell \sigma} > \frac{420}{147}$ is more restrictive.

The other cases $(\rho,\ell;\ \rho,c;\ c,\ell)$ cannot be solved by means of Biot's method while they can by the H.B.I.M. whenever the data satisfy $\frac{1}{2} < \mu_o = \frac{k\theta_o}{2h_o\sigma} < 1$.

This condition is more restrictive than the one imposed by the exact problem: $\mu_o < 1$.

The advantage of these methods is that we doesn't need to solve a trascendental equation as in the exact case.

We applied these methods in an example. We consider, as in 2.4:

$\theta_0=15°C$, $c=1$ cal/gr°C , $\rho=1$ gr/cm³ , $\ell=79,7$ cal/gr , $k=0.00144$ cal/seg cm°C , $\sigma=0.0123$ cm/seg$^{1/2}$

We give in each case three of the first five data, the value of σ and a range of variation for h_0.

The results obtained for case 1,2,3,4,5 and 6 are shown in Fig.4,5,6,7,8 and 9, respectively.

We obtain very good approximations for cases 1 and 3 except for the variational method (Fig 4 and 6)

In case 2 (Fig.5), the H.B.I.M. and the exact solutions are almost the same for c but not for k. However, for $h_0 \cong 1$ we obtain approximately k and c of water in both graphs.

We see in Fig.7, 8 and 9, that for the cases 4,5 and 6 the results are not the same for the H.B.I.M. and the exact problem.

Note that, at $h_0 \gtrsim 1$, the H.B.I.M. solution is nearer to the experimental thermal coefficient for water (pointed out with x) [2]. than the exact result.

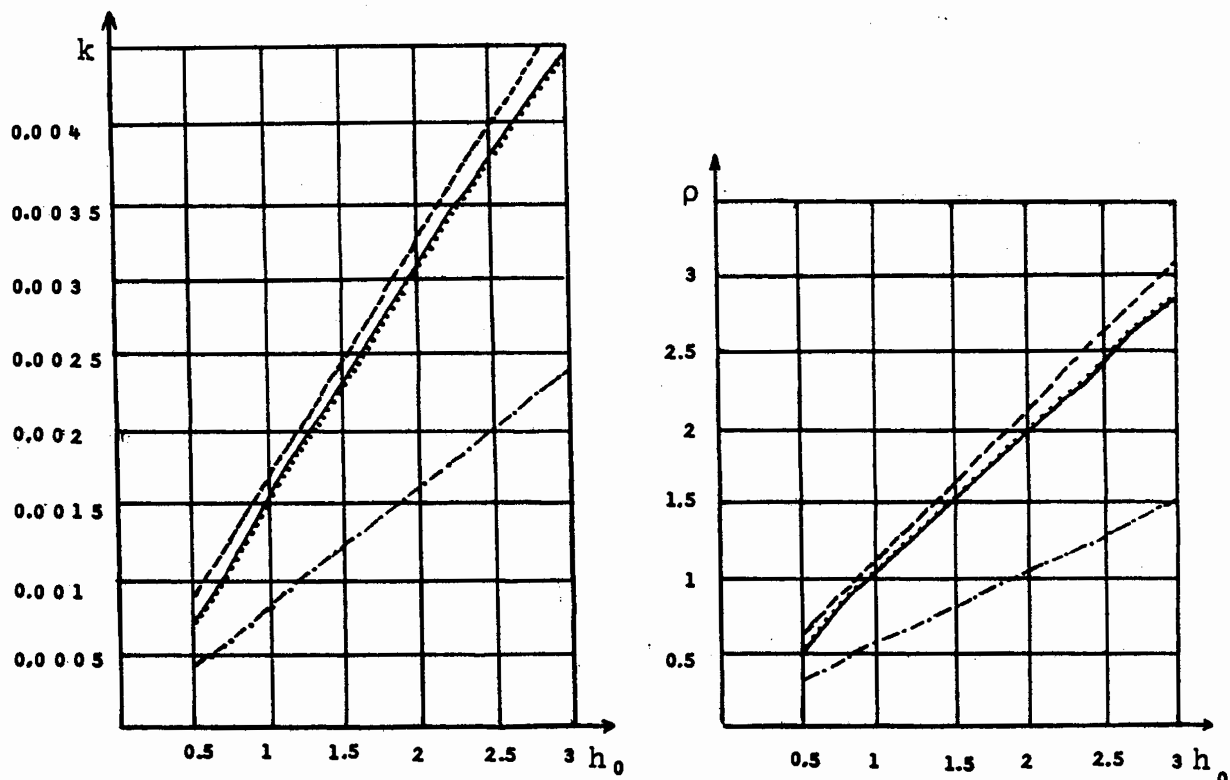

FIG.4

k(cal/seg cm°C) and ρ(gr/cm³)vs.h_0(°C seg$^{1/2}$/cm)

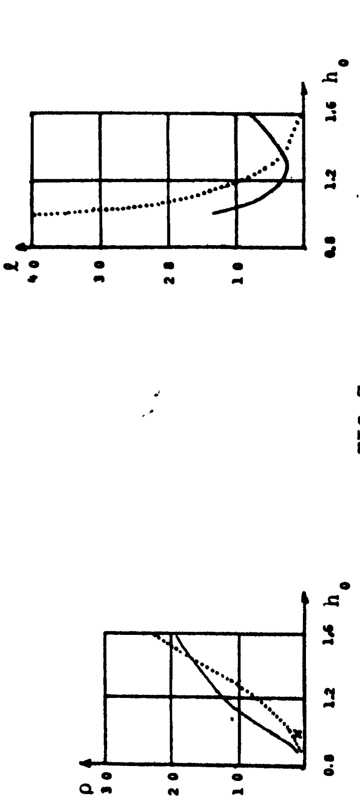

FIG.7 $\rho(gr/cm^3)$ and $\ell(cal/gr)$ vs. $h_0(^{\circ}C\ seg^{1/2}/cm)$

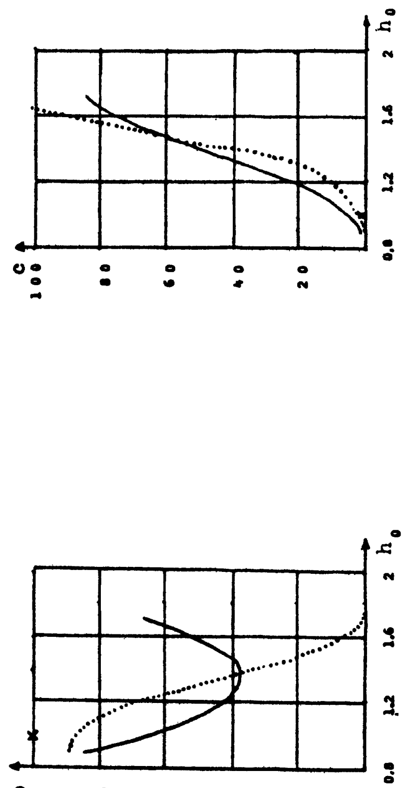

FIG.8 $\rho(gr/cm^3)$ and $c(cal/gr^{\circ}C)$ vs. $h_0(^{\circ}C\ seg^{1/2}/cm)$

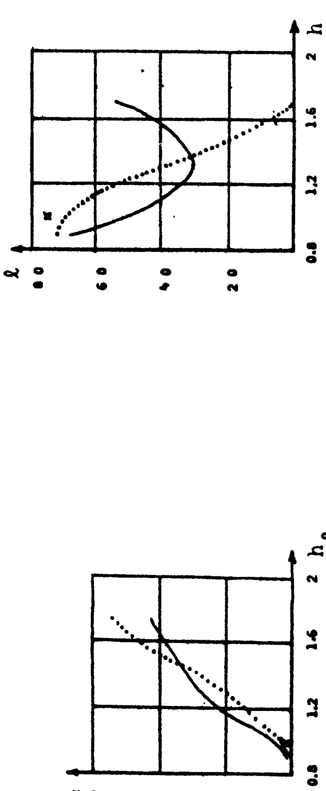

FIG.9 $c(cal/gr^{\circ}C)$ and $\ell(cal/gr)$ vs. $h_0(^{\circ}C\ seg^{1/2}/cm)$

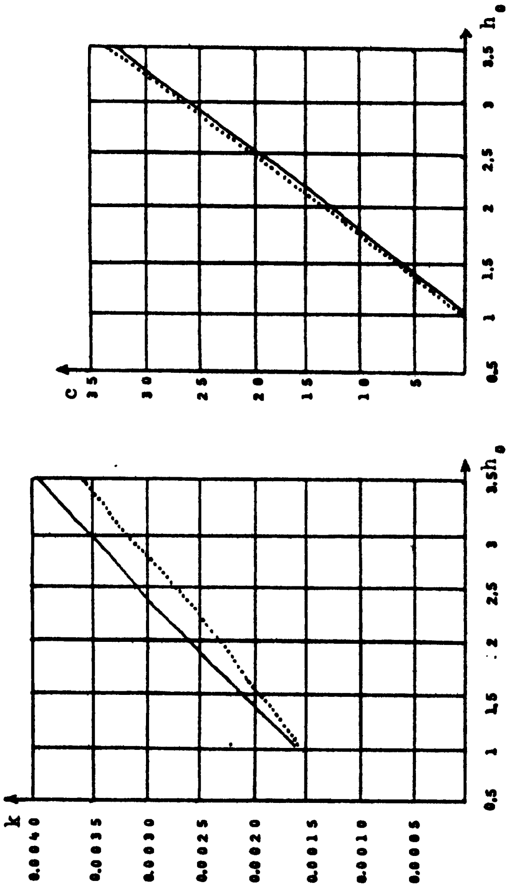

FIG. 5 $k(cal/seg\ cm^{\circ}C)$ and $c(cal/gr^{\circ}C)$ vs. $h_0(^{\circ}C\ seg^{1/2}/cm)$

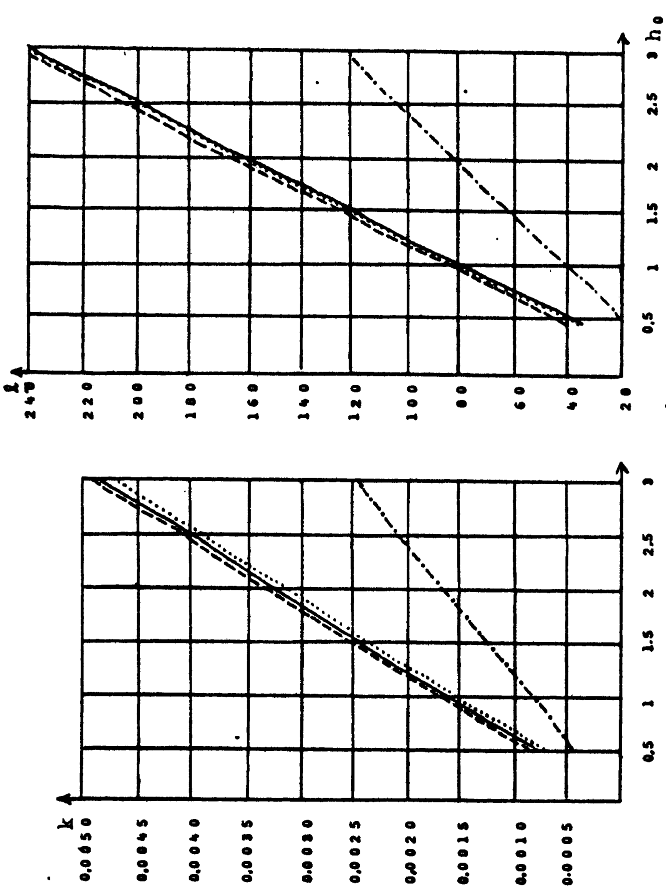

FIG. 6 $k(cal/seg\ cm^{\circ}C)$ and $\ell(cal/gr)$ vs. $h_0(^{\circ}C\ seg^{1/2}/cm)$

TABLE 4

Determination of two coefficients using H.B.I.M.

Case	Unknown coeffic.	Complementary condition.	Solution
1	k,ρ	—	$k = \frac{2ch_o\sigma}{\ell\gamma(\gamma-1)}$ $\quad \rho = \frac{6h_o}{\ell\sigma(4+\gamma+\gamma^2)}$
2	k,c	$\frac{h_o}{\rho\ell\sigma} > 1$	$k = \frac{h_o\sigma(\xi+1)}{\theta_o\xi}$ $\quad c = \frac{\ell(\xi^2-1)}{2\theta_o}$ where ξ is the unique solution of $\begin{cases}\rho\ell\sigma\xi^2+\rho\ell\sigma\xi+(4\rho\ell\sigma-6h_o) = 0\\ \xi > 1\end{cases}$
3	k,ℓ	$\frac{h_o}{\rho c\theta_o\sigma} > \frac{1}{3}$	$k = \frac{h_o\sigma(\xi+1)}{\theta_o\xi}$ $\quad \ell = \frac{2\theta_o c}{\xi^2-1}$ where ξ is the unique solution of $\begin{cases}(\rho c\theta_o\sigma-3h_o)\xi^2+\rho c\theta_o\sigma\xi+(4\rho c\theta_o\sigma+3h_o)=0\\ \xi > 1\end{cases}$
4	ρ,ℓ	$\frac{1}{2}<\mu_o=\frac{k\theta_o}{2h_o\sigma}<1$	$\rho = \frac{3k(1-\mu_o)}{\sigma^2c(8\mu_o^2-7\mu_o+2)}$ $\quad \ell = \frac{\theta_oc(2\mu_o-1)^2}{2\mu_o(1-\mu_o)}$
5	ρ,c	$\frac{1}{2}<\mu_o=\frac{k\theta_o}{2h_o\sigma}<1$	$\rho = \frac{3h_o(2\mu_o-1)^2}{\sigma\ell(8\mu_o^2-7\mu_o+2)}$ $\quad \ell = \frac{2\mu_o(1-\mu_o)\ell}{(2\mu_o-1)^2\theta_o}$
6	c,ℓ	$\frac{1}{2}<\mu_o=\frac{k\theta_o}{2h_o\sigma}<1$	$c = \frac{3k(1-\mu_o)}{\sigma^2\rho(8\mu_o^2-7\mu_o+2)}$ $\quad \ell = \frac{3h_o(2\mu_o-1)^2}{\sigma\rho(8\mu_o^2-7\mu_o+2)}$

TABLE 5

Determination of two coefficients using Biot's Variational Method

Case	Unknown Coeffic.	Complementary condition for the existence and unicity of solution	Solution
1	k,ρ	—	$k = \frac{h_o\sigma}{\theta_o}$ $\quad \rho = \frac{h_o\ell(147Ste + 630)}{4\sigma(13Ste^2+105\,Ste+315)}$
2	k,c	$\frac{h_o}{\rho\ell\sigma} > \frac{420}{147}$	$k = \frac{h_o\sigma}{\theta_o}$ c is the unique solution of $\begin{cases}52\frac{\theta_o}{\ell}c^2+(420-147\frac{h_o}{\rho\ell\sigma})c+(1260-630\frac{h_o}{\rho\ell\sigma})\frac{\ell}{\theta_o} = 0\\ c > 0\end{cases}$
3	k,ℓ	$\frac{h_o}{\rho c\theta_o\sigma} > \frac{52}{147}$	$k = \frac{h_o\sigma}{\theta_o}$ ℓ is the unique solution of $\begin{cases}\frac{1260}{c\theta_o}\ell^2+(420-630\frac{h_o}{\rho c\theta_o\sigma})\ell+(52-147\frac{h_o}{\rho c\theta_o\sigma})c\theta_o = 0\\ \ell > 0\end{cases}$

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