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# A HEAT CONDUCTION PROBLEM INVOLVING PHASE CHANGE AND ITS NUMERICAL SOLUTION BY FINITE DIFFERENCE METHODS

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## 1. Introduction

It is well known that steel is a very complicated material. At certain critical temperatures its internal energy state changes abruptly. In this study different internal energy states are called phases. Every phase change process involves a latent heat which is absorbed or liberated depending on the direction of the phase change process. One well-understood example is the solidification (or melting) of steel.

At temperatures below the melting point of steel, several recrystallizations which are solid-solid phase change processes occur. Such structural changes involve a latent heat, one power of ten less than the latent heat of melting. All phase change processes of steel are very complex in that they may be accompanied by diffusion of carbon or carbon compounds.

Among the structural changes of steel the phase change process in a temperature range $U_1 \leqslant u \leqslant U_2$ which involves the three phases of pearlite, ferrite and austenite called austenitizing treatment is of great importance. Throughout the paper steel is assumed to be ferrite containing uniformly distributed grains of pearlite. In the following sections a mathematical model is developed for the description of the local temperature field in the neighbourhood of a pearlite grain during the austenitizing treatment. The size of a pearlite grain is approximately of the order of $10^{-5}$ metres. For the sake of simplicity a simple concept of carbon diffusion is used in the model.

## 2. Assumptions of the model

In the model the structural change into austenite is considered in a grain of pearlite and its surroundings of ferrite. Let the steel be preheated

in such a way that its initial temperature is a constant $U_0$, $U_0 < U_1$ throughout. As a consequence of internal heat sources the temperature rises with time during heat treatment. The structural change into austenite absorbs latent heat (recrystallization heat) in two steps. In the first step the grain of pearlite changes into austenite at temperature $U_1$. The corresponding latent heat $\lambda_1$ is a constant. The second is the phase change of ferrite into austenite at the moving boundary of the growing grain of austenite in a temperature range of $U_1 \leqslant u \leqslant U_2$. The structural change stops if all ferrite is replaced by austenite.

The mathematical model assumes that pearlite, ferrite and austenite are homogeneous materials with constant density $\varrho_{pe}, \varrho_{fe}, \varrho_{au}$, with constant heat conductivity $k_{pe}, k_{fe}, k_{au}$, and constant heat capacity $c_{pe}, c_{fe}, c_{au}$ respectively. The density differences between the three phases are ignored and a common density $\varrho = \frac{1}{3}(\varrho_{pe} + \varrho_{fe} + \varrho_{au})$ is used.

The considered austenitizing treatment is accompanied by carbon diffusion. The assumptions stated here are that the carbon concentration of pearlite is constant and equals $C_1$ while the carbon content of ferrite is neglected. In the following the shapes of the grains and its surroundings are supposed to be concentric spherical domains of radius $R_1$ and $R_2$ with a temperature field of spherical symmetry.

In the second step, the phase change temperature of ferrite into austenite depends on the carbon concentration in austenite. The latter is assumed to be only time dependent. Conservation of mass applied to the carbon content of the growing austenite ball of radius $s(t)$ gives

$$C_1 R_1^3 = c(t)s^3(t) = C_0 R_2^3.$$

Now the iron-carbon diagram shows that the phase change temperature decreases from $U_3$ for pure iron to $U_1$ for steel of a carbon concentration of $C_1$ (see Fig. 1). The linear function

$$U = U_3 - \frac{U_3 - U_1}{C_1} C$$

is a good approximation for this type of temperature-concentration dependence. From the above relations, the variable phase change tem-

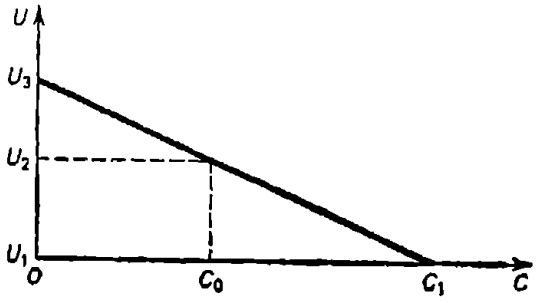


Fig. 1

perature is obtained by

$$U = U_3 - \frac{U_3 - U_1}{s^3(t)} R_1^3, \qquad R_1 \leqslant s(t) \leqslant R_2.$$

This phase change involves the constant latent heat $\lambda_2$.

### 3. Mathematical model

The mathematical model consists of two one-dimensional boundary value problems.

PROBLEM 1. *Find two functions $u(r, t)$ and $\bar{u}(r, t)$ so that the following equations hold:*

$$\varrho\left(c(u) + \lambda_1 \delta(u - U_1)\right)\frac{\partial u}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k(u)\frac{\partial u}{\partial r}\right) + f(u),$$

$$0 < r < R_1, \quad 0 < t \leqslant T_1,$$

$$\varrho c_{\mathrm{fe}}\frac{\partial \bar{u}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 k_{\mathrm{fe}}\frac{\partial \bar{u}}{\partial r}\right) + f_{\mathrm{fe}},$$

$$R_1 < r < R_2, \quad 0 < t \leqslant T_1,$$

$$u(r, 0) = U_0, \qquad 0 \leqslant r \leqslant R_1,$$

$$\bar{u}(r, 0) = U_0, \qquad R_1 \leqslant r \leqslant R_2,$$

$$\left.\frac{\partial u}{\partial r}\right|_{r=0} = 0,$$

$$u(R_1, t) = \bar{u}(R_1, t), \qquad 0 \leqslant t \leqslant T_1,$$

$$k(u)\left.\frac{\partial u}{\partial r}\right|_{r=R_1-0} = k_{\mathrm{fe}}\left.\frac{\partial \bar{u}}{\partial r}\right|_{r=R_1+0},$$

$$\left.\frac{\partial \bar{u}}{\partial r}\right|_{r=R_2} = 0,$$

*where*

$$c(u) = \begin{cases} c_{\mathrm{pe}}, & u \leqslant U_1, \\ c_{\mathrm{au}}, & u > U_1, \end{cases}$$

$$k(u) = \begin{cases} k_{\mathrm{pe}}, & u \leqslant U_1, \\ k_{\mathrm{au}}, & u > U_1. \end{cases}$$

The heat source terms are expressed by

$$f(u) = \begin{cases} f_{\mathrm{pe}}, & u \leqslant U_1, \\ f_{\mathrm{au}}, & u > U_1, \end{cases} \quad \text{and} \quad f_{\mathrm{fe}}.$$

By $\delta(u)$ the Dirac delta function is denoted.

At the time level $t = T_1$ defined by

$$T_1 = \min_{t>0} \{t: \min_{0 \leqslant r \leqslant R_1} u(r, t) > U_1\}$$

the pearlite has changed into austenite. The initial distribution of the second step is then defined by

$$\varphi(r) = u(r, T_1), \quad 0 \leqslant r \leqslant R_1,$$

$$\bar{\varphi}(r) = \bar{u}(r, T_1), \quad R_1 < r \leqslant R_2.$$

PROBLEM 2. *Find functions* $u(r, t)$, $s(t)$, $\bar{u}(r, t)$ *satisfying the equations*

$$\varrho c_{\mathrm{au}} \frac{\partial u}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k_{\mathrm{au}} \frac{\partial u}{\partial r} \right) + f_{\mathrm{au}},$$

$$0 < r < s(t), \; T_1 < t \leqslant T_2,$$

$$\varrho c_{\mathrm{fe}} \frac{\partial \bar{u}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 k_{\mathrm{fe}} \frac{\partial \bar{u}}{\partial r} \right) + f_{\mathrm{fe}},$$

$$s(t) < r < R_2, \; T_1 < t \leqslant T_2,$$

$$u(r, T_1) = \varphi(r), \quad 0 \leqslant r \leqslant R_1,$$

$$\bar{u}(r, T_1) = \bar{\varphi}(r), \quad R_1 < r \leqslant R_2,$$

$$\left. \frac{\partial u}{\partial r} \right|_{r=0} = 0, \quad T_1 \leqslant t \leqslant T_2,$$

$$u(s(t), t) = \bar{u}(s(t), t) = U_3 - \frac{U_3 - U_1^*}{s^3(t)} R_1^3, \quad T_1 < t \leqslant T_2,$$

$$\varrho \lambda_2 s'(t) = k_{\mathrm{fe}} \left. \frac{\partial \bar{u}}{\partial r} \right|_{r=s+0} - k_{\mathrm{au}} \left. \frac{\partial u}{\partial r} \right|_{r=s-0}, \quad T_1 < t \leqslant T_2,$$

$$\left. \frac{\partial \bar{u}}{\partial r} \right|_{r=R_2} = 0, \quad T_1 \leqslant t \leqslant T_2,$$

$$s(T_1) = R_1.$$

At the time level $T_2$ defined by $s(T_2) = R_2$ the ball of radius $R_2$ has changed into austenite.

Generally $\varphi(R_1) = U_1$ cannot be expected. To guarantee the continuity of the solution at the time level $t = T_1$ the temperature $U_1$ is replaced by $U_1^* = \varphi(R_1)$. Problem 2 is a two-phase Stefan problem with variable temperature at the moving boundary.

Three situations of the mathematical model at different time levels of the structural change into austenite are illustrated in Figure 2.

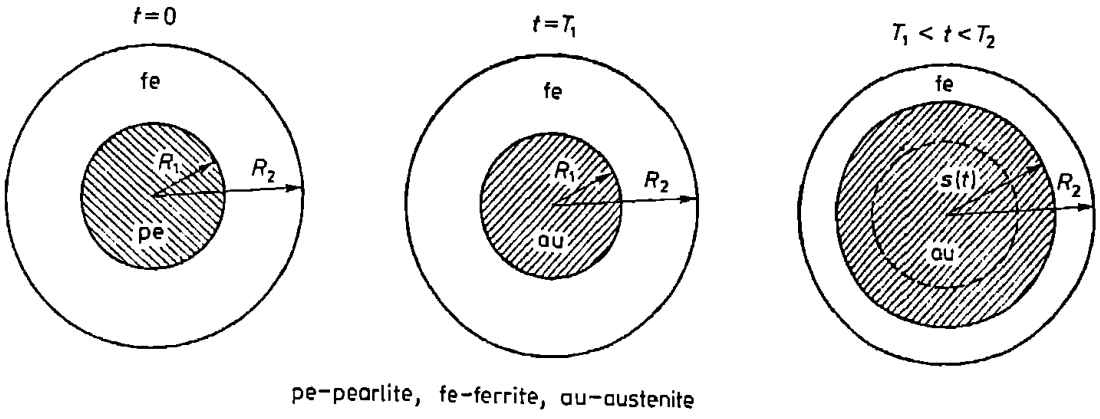


Fig. 2

## 4. Numerical solution by finite difference methods

Let $\overline{\omega}_{h\tau}$ be a mesh defined by the mesh points $(r_i, t_n)$:

$$\overline{\omega}_{h\tau} = \Big\{(r_i, t_n),\ r_i = ih,\ i = 0, \ldots, N_1, \ldots, N_2,\ N_1 h = R_1,\ N_2 h = R_2,$$

$$t_n = n\tau,\ n = 0, \ldots, M_1,$$

$$t_n = t_{M_1} + \sum_{M_1+1 \leqslant j \leqslant n} \tau_{j-M_1},\ n = M_1+1, \ldots, M_1+N_2-N_1\Big\},$$

where $M_1$ is a priori unknown.

The numerical solution of Problem 1 is based on implicite difference methods. For numerical reasons, the Dirac delta function $\delta(u-U_1)$ is approximated by a function $\delta_\Delta(u) \geqslant 0$ with

$$\delta_\Delta(u) = 0 \quad \text{for} \quad |u-U_1| > \Delta,$$

$$\int_{U_1-\Delta}^{U_1+\Delta} \delta_\Delta(u)\,du = 1.$$

There are several ways of choosing $L_2$ or $C^k$ $(k \geqslant 0)$ approximations for the delta function. Such an approximation can be interpreted as a distribution of the latent heat in the first step over the interval $U_1-\Delta < u < U_1+\Delta$. Thus the phase-change region consists of all mesh points $r_i$ for which the approximate values $y_{i,n}$ of the temperature $u(r_i, t_n)$ satisfy $U_1-\Delta < y_{i,n} < U_1+\Delta$. The crucial point of the method is the choice of the parameter $\Delta$. It must be great enough to ensure that sufficiently many mesh points are in the phase change region and, on the other hand, $\delta_\Delta(u)$ must be a good approximation of the delta function. Similar questions occur using $C^k$ $(k \geqslant 0)$ approximations for $c(u)$ and $k(u)$.

The approximation of Problem 1 by a system of finite difference equations is given in Problem 1′.

PROBLEM 1'.

$$\varrho\left(c(y_{i,n})+\lambda_1\delta_\Delta(y_{i,n})\right)y_{\bar{t},i,n}=\frac{1}{r_i^2}\left(r_{i-1/2}^2 k\left(\frac{y_{i-1,n}+y_{i,n}}{2}\right)y_{\bar{r},i}\right)_{r,i,n}+f(y_{i,n}),$$

$$i=1,\ldots,N_1-1,\ n=1,\ldots,M_1,$$

$$\varrho c_{\mathrm{fe}}\bar{y}_{\bar{t},i,n}=\frac{1}{r_i^2}\left(r_{i-1/2}^2 k_{\mathrm{fe}}\bar{y}_{\bar{r},i}\right)_{r,i,n}+f_{\mathrm{fe}},$$

$$i=N_1+1,\ldots,N_2-1,\ n=1,\ldots,M_1,$$

$$y_{i,0}=U_0,\quad i=0,\ldots,N_1,$$

$$\bar{y}_{i,0}=U_0,\quad i=N_1+1,\ldots,N_2,$$

$$y_{r,0,n}=0,$$

$$k\left(\frac{y_{N_1-1,n}+y_{N_1,n}}{2}\right)y_{\bar{r},N_1,n}=k_{\mathrm{fe}}\bar{y}_{r,N_1,n},\quad n=1,\ldots,M_1,$$

$$y_{N_1,n}=\bar{y}_{N_1,n},$$

$$\bar{y}_{\bar{r},N_2,n}=0.$$

Using through-count finite difference schemes ([1], [2]), the nonlinear system of difference equations in Problem 1' is solved by iterative methods for quasilinear parabolic equations, see [1]. Then the integer $M_1$ is defined by

$$M_1=\min_n\left(n:\ \min_{1\leqslant i\leqslant N_1}y_{i,n}>U_1+\Delta\right)$$

and $t=t_{M_1}$ may be regarded as an approximation of $T_1$. The discrete initial distribution for the numerical solution of Problem 2 is given by

$$\varphi_i=y_{i,M_1},\quad i=0,\ldots,N_1,$$

$$\bar{\varphi}_i=\bar{y}_{i,M_1},\quad i=N_1,\ldots,N_2.$$

The finite difference method for Problem 2 is based on a well-known front tracking approach studied in many previous papers. The time steps $\tau_{n-M_1}$ have to be determined so that the free boundary moves from the mesh point $r_{N_1+n-M_1-1}$ to $r_{N_1+n-M_1}$ during the time $\tau_{n-M_1}=t_n-t_{n-1}$, $n=M_1+1,\ldots,M_1+N_2-N_1$.

PROBLEM 2'.

$$\varrho c_{\mathrm{au}}\frac{y_{i,n}-y_{i,n-1}}{\tau_{n-M_1}}=\frac{1}{r_i^2}\left(r_{i-1/2}^2 k_{\mathrm{au}}y_{\bar{r},i}\right)_{r,i,n}+f_{\mathrm{au}},$$

$$i=1,\ldots,N_1+n-M_1-1,$$

$$n=M_1+1,\ldots,M_1+N_2-N_1,$$

$$\varrho c_{\mathrm{fe}} \frac{\bar{y}_{i,n}-\bar{y}_{i,n-1}}{\tau_{n-M_1}} = \frac{1}{r_i^2}\left(r_{i-1/2}^2 k_{\mathrm{fe}} \bar{y}_{\bar{r},i}\right)_{r,i,n} + f_{\mathrm{fe}},$$

$$i = N_1+n-M_1+1, \ldots, N_2-1,$$

$$n = M_1+1, \ldots, M_1+N_2-N_1-2,$$

$$y_{i,M_1} = \varphi_i, \quad i = 0, \ldots, N_1,$$

$$\bar{y}_{i,M_1} = \bar{\varphi}_i, \quad i = N_1, \ldots, N_2,$$

$$y_{r,0,n} = 0, \quad n = M_1+1, \ldots, M_1+N_2-N_1,$$

$$y_{N_1+n-M_1,n} = \bar{y}_{N_1+n-M_1,n} = U_3-(U_3-U_1^*)\left(\frac{r_{N_1}}{r_{N_1+n-M_1}}\right)^3,$$

$$\varrho\lambda_2 \frac{h}{\tau_{n-M_1}} = k_{\mathrm{fe}} \bar{y}_{r,N_1+n-M_1,n} - k_{\mathrm{au}} y_{\bar{r},N_1+n-M_1,n},$$

$$n = M_1+1, \ldots, M_1+N_2-N_1-1,$$

$$\bar{y}_{\bar{r},N_2,n} = 0, \quad n = M_1+1, \ldots, M_1+N_2-N_1-1,$$

$$\tau_{M_1+N_2-N_1} = \tau_{M_1+N_2-N_1-1}.$$

The algorithm proposed in Problem 2′ has been investigated for a more general Stefan problem, characterized by variable temperature at the moving boundary and inhomogeneous heat equations formulated by cartesian coordinates in [3]. The system of nonlinear difference equations may be solved by well-known iterative techniques, used in [3], or by the application of Newton's method [4].

## 5. Results

The proposed mathematical model for a local temperature field of a structural change into austenite in a small spherical grain has been used to compute the time-delay of temperature growth. Because the diameters of the considered balls are small, the computed approximate values $y_{i,n}$ and $\bar{y}_{i,n}$ for the temperature differ only in the last decimal places, i.e. the temperature over one such spherical grain is at any time level virtually constant. If a constant growth of the temperature is assumed, then, as a consequence of the phase change in the first step, the temperature growth stops temporarily at the temperature $U_1$. After the first step the slope of the temperature growth is smaller than the original one because part of the supplied heat is absorbed at the moving boundary. At time level $t_{M_1+N_2-N_1}$, which may be considered as an approximation

of $T_2$, all ferrite is replaced by austenite and subsequently the growth of the temperature is the same as before (see Fig. 3).

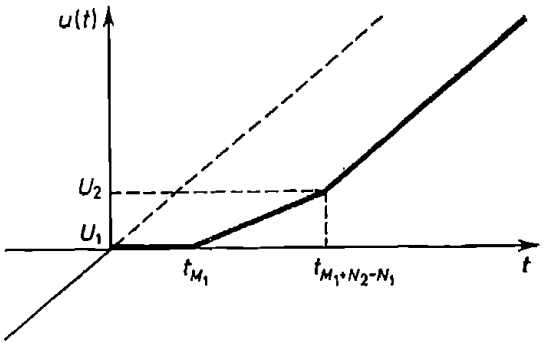


Fig. 3

From measurements of the interior of the samples during the austenitizing treatment, it is known that the temperatures $u(t)$ alter in the above manner.

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