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Analysis of a One-Dimensional Solidification Problem with Two-Phase Moving Boundaries

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ABSTRACT

This paper analyzes a one-dimensional temperature field problem on solidification with two moving boundaries. The theoretical results are compared with those obtained from the finite element analysis and a satisfactory agreement is obtained. It is further extended to a 2-D case of welding on a thin plate to show the movement of the solidus and liquidus interfaces in the material during the phase change.

INTRODUCTION

The transient heat conduction problem involving melting and solidification is often referred to as a phase change or a moving boundary problem. A moving boundary problem, for instance, is encountered in the process of solidification of ice making and casting, of melting and solidification during welding, of the freezing of food, etc. When a material undergoes the transition from liquid state to solid state, or vise versa, it will release or absorb heat energy isothermally through the phase change. The difficulty in analyzing such a problem lies in the fact that the locations of liquid-solid transition vary with time, i.e. the interfaces of solid and liquid are movable and there also exists the problem of release and absorption of latent heat. For a pure metal during melting or solidification, the phase change occurs at a certain discrete temperature (fusion point) with liquid and solid phases separated distinctly by a sharp moving interface. The latent heat is released or absorbed right in this surface layer which moves with time. But for most alloys and mixed materials, the phase change takes place in a transition zone (or two-phase region), where both phases exist simultaneously, while solid and liquid are separated by a solidus front and a liquidus front, respectively, shown in Figure 1. In engineering practice, it is the latter case that we often meet with.

Most of the exact solutions of phase change problems with a sharp moving interface are discussed in detail by Ozisik (1980, pp.397-438). There exists, however, a limited amount of literature on two moving boundary problems (Tien and Geiger, 1967; Ozisik and Uzzell, 1979). This paper presents an exact solution to the semi-infinite freezing problem with two moving boundaries. The result is compared with that obtained from the finite element analysis. The phase change model is further used in analyzing a more complicated 2-D temperature field of welding caused by a moving torch.

THEORETICAL ANALYSIS

Consider a semi-infinite body of one dimensional space. At the beginning (t=0), the entire body is in a liquid state and has the temperature T_i which is above the liquidus front T_2. Then a constant temperature T_0, lower than the solidus front T_1, is suddenly imposed on the surface at x=0. Consequently the liquid begins to condense to solid continuously through a solidification zone while T_i is maintained at infinity. Heat is removed through the surface of x=0. The solidification zone between T_1 and T_2 expands continuously and travels to the right with increasing time, as illustrated in Figure 1. The solidus interface $S_1(t)$ and liquidus interface $S_2(t)$ move accordingly.

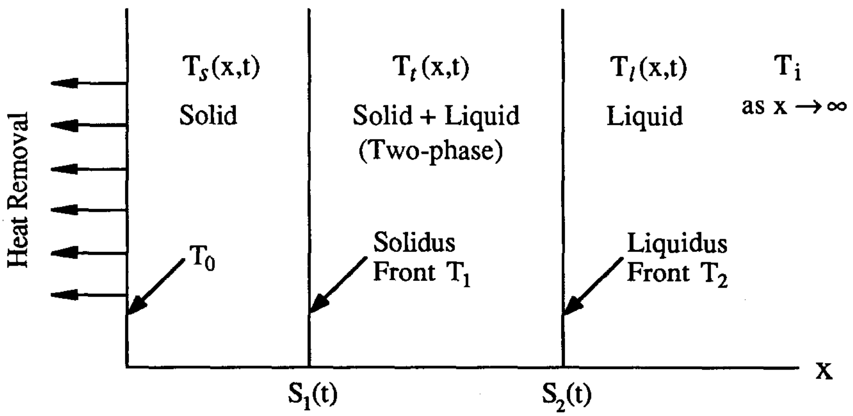


Figure 1. Various Phases during the solidification of a binary system

For simplicity, the following assumptions have been made:

1) the physical properties of the solid and liquid part do not change with temperature, but may have different values in the three zones,
2) the volume of the body does not undergo any change through the whole period of phase change, therefore, the density is a constant,
3) heat conduction prevails in all the three different regions, even in the liquid zone, and
4) in the phase change zone, the fraction of solid is directly proportional to temperature (Tien and Geiger, 1967; Ozisik and Uzzell, 1979), that is,

$$f_s = f_{su}\left(1 - \frac{T_t - T_1}{T_2 - T_1}\right) \tag{1}$$

where,

f_s solid fraction in the two-phase zone
f_{su} solid fraction at the solidus front of the two-phase zone
T_t temperature in the two-phase zone
T_1 temperature at the solidus front, and
T_2 temperature at the liquidus front

f_{su}=1 corresponds to a balanced condensation, solid and liquid have infinite diffusivities. $0 < f_{su} < 1$ corresponds to an unbalanced condensation, diffusivity of liquid is infinite, of solid is zero.

The heat energy generated per unit volumn per unit time in the two-phase zone due to latent heat can be described as

$$Q(x,t) = \rho L \frac{df_s}{dt} \tag{2}$$

where L is the energy released or absorbed per unit mass (J/kg) during the phase change, and ρ is the density of material.

Based on the above assumptions, the governing energy equations in the three zones can be given as

$$\frac{\partial^2 T_s}{\partial x^2} = \frac{1}{\alpha_s}\frac{\partial T_s}{\partial t} \qquad \text{in } 0 < x < S_1(t) \tag{3}$$

$$\frac{\partial^2 T_t}{\partial x^2} + \frac{Q}{k_t} = \frac{1}{\alpha_t}\frac{\partial T_t}{\partial t} \qquad \text{in } S_1(t) < x < S_2(t) \tag{4}$$

$$\frac{\partial^2 T_l}{\partial x^2} = \frac{1}{\alpha_l}\frac{\partial T_l}{\partial t} \qquad \text{in } x > S_2(t) \tag{5}$$

in which $S_1(t)$ and $S_2(t)$ are the locations of solidus and liquidus fronts, or moving boundaries, which are the function of time, k and α represent thermal conductivity and diffusivity of material, and the subscripts *s*, *t* and *l* indicate solid, two-phase and liquid, respectively. The boundary conditions at the solidus front are

$$T_s(x,t) = T_t(x,t) = T_1 \qquad \text{at } x = S_1(t),\ t > 0 \tag{6}$$

$$k_s \frac{\partial T_s}{\partial x} - k_t \frac{\partial T_t}{\partial x} = \rho L(1-f_{su}) \frac{dS_1(t)}{dt} \qquad \text{at } x = S_1(t), t > 0 \qquad (7)$$

and at the liquidus front

$$T_t(x,t) = T_l(x,t) = T_2 \qquad \text{at } x = S_2(t), t > 0 \qquad (8)$$

$$k_t \frac{\partial T_t}{\partial x} = k_l \frac{\partial T_l}{\partial x} \qquad \text{at } x = S_2(t), t > 0 \qquad (9)$$

Equations (7) and (9) are derived from the principle of conservation of energy. The right hand side of Eq.(7) represents the heat energy produced at the solidus front by the remaining part of liquid during the isothermal change to solid. The boundary conditions at $x=0$ and $x \rightarrow \infty$ are defined as

$$T_s(x,t) = T_0 \qquad \text{at } x = 0, t > 0 \qquad (10)$$

$$T_l(x,t) = T_i \qquad \text{as } x \rightarrow \infty, t > 0 \qquad (11)$$

and the initial condition is

$$T(x,t) = T_i \qquad \text{for } t = 0, \text{ in } x > 0 \qquad (12)$$

The expression for the internal heat source Q of Eq.(4), due to the latent heat, can be obtained by substituting Eq.(1) into Eq.(2)

$$Q(x,t) = \frac{\rho L f_{su}}{T_2 - T_1} \frac{\partial T_t(x,t)}{\partial t} \qquad (13)$$

The energy equation in the two-phase zone can then be simplified by combining Eq.(4) and (13), as

$$\frac{\partial^2 T_t}{\partial x^2} = \frac{1}{\alpha^*_t} \frac{\partial T_t}{\partial t} \qquad \text{in } S_1(t) < x < S_2(t) \qquad (14)$$

where α^*_t is the modified thermal diffusivity in the two-phase region in which the effect of latent heat is included,

$$\frac{1}{\alpha^*_t} = \frac{\rho L f_{su}}{k_t(T_2 - T_1)} + \frac{1}{\alpha_t} \qquad (15)$$

Thus, the governing equations (3-5) for these three regions can share a simple form with three different thermal diffusivities,

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t} \qquad \text{for } t > 0 \qquad (16)$$

$$\alpha = \begin{cases} \alpha_s & \text{in } 0 < x < S_1(t) \\ \alpha^*_t & \text{in } S_1(t) < x < S_2(t) \\ \alpha_l & \text{in } x > S_2(t) \end{cases} \qquad (17)$$

The three general solutions for the three different zones can be obtained with these diffusivities

$$T_s(x,t) = C_1 \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_s t}}\right) + C_2 \qquad \text{in } 0 < x < S_1(t) \tag{18}$$

$$T_t(x,t) = C_3 \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha^*_t t}}\right) + C_4 \qquad \text{in } S_1 < x < S_2(t) \tag{19}$$

$$T_l(x,t) = C_5 \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_l t}}\right) + C_6 \qquad \text{in } x > S_2(t) \tag{20}$$

where erf(x) is an error function, or probability integral function,

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2}du \tag{21}$$

and C_1, C_2, ……, C_6 are integral constants which can be solved with the boundary conditions, Eqs.(6), (8), (10) and (11)

$$C_1 = \frac{T_1 - T_0}{\operatorname{erf}(\lambda)} \qquad C_4 = \frac{T_1\operatorname{erf}(\eta) - T_2\operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)}{\operatorname{erf}(\eta) - \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)}$$

$$C_2 = T_0 \qquad C_5 = \frac{T_i - T_2}{\operatorname{erfc}\left(\eta\sqrt{\frac{\alpha^*_t}{\alpha_l}}\right)} \tag{22}$$

$$C_3 = \frac{T_2 - T_1}{\operatorname{erf}(\eta) - \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)} \qquad C_6 = T_i - \frac{T_i - T_2}{\operatorname{erfc}\left(\eta\sqrt{\frac{\alpha^*_t}{\alpha_l}}\right)}$$

where erfc(x)=1-erf(x) is a complementary error function.

The temperature distributions in the three zones can be established and have the form

$$T_s(x,t) = T_0 + \frac{T_1 - T_2}{\operatorname{erf}(\lambda)}\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_s t}}\right) \qquad \text{in } 0 < x < S_1(t) \tag{23}$$

$$T_t(x,t) = \frac{T_1\operatorname{erf}(\eta) - T_2\operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)}{\operatorname{erf}(\eta) - \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)} + \frac{T_2 - T_1}{\operatorname{erf}(\eta) - \operatorname{erf}\left(\lambda\sqrt{\frac{\alpha_s}{\alpha^*_t}}\right)}\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha^*_t t}}\right)$$

$$\text{in } S_1(x) < x < S_2(t) \tag{24}$$

$$T_l(x,t) = T_i - \frac{T_i - T_2}{\text{erfc}(\eta\sqrt{\frac{\alpha_t^*}{\alpha_l}})}\ \text{erfc}(\frac{x}{2\sqrt{\alpha_l t}}) \qquad \text{in } x > S_2(t) \tag{25}$$

in which

$$\lambda = \frac{S_1(t)}{2\sqrt{\alpha_s t}} \qquad \text{or} \qquad S_1(t) = 2\lambda\sqrt{\alpha_s t} \tag{26}$$

$$\eta = \frac{S_2(t)}{2\sqrt{\alpha_l t}} \qquad \text{or} \qquad S_2(t) = 2\eta\sqrt{\alpha_l t} \tag{27}$$

Since equations (26-27) should be satisfied for all times, the parameters λ and η must be constant, which are determined by equations (7) and (9). Substituting the above two equations into energy equations, we obtain the implicit expressions for λ and η as

$$\frac{T_1 - T_0}{T_2 - T_1}\frac{e^{-\lambda^2}}{\text{erf}(\lambda)} - \frac{k_t}{k_s}\sqrt{\frac{\alpha_s}{\alpha_t^*}}\frac{e^{-\lambda^2\frac{\alpha_s}{\alpha_t^*}}}{\text{erf}(\eta) - \text{erf}(\lambda\sqrt{\frac{\alpha_s}{\alpha_t^*}})} = \frac{\sqrt{\pi}\lambda(1 - f_{su})L}{c_s(T_2 - T_1)} \tag{28}$$

$$\frac{T_i - T_2}{T_2 - T_1}\frac{e^{-\lambda^2\frac{\alpha_t^*}{\alpha_t}}}{\text{erfc}(\eta\sqrt{\frac{\alpha_t^*}{\alpha_l}})} - \frac{k_t}{k_l}\sqrt{\frac{\alpha_l}{\alpha_t^*}}\frac{e^{-\eta^2}}{\text{erf}(\eta) - \text{erf}(\lambda\sqrt{\frac{\alpha_s}{\alpha_t^*}})} = 0 \tag{29}$$

The parameters λ and η can be solved from the above two equations, hence the positions $S_1(t)$ and $S_2(t)$ of the two phase moving boundaries at any time are known and the whole temperature field is thus completely defined.

To illustrate the validity of the above analyses, we take an example of the solidification of an aluminum-copper alloy containing five percent copper. The physical properties and concerned parameters of this material are obtained from Ozisik an Uzzell (1979),

$k_s = 197.3\ \frac{w}{m\cdot°C}$ $\qquad$ $k_l = 181.7\ \frac{w}{m\cdot°C}$

$c_s = 1{,}046.7\ \frac{J}{kg\cdot°C}$ $\qquad$ $c_l = 1{,}256.0\ \frac{J}{kg\cdot°C}$

$\rho = 27{,}232.2\ \frac{kg}{m^3}$ $\qquad$ $L = 395{,}403\ \frac{J}{kg}$

$T_1 = 547.8\ °C$ $\qquad$ $T_2 = 642.2\ °C$

$f_{su} = 0.8952$

and k_t and c_t for the two-phase region can be approximately taken as an average value of that of liquid and solid.

It is assumed that the initial temperature T_i of liquid is 646°C and several boundary temperatures are chosen for calculation: T_0 = 530°C, 500°C, 400°C, 300°C and 100°C, respectively. The values of the parameters λ and η are solved from the simultaneous equations (28-29), and are listed in Table 1.

TABLE 1

The variation of λ and η with different boundary temperatures T_0 (T_i = 646°C)

T_0 (°C)	λ	η
530	0.06519	1.8147
500	0.14382	1.8766
400	0.30703	2.0324
300	0.41192	2.1506
100	0.55408	2.3309

The locations of solidus and liquidus moving boundaries can be determined from equations (26-27), if λ and η are known. Thus according to equations (23-25), one dimensional temperature field with the variation of time is established. Figure 2 shows the variation of location of the solidus and liquidus fronts with time (T_0 = 530°C). Figure 3 and Figure 4 show the temperature distributions, with (a), (b) and (c) corresponding to T_0 = 530°C, 300°C and 100°C, respectively. The former shows the variation of temperature with time at fixed locations, and the latter shows the variations of temperature with location at fixed times.

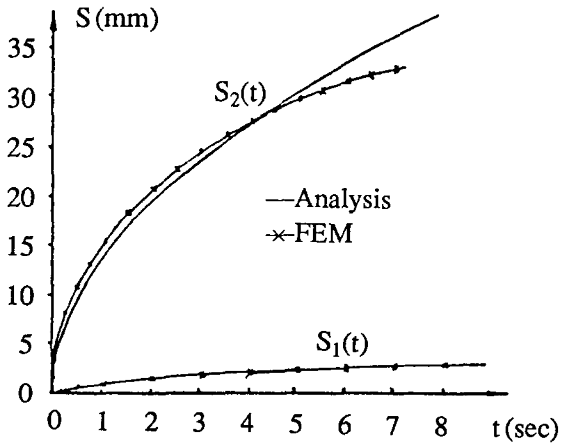
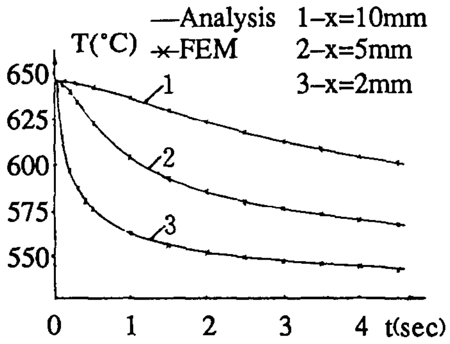
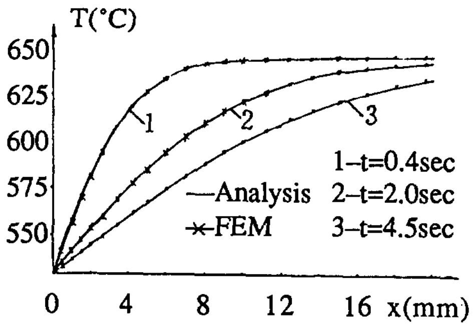


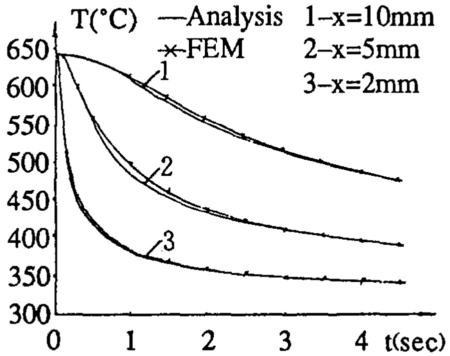
Figure 2. The variation of locations of solidus and liquidus fronts with time for T_0 = 530°C



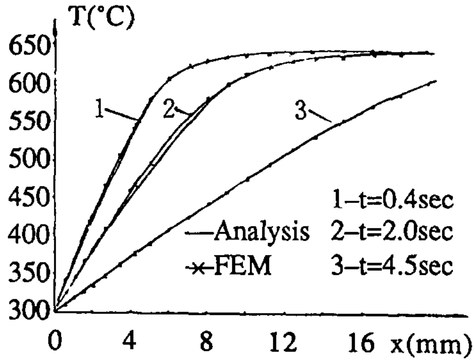
(a) T_0=530°C



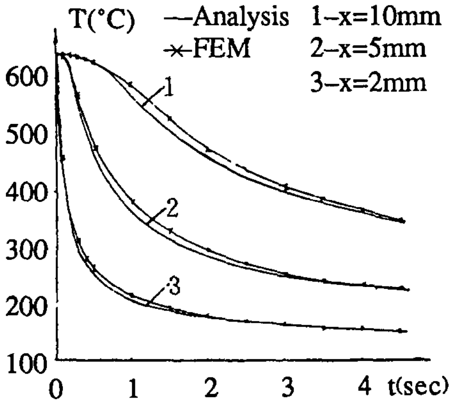
(a) T_0=530°C



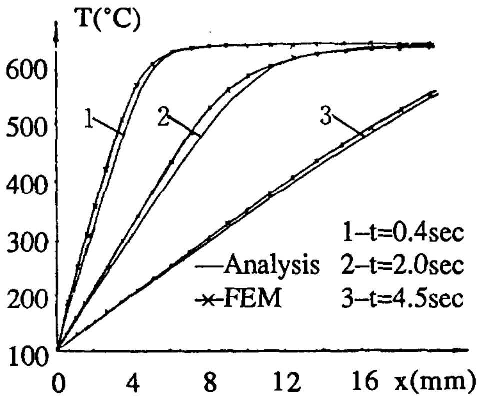
(b) T_0=300°C



(b) T_0=300°C



(c) T_0=100°C



(c) T_0=100°C

Figure 3. The variation of temperature with time at fixed locations for T_i = 646°C

Figure 4. The cariation of temperature with location at fixed times for T_i = 646°C

NUMERICAL SOLUTIONS AND DISCUSSTION

In addition to the theoretical analysis, we also carried out a finite element analysis on this problem for comparison. The model of Eq.(17) was applied in the numerical calculation. The finite element mesh used is 40 × 1 mm, as shown in Figure 5. The numerical results relevant to the exact solutions are plotted on the same figures as the analytical ones (Figures 2-4).

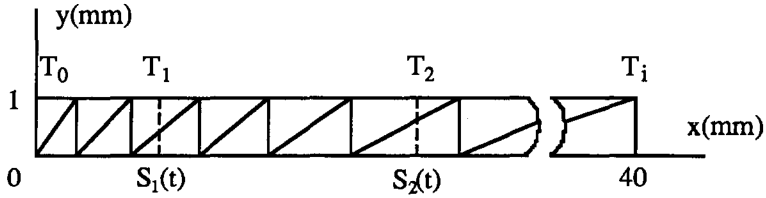


Figure 5. Finite element mesh of one-dimenstional freezing problem

It can be seen from the curves in Figures 2-4 that the finite element results agree well with the exact solutions. The temperature difference on the liquidus front in Figure 2 (T_0=530°C) is due to the limited length of the finite element mesh (40 mm). If the length were infinite, the difference would be hardly seen, which can be explained by reference to the solidus front. There is almost no difference shown in the figure between analytical and numerical solutions on the solidus interface. It implies that the phase change model of Eq.(1) can be used not only in one dimensional analysis, but applied to two or three dimensional cases and more complicated boundaries as well with the aid of numerical methods.

Welding on a thin plate is a two dimensional case. According to Krutz and Segerlind (1978), there exist two interfaces in a mild steel, a liquidus front and a solidus front, with a transition zone in-between where the latent heat is absorbed or released. The solidus front is represented by a 1700 K isotherm while the liquidus front has a 1755 K isotherm. According to Wang (1984), the equation of 2-D heat conduction in a thin plate with upper and lower surfaces exposed to air can be expressed as

$$\frac{\partial}{\partial x}(k_x\frac{\partial T}{\partial x}) + \frac{\partial}{\partial y}(k_y\frac{\partial T}{\partial y}) - \frac{2h_\infty}{\delta}(T-T_\infty) + \dot{q} = \rho c_p^* \frac{\partial T}{\partial t} \qquad (30)$$

where

h_∞ average heat transfer coefficient of the upper and lower surfaces of the plate,

T_∞ temperature of the surroundings, and

$c_p^* = c_l + \frac{L}{T_2 - T_1}$ is the modified specific heat in the transition zone ($T_1 < T < T_2$), which means the effect of latent heat is taken into account by increasing the value of specific heat. When The temperature of an element is below T_1 or above T_2, the c_s of solid or c_l of liquid will be adopted.

The heat energy per unit volumn absorbed by the plate can be modeled as

$$\dot{q}(x,y,t) = \frac{3G}{\pi\bar{r}^2\delta} \exp[-3\frac{x^2 + (y - \nu t)^2}{\bar{r}^2}] \tag{31}$$

where

G total effective power input (Watts) from the welding torch,

$\bar{r}$ effective heating radius,

δ thickness of the plate, and

ν travel speed of the torch.

Applying the finite element method to a mild steel plate (see Figure 6) of dimensions

$$L = 240 \text{ mm}, \quad b = 80 \text{ mm}, \quad \delta = 2 \text{ mm},$$

with the finite element mesh drawn in Figure 7, and the travel speed of the torch of 5 mm/sec, a set of isotherms can be drawn at different locations along the path of the arc, which are shown in Figure 8. Since the fusion of steel occurs in a temperature range from 1700 K to 1755 K, the travel of the interfaces can be readily determined as illustrated in Figure 9.

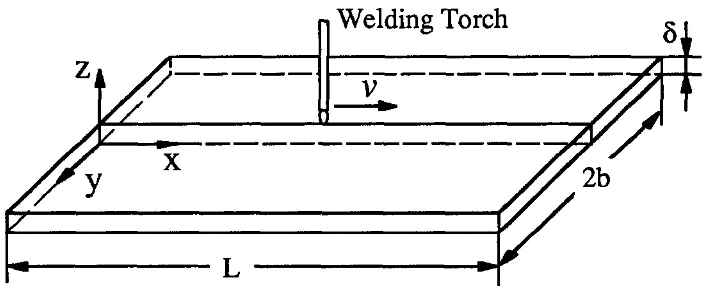


Figure 6. Schematic sketch of welding on a thin plate of mild steel

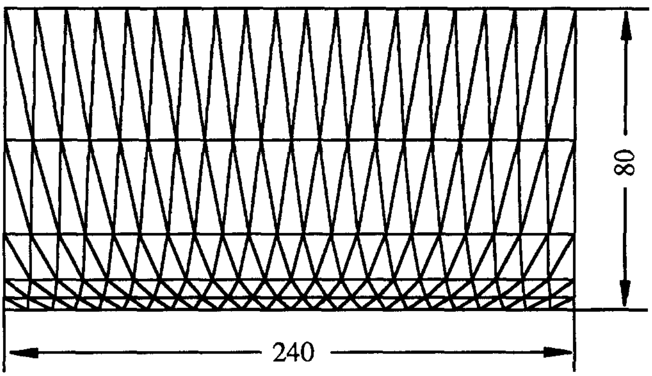
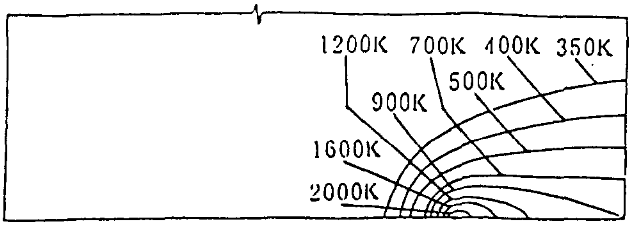
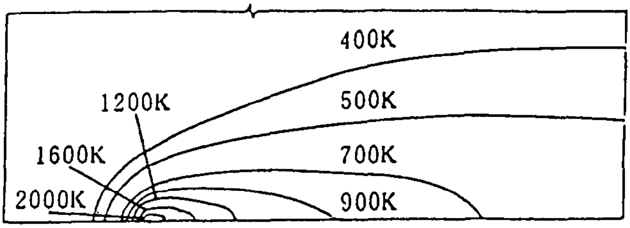


Figure 7. Finite element mesh of the thin plate



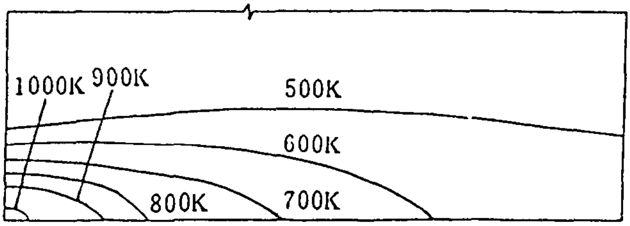
← Direction of the torch movement

(a) Isotherms at x=64 mm time=12.8 sec.



← Direction of the torch movement

(b) Isotherms at x=184 mm time=36.8 sec.



← Direction of the torch movement

(c) Isotherms at x=240 mm time=48 sec.

Figure 8. Temperature distributions as the arc travels along the plate

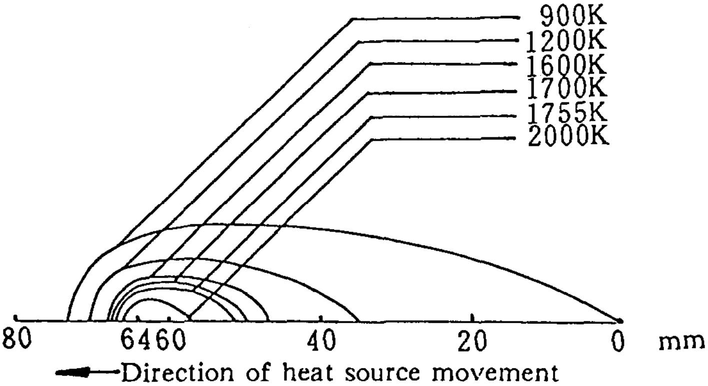


Figure 9. Position of interfacial moving boundaries at x=64 mm and time=12.8 sec. (enlargement of Figure 8(a))

CONCLUSION

From the above analysis of the one-dimensional heat conduction problem, it can be seen that the method of finite element analysis can be used to determine the movement of the interfacial boundaries of a material under a transient change of temperature with sufficient accuracy. It has been further applied to a two-dimensional case of welding plates. The calculated results are found to be in a satisfactory agreement with the experiment (Wang, 1984). Hence it can be concluded that, this method of analysis can also be used for the two-dimensional case. Further investigations will show that it can be used for three-dimensional problems as well.

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