

A Comparative Study of Methods Used for the Prediction of Nonisothermal Austenite Decomposition

T. Réti, L. Horváth, and I. Felde

In this paper, different phenomenological procedures applied to the prediction of the progress of nonisothermal austenite transformation are analyzed and compared. It is shown, that by formal generalization of the isothermal Avrami kinetic function, various types of kinetic differential equations can be generated. These are suitable for the phenomenological description of nonisothermal, diffusion-controlled, transformation processes. First, fundamental features of generalized kinetic differential equations and the additivity rule are discussed. Next, practical applications for prediction purposes are tested on the basis of dilatometric experiments.

When studying the austenite/pearlite transformation in a low alloy eutectoid steel, transformation kinetics were measured under isothermal and nonisothermal conditions. Dilatometric measurements verified that both the "semiadditive" kinetic differential equations and the additivity rule can be successfully applied to predict the progress of nonisothermal austenite/pearlite transformation. It was found that the selected Avrami type semiadditive differential equation and the application of the additivity rule furnish practically identical results. This is due to the fact that there is a close theoretical relationship between the kinetic differential equations of separable types and the additivity principle.

Keywords distortion prediction, phase transformation, process modeling, transformation modeling

1. Introduction

Starting with theoretical considerations, five prediction methods (based on the use of differential equations, the additivity principle, and an integro-differential equation of special form) are discussed and compared. The validity of different phenomenological methods applied to the prediction of the progress of austenite/pearlite transformation are critically examined.

For this purpose, isothermal and nonisothermal dilatometric measurements are performed on a low alloy eutectoid steel. Comparing the five methods, it is shown that the kinetics of nonisothermal austenite/pearlite transformation in the selected eutectoid steel can be successfully predicted using both the Avrami type generalized "semiadditive" kinetic differential equation and the additivity principle.

2. Theoretical Background

Before presenting the description of the investigations based on dilatometric experiments and computer simulation, the theoretical background of prediction methods applied are outlined and definitions and notations are introduced. They concern the basic properties of kinetic differential equations, the additivity rule, and the integro-differential equations selected for the description of the diffusional austenite decomposition.

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2.1 Kinetic Differential Equations

In general, a mathematical model of transformation kinetics consists of a set of algebraic or differential equations that quantitatively represent the progress of the process as a function of time.

As a first step, the traditional isothermal kinetic function is defined as:

$$F(t, y, \dot{T}) = 0 \quad (\text{Eq 1})$$

where t is the time, y is the amount of material transformed, T is the temperature, and F is an appropriately selected real function. The kinetic function given by Eq 1 should ensure the satisfaction of the following conditions:

$$y(t, T) = 0 \quad \text{if} \quad t \leq t_T \quad (\text{Eq 2.1})$$

$$\frac{dy}{dt} \geq 0 \quad \text{if} \quad t \geq t_T \quad (\text{Eq 2.2})$$

$$\lim y(t, T) = Y_e \quad \text{if} \quad t \rightarrow \infty \quad (\text{Eq 2.3})$$

where t_T is the incubation time at a specific temperature and $Y_e = Y_e(T)$ is the total amount of transformation product at the condition of equilibrium. If $Y_e = 1$, the reaction complete; if $Y_e < 1$, then it is incomplete by definition.

In many cases, the modeling and the phenomenological description of nonisothermal transformations are based on the application of an ordinary differential equation given by:

$$\frac{dy}{dt} = f_0(t, y, T) f_1(t, y, T, \dot{T})$$

$$y(t_T) = 0 \quad (\text{Eq 3})$$

where $\dot{T} = dT/dt$ is the rate of temperature change, and f_0 and f_1 are nonnegative functions. It is assumed in Eq 3 that

$$f_1(t, y, T, \dot{T}) \equiv 1$$

if the temperature is constant, that is, $\dot{T} = 0$.

Most kinetic differential equations can be classified into two main categories: additive differential equations and semiadditive differential equations (Ref 1-3).

A kinetic differential equation is said to be additive if it has the form:

$$\frac{dy}{dt} = K_A(T)H_A(y) \quad (\text{Eq 4})$$

A kinetic differential equation is called semiadditive if it can be written in the form:

$$\frac{dy}{dt} = H(y, T) \quad (\text{Eq 5})$$

Consequently, a transformation process described by Eq 4 or 5 is called an additive or semiadditive process, respectively.

According to the definitions stated above, every additive kinetic differential equation is semiadditive. The special characteristic of Eq 4 and 5 are that the instantaneous transformation rate is solely a function of the fraction transformed y and the transformation temperature T . The main property of additive kinetic differential equations is that they are separable with respect to T and y .

In the majority of cases, kinetic differential equations can be formulated in the following factorized form (Ref 4):

$$\frac{dy}{dt} = [Y_e(T) - y]H_B(t, y, T) \\ y(t_T) = 0 \quad (\text{Eq 6})$$

where H_B is a nonnegative function and $H_B(t, y, T) = 0$ if $t = t_T$ at constant temperature. The term $[Y_e(T) - y]$ is referred to as the "impingement" factor (Ref 2).

Kinetic differential equations of practical interest can be written in the following generalized form:

$$\frac{dy}{dt} = K_R[Y_e - y]^\alpha y^\beta \left[\ln \frac{Y_e}{y_e - y} \right]^\gamma \left[\left(\frac{Y_e}{y_e - y} \right)^\epsilon - 1 \right]^\eta \quad (\text{Eq 7})$$

where $\alpha, \beta, \gamma, \epsilon, \eta$, and K_R are appropriately selected composition, microstructure, and temperature dependent parameters (Ref 5). Generally, the differential equation represented by formula in Eq 7 cannot be integrated in a closed form. From this, it follows that their parameters can be determined only by measuring y and dy/dt values simultaneously. The temperature dependent parameters $\alpha, \beta, \gamma, \epsilon, \eta$, and K_R can be calculated more easily if the values y and dy/dT (i.e., the derivative of y

with respect to temperature) are directly measured by performing nonisothermal dilatometric investigations. A concrete practical application of this method is demonstrated in Ref 6.

In some special cases, by applying appropriately selected parameters, the differential equation (Eq 7) can be integrated in a closed form. For example, by selecting the following parameters in Eq 7:

$$\begin{aligned} \alpha &= p + 1 \quad (p > 0) \\ \beta &= \gamma = 0 \\ \epsilon &= p \\ \eta &= \frac{m-1}{m} \quad (m \geq 1) \\ K_R &= \frac{m}{p} \frac{K_T^{1/m}}{Y_e^p} \end{aligned} \quad (\text{Eq 8})$$

The differential Eq 7 can be transformed into a simplified form:

$$\frac{dy}{dt} = \frac{m}{p} \frac{K_T^{1/m}}{Y_e^p} [Y_e - y]^{p+1} \left[\left(\frac{Y_e}{Y_e - y} \right)^p - 1 \right]^{(m-1)/m} \quad (\text{Eq 9})$$

Originally Eq 9 was used for predicting the nonisothermal austenite/ferrite reaction in hypoeutectoid steels (Ref 7, 8). If the kinetic parameters in Eq 9 are considered to be constant, its solution is given as:

$$y(t) = Y_e \left\{ 1 - [1 + K_T t^m]^{-1/p} \right\} \quad (\text{Eq 10})$$

If $p = 1$, then Eq 10 reduces to the well known Austin-Rickett's kinetic function (Ref 9, 10). Due to this fact, Eq 10 is referred to as a generalized Austin-Rickett's kinetic equation.

It follows from the previous considerations, that differential Eq 7 is semiadditive if their parameters $\alpha, \beta, \gamma, \epsilon, \eta$, and K_R are independent of time, and it is additive if $\alpha, \beta, \gamma, \epsilon, \eta$, and K_R are constant. As previously mentioned, differential Eq 7 can be solved generally by using numerical methods, for example, by applying the generalized recursive algorithm (Ref 11).

2.2 Avrami Type Generalized Kinetic Differential Equations

Kinetic differential equations can be derived from basic physical laws, but it is possible to generate them on the basis of the known isothermal kinetic functions (Ref 1). When constructing kinetic differential equations for prediction purposes, the study concentrated on the commonly used Avrami equation defined as:

$$y(t) = Y_e \left\{ 1 - \exp [-K t^n] \right\} \quad (\text{Eq 11})$$

where K, n , and Y_e are the temperature and composition dependent parameters (Ref 3, 12, 13).

The Avrami Eq 11 can be extended to a nonisothermal condition in several other manners. The simplest way of generat-

ing a kinetic differential equation from Avrami's law is to differentiate Eq 11 with respect to time. Thus (Ref 14):

$$\frac{dy}{dt} = Y_e n K t^{n-1} \exp \{-K t^n\} \quad (\text{Eq 12})$$

Another type of generalized kinetic differential equation is given as:

$$\frac{dy}{dt} = n K^{1/q} t^{(n-q)/q} [Y_e - y] \left[\ln \frac{Y_e}{Y_e - y} \right]^{(q-1)/q} \quad (\text{Eq 13})$$

where n and q are nonnegative temperature dependent parameters.

Differential equations (Eq 12, 13) are referred to as the Avrami type generalized kinetic functions because by solving them under isothermal conditions, the Avrami equation (Eq 11) can be obtained as a special case. Some typical properties of Eq 13 are parameters n and K can be estimated from isothermal measurements, but in order to compute the parameter q , it is necessary to perform experiments at varying temperatures (i.e., by using linear cooling or heating). Because the right-hand side of Eq 13 depends on time explicitly, Eq 13 is not semiadditive. The function $\delta(T)$, defined as:

$$\delta(T) = \frac{n(T)}{q(T)} \quad (\text{Eq 14})$$

can be considered a quantitative measure of semiadditivity. It follows that the kinetic differential equation (Eq 13) is semiadditive if $\delta(T) \equiv 1$. If q is constant and $Y_e = 1$, the solution of Eq 13 is

$$y(t) = 1 - \exp \left\{ - \left[\frac{1}{q} \int_0^t n K^{1/q} t_u^{(n-q)/q} dt_u \right]^q \right\} \quad (\text{Eq 15})$$

If q and n are constant and $q = n$, and $Y_e = 1$, then Eq 13 will be additive. In this case, the solution can be reduced to the form

$$y(t) = 1 - \exp \left\{ - \left[\int_0^t K^{1/n} dt_u \right]^n \right\} \quad (\text{Eq 16})$$

2.3 Additivity Rule

The additivity rule was proposed by Scheil (Ref 15) to predict the start of transformation, that is, the incubation time under nonisothermal conditions. Later, it was extended to the entire range of transformed fractions (Ref 2, 3, 16-19).

The additivity rule is considered a special algorithm for predicting the nonisothermal transformation (CCT curves) on the basis of the previously known isothermal kinetic function (TTT curves) (Ref 20-23). It can be formulated by the following equation. Consider the isothermal time $\tau(y, T)$ at which the re-

action reached a certain fraction of completion y . On changing the temperature as a function of time, the integral:

$$G(t, y) = \int_0^t \frac{dt_u}{\tau(y, T)} \quad (\text{Eq 17})$$

equals unity in that time $t = t_f$ when the fraction transformed reaches the preselected y_f , that is, $G(t_f, y_f) = 1$.

Beginning with Eq 17, several conclusions can be drawn. It can be proven that if a kinetic differential equation is additive, the same fraction y is predicted by applying the additivity rule and by solving the differential equation (Eq 4) (Ref 2, 3, 24-26). From this, it immediately follows that the use of Eq 4 and the application of the additivity rule lead to identical results. Conversely, if a kinetic differential equation is nonadditive, the results computed by the two methods will be theoretically different.

The traditional additivity rule given by Eq 17 can be generalized in the following form:

$$G(t, y) = \int_0^t \frac{dt_u}{\tau(y, T) f_2(t_u, T, \dot{T})} \quad (\text{Eq 18})$$

where f_2 is a nonnegative weighting function for which:

$$f_2(t, T, \dot{T}) \equiv 1$$

is fulfilled if $\dot{T} = 0$ (Ref 27). Function f_2 , which takes into account the influence of rate of temperature change on the rate of nonisothermal transformation, can be defined in several ways. In practice, it can be given in the form:

$$f_2(t, T, \dot{T}) \equiv 1 + \kappa \dot{T} \quad (\text{Eq 19.1})$$

or

$$f_2(t, T, \dot{T}) \equiv \exp(-\kappa \dot{T}) \quad (\text{Eq 19.2})$$

where κ is a constant or a temperature and/or time dependent parameter. If $f_2(t, T, \dot{T}) \equiv 1$, then the conventional additivity principle represented by Eq 17 is a special case.

Based on the generalized additivity formula (Eq 18), a nonisothermal kinetic differential equation can be generated in the form (Ref 27):

$$\frac{dy}{dt} = - \frac{\frac{\partial G}{\partial t}}{\frac{\partial G}{\partial y}} = - \frac{\left[\frac{\partial}{\partial y} \int_0^t dt_u / [\tau(y, T) f_2(t_u, T, \dot{T})] \right]^{-1}}{\tau(y, T) f_2(t, T, \dot{T})} \quad (\text{Eq 20})$$

where $G(t, y) = 1$ and $y(0) = 0$.

If the function $\tau(y, T)$, characterizing the isotherm transformation time, is separable with respect to y and T , then the solution of the differential equation can be easily generated. In this case, $\tau(y, T)$ can be written as:

$$\tau(y, T) = \tau_1(y)\tau_2(T) \quad (\text{Eq 21})$$

and the differential equation (Eq 20) is simplified to the form:

$$\frac{dy}{dt} = \frac{[d\tau_1(y)/dy]^{-1}}{\tau_2(T)f_2(t, T, \dot{T})} \quad (\text{Eq 22})$$

Integrating this formula:

$$\tau_1(y) = \int_0^t \frac{dt_u}{\tau_2(T)f_2(t_u, T, \dot{T})} \quad (\text{Eq 23})$$

where $\tau_1(0) = 0$. Assuming that the inverse function τ_1^{inv} exists, the solution $y(t)$ can be generated as (Ref 27):

$$y(t) = \tau_1^{\text{inv}} \left\{ \int_0^t \frac{dt_u}{\tau_2(T)f_2(t_u, T, \dot{T})} \right\} \quad (\text{Eq 24})$$

Equation 24 makes it possible to derive nonisotherm kinetic equations from known isotherm kinetic functions. The method can generally be applied to every transformation process for which Eq 21 is fulfilled. For example, beginning with the Avrami function (Eq 11) and then supposing that $Y_e = 1$ and n is constant, the following Avrami type generalized kinetic function is:

$$y(t) = 1 - \exp \left\{ - \left[\int_0^t \frac{K^{1/n}}{f_2(t_u, T, \dot{T})} dt_u \right]^n \right\} \quad (\text{Eq 25})$$

If $f_2(t, y, T, \dot{T}) \equiv 1$, then Eq 25 will be identical to Eq 16. It must be noted that the parameters of weighting function f_2 in Eq 25 can be estimated only by performing nonisothermal experiments.

2.4 Integro-Differential Equations Used for the Prediction of Nonisothermal Transformation

Some authors use integro-differential equations for prediction purposes (Ref 2, 29-32). In many practical cases, these equations are formulated in the following form:

$$\frac{dy}{dt} = (Y_e - y) \cdot J[t, y, T] \\ y(0) = 0 \quad (\text{Eq 26})$$

where $J[t, y, T]$ is a definite integral over the time interval $(0, t)$.

The integro-differential equation of the simplest type can be obtained from the Avrami's transformation theory (Ref 3, 12, 13, 33), and it can be written as:

$$\frac{dy}{dt} = (Y_e - y) \int_0^t n[n - 1]K(T)[t - t_u]^{n-2} dt_u \quad (\text{Eq 27})$$

where $n = n(T) > 1$.

The solution of Eq 27 can be obtained by transforming the integral into the following form:

$$\int_0^t n[n - 1]K(T)[t - t_u]^{n-2} dt_u = \int_0^t nK(T) \frac{\partial}{\partial t} \{[t - t_u]^{n-1}\} dt_u \\ = \frac{d}{dt} \int_0^t nK(T)[t - t_u]^{n-1} dt_u \quad (\text{Eq 28})$$

By inserting the formula of Eq 28 in Eq 27, and integrating with respect to time:

$$y(t) = Y_e \left\{ 1 - \exp \left[- \int_0^t nK(T)[t - t_u]^{n-1} dt_u \right] \right\} \quad (\text{Eq 29})$$

It can be easily verified, that with constant temperature, Eq 29 is identical to the Avrami law (Eq 11, Ref 11). A special form of the kinetic function (Eq 29) has been used mainly by Japanese authors for predicting nonisothermal diffusion controlled transformations (Ref 28-30).

Integro-differential equations can also be constructed from isothermal kinetic functions by using the differential equation (Eq 20), which was generated on the basis of the extended additivity principle given by Eq 18. This method is demonstrated by the following example. Starting with the Avrami equation (Eq 11, Ref 11), and assuming that $Y_e = 1$ and n is constant (Eq 20), then:

$$\frac{dy}{dt} = V(t, y) \frac{K^{1/n}}{f_2(t, T, \dot{T})} [1 - y] \left\{ \ln \left(\frac{1}{1 - y} \right) \right\}^{1-1/n} \quad (\text{Eq 30})$$

where $V(t, y)$ is defined as:

$$V(t, y) = \left[\int_0^t \frac{dt_u}{n(T)\tau(y, T)f_2(t_u, T, \dot{T})} \right]^{-1} \quad (\text{Eq 31})$$

and $G(t, y_s) = 1$. Consequently, if the Avrami exponent n is constant, it follows from Eq 30 and 31 that $V(t, y) = n$. In this case, integro-differential Eq 30 will simplify to the form:

$$\frac{dy}{dt} = \frac{nK^{1/n}}{f_2(t, T, \dot{T})} [1 - y] \left\{ \ln \left(\frac{1}{1 - y} \right) \right\}^{1-1/n} \quad (\text{Eq 32})$$

From the preceding equations, it follows that in the case of constant Avrami exponent n , the solution of differential Eq 32 will be identical to the formula of Eq 25.

3. Investigations Based on Dilatometric Measurements and Computer Simulation

3.1 Experimental Analysis of Kinetics of Austenite-Pearlite Transformation

To compare the different phenomenological models selected for predicting the progress of nonisothermal austenite decomposition, experiments were performed on a low alloy eutectoid steel (0.78% C-0.31% Si-0.41% Mn-0.96% Ni-0.28% Cr). The basic material, a hot rolled steel bar, was homogenized in oxygen-free argon at 1200 °C for 10 h to remove the banding by high temperature treatment. To study the pearlite transformation behavior, specimens were austenitized at 1000 °C for 20 min and cooled by argon according to specified time-temperature programs. The progress of pearlite transformation during isothermal holding in the 598 to 646 °C temperature range and continuous cooling was measured in a vacuum dilatometer, with argon rinsing, using a highly accurate temperature control.

When studying the isothermal austenite decomposition, the austenitized specimens were immediately cooled by argon to various temperatures below the eutectoid temperature ($A_{e1} = 688$ °C) and held at these temperatures to transform into pearlite. Figure 1 shows isothermal kinetic curves for specimens transformed at temperatures of 598, 617, and 638 °C.

To describe the isothermal austenite/pearlite transformation in the temperature range of 598 to 646 °C, the authors chose the Avrami kinetic function. Taking into consideration that the austenite-pearlite transformation is complete, and that $Y_e = 1$, the Avrami function can be given in a simplified form:

$$y(t) = 1 - \exp \{-K(T)t^n(T)\} \quad (\text{Eq 33})$$

Parameters K and n were estimated by nonlinear regression analysis, using the measured reaction fractions obtained from isothermal dilatometric tests.

Table 1 gives the measured values of the Avrami exponent. As can be observed, parameter n is not constant in the investigated temperature interval, but it is a monotonic decreasing function of temperature.

The temperature-dependent kinetic parameters of the Avrami equation were approximated by continuous exponential type functions defined as:

$$K(T) = \exp \left[A_0 + A_1(T - 562)^2 + A_2 \frac{1}{(T - 688)^2 T} \right] \quad (\text{Eq 34})$$

and

$$n(T) = 3.4 + \exp[N_0 + N_1 T + N_2 T^2] \quad (\text{Eq 35})$$

where $A_0 = -14.2144$, $A_1 = 1.0388 \times 10^{-3}$, $A_2 = -8927517$, $N_0 = -389$, $N_1 = 1.3115$, and $N_2 = -1.10517 \times 10^{-3}$. Table 1 also gives values of the Avrami exponent calculated by Eq 33. Figure 2 shows the TTT diagram describing the isothermal,

austenite-pearlite transformation. It was calculated using Eq 33 to 35.

To analyze the pearlite formation during continuous cooling with constant rates of temperature, specimens held at the austenitizing temperature were first gas cooled to 684 ± 3 °C and cooled with the following cooling rates: 0.17, 0.38, 0.85, and 1.1 K/s. Figure 3 illustrates the kinetics of pearlite transformation for different cooling rates. Transformation kinetics related to the cooling rate of 1.1 K/s were excluded from investigations because a considerable amount of austenite transformed into bainite during cooling.

3.2 Computer Simulation Performed for the Prediction of Nonisothermal Austenite-Pearlite Transformation

To predict the austenite-pearlite transformation during linear cooling, the following methods were selected for testing:

- Additivity rule represented by Eq 17
- Integro-differential equation given by Eq 27
- Three kinetic differential equations generated from Eq 12 and 13

It is important to note that all five methods are based on the use of the Avrami law given by Eq 33. The solution of the selected integro-differential equation results from the formula of Eq 29, as a special case, assuming that $Y_e = 1$ for pearlitic reaction in a eutectoid steel:

$$y_A(t) = 1 - \exp \left[- \int_0^t nK(T)[t - t_u]^{n-1} dt_u \right] \quad (\text{Eq 36})$$

Table 1 Measured and calculated values of Avrami exponent, n

Method	Avrami exponent, n					
	598 °C	609 °C	617 °C	630 °C	638 °C	688 °C
Measured values	4.48	4.21	3.97	3.65	3.52	...
Calculated by Eq 35	4.466	4.233	3.988	3.647	3.521	3.4

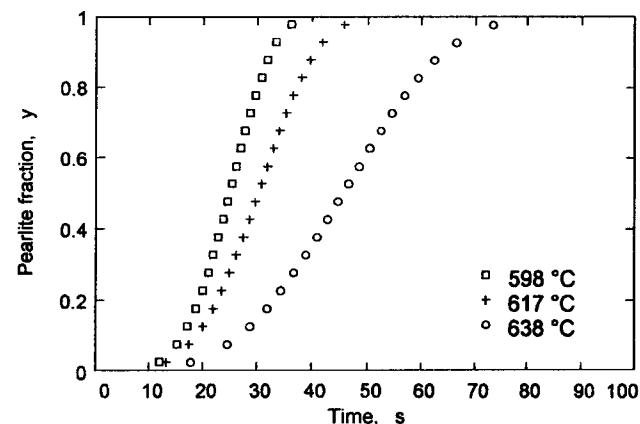


Fig. 1 Isothermal kinetic curves for specimens transformed at different temperatures

The selected kinetic differential equations were the following:

$$\frac{dy_B}{dt} = nKt^{n-1} \exp \{-Kt^n\} \quad (\text{Eq 37})$$

$$\frac{dy_C}{dt} = nKt^{n-1}(1 - y_C) \quad (\text{Eq 38})$$

$$\frac{dy_D}{dt} = nK^{1/n} [-\ln(1 - y_D)]^{(n-1)/n} (1 - y_D) \quad (\text{Eq 39})$$

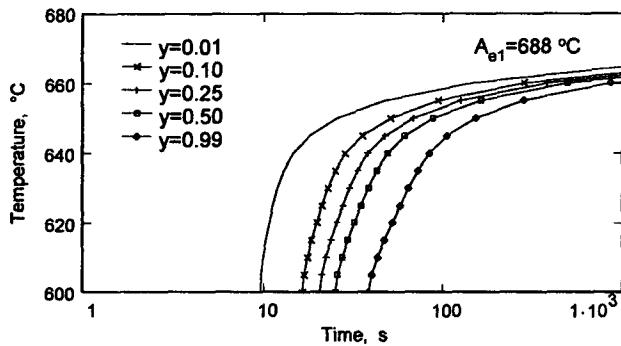


Fig. 2 TTT diagram of the eutectoid steel investigated

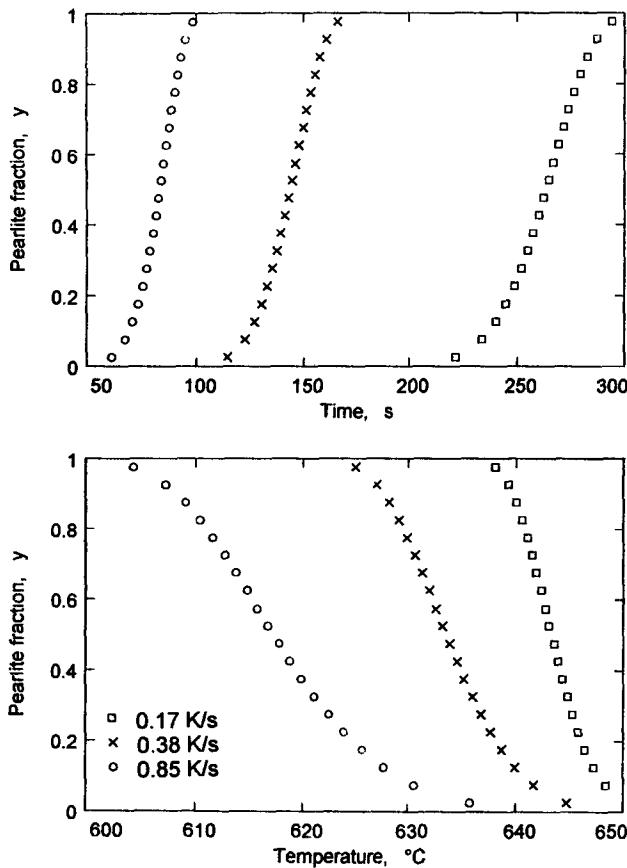


Fig. 3 Nonisothermal transformation kinetics related to different cooling rates

In the case of $Y_e = 1$, Eq 37 is identical to Eq 12. Equations 38 and 39 are considered to be special cases of Eq 13. Starting with Eq 13 and assuming that $Y_e = 1$, Eq 38 can be obtained by selecting $q(T) = 1$, while Eq 39 can be obtained if $q(T) = n(T)$ is fulfilled. Parameters K and n in Eq 37 to 39 were calculated by means of the formulas in Eq 34 and 35.

Because Eq 37 to 39 have been used by several authors for prediction purposes (Ref 13, 14, 33-35), the following facts must be taken into account:

- Since K and n are temperature dependent, the solution of differential equations (Eq 37-39) can be determined by numerical methods only. For numerical calculations the authors used the computational algorithms given in Ref 19.
- Under isothermal conditions, the solution of Eq 37 to 39 results in the traditional Avrami equation (Eq 33) as a special case.
- Kinetic differential Eq 39 can be generated not only from Eq 13 but also from Eq 7 or Eq 30. This can be easily verified by substituting $\alpha = 1$, $\beta = 0$, $\gamma = (n - 1)/n$, $\eta = 0$, and $K_R = nK^{1/n}$ into Eq 7 or by substituting $f_2(t, T, \dot{T}) \equiv 1$ into Eq 32, respectively. It is semiadditive because n is temperature-dependent. If $n = 1$, Eq 38 and 39 are simplified into the same form.

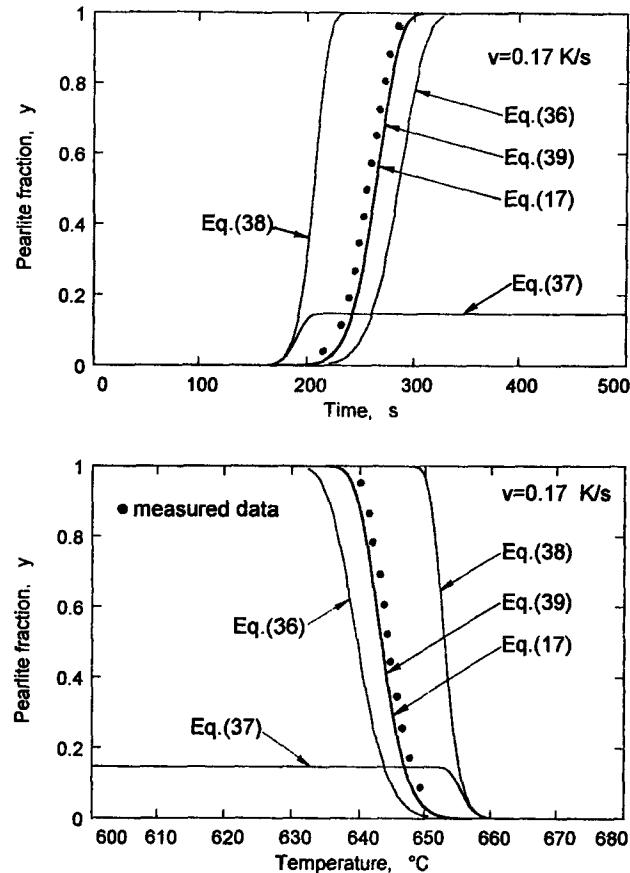


Fig. 4 Transformation kinetics predicted by five different methods (cooling rate: 0.17 K/s)

- For cooling rates 0.17, 0.38, and 0.85 K/s, the measured data and the results of computer simulation obtained by the five methods of prediction are shown in Fig. 4 to 6.

3.3 Comparison of Methods Used for Predicting the Austenite-Pearlite Transformation

From the comparison between the calculated results and experiments, the following conclusions can be drawn (Fig. 4-6):

- The pearlite fractions predicted by Eq 39 and the additivity rule agree with experimental results obtained by dilatometric measurements. The kinetic differential Eq 39 and the application of the additivity rule lead to the similar results. This is because the structure of the differential equations (Eq 30, 39) seems to be similar.
- Pearlite amounts calculated by Eq 36 and 38 differ considerably from those obtained by measurements. As can be seen from diagrams, the pearlite fraction predicted by Eq 38 is overestimated, while Eq 36 underestimates the measured amount of pearlite.
- As demonstrated in Fig. 4 to 6, a special property of Eq 37 is $\lim y_B(t)$ is not equal to 1, if the transformation time tends toward infinity. Due to this fact, which is verified

theoretically in Appendix 1, the requirement formulated by Eq 2.3 is not fulfilled. From this, it follows that the kinetic equation represented by Eq 37 cannot be applied to predict nonisothermal transformation (Ref 14).

4. Summary and Conclusions

Several approaches devoted to the prediction of nonisothermal transformation were analyzed and compared, taking into consideration the generalization of phenomenological methods of various types. Starting with the Avrami function, it was demonstrated that conventional isotherm kinetic functions can be extended in several ways to describe the diffusional transformation processes occurring at varying temperatures.

After studying the austenite decomposition in a low alloy eutectoid steel, kinetic pearlite transformation was measured under isothermal and nonisothermal conditions using a dilatometer.

For predicting the progress of nonisothermal pearlite transformation, five methods—the additivity rule represented by Eq 17, the integro-differential equation (Eq 27), and three different types of kinetic differential equations (Eq 37-39)—were analyzed and tested.

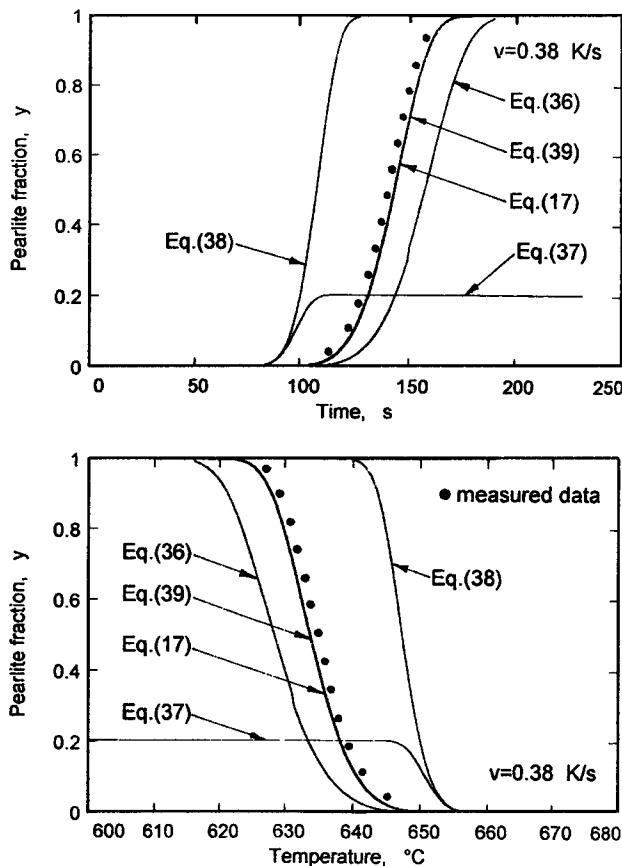


Fig. 5 Transformation kinetics predicted by five different methods (cooling rate: 0.38 K/s)

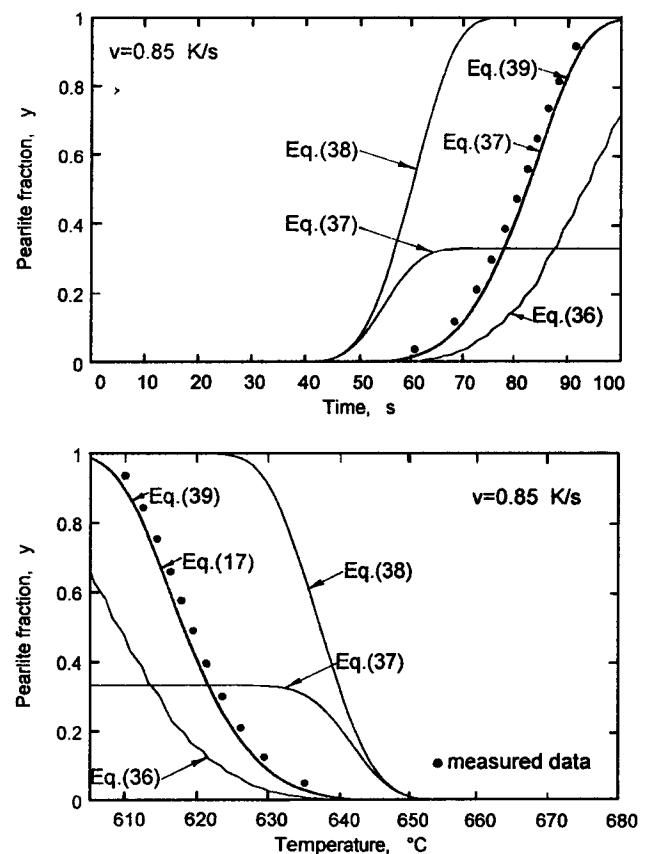


Fig. 6 Transformation kinetics predicted by five different methods (cooling rate: 0.85 K/s)

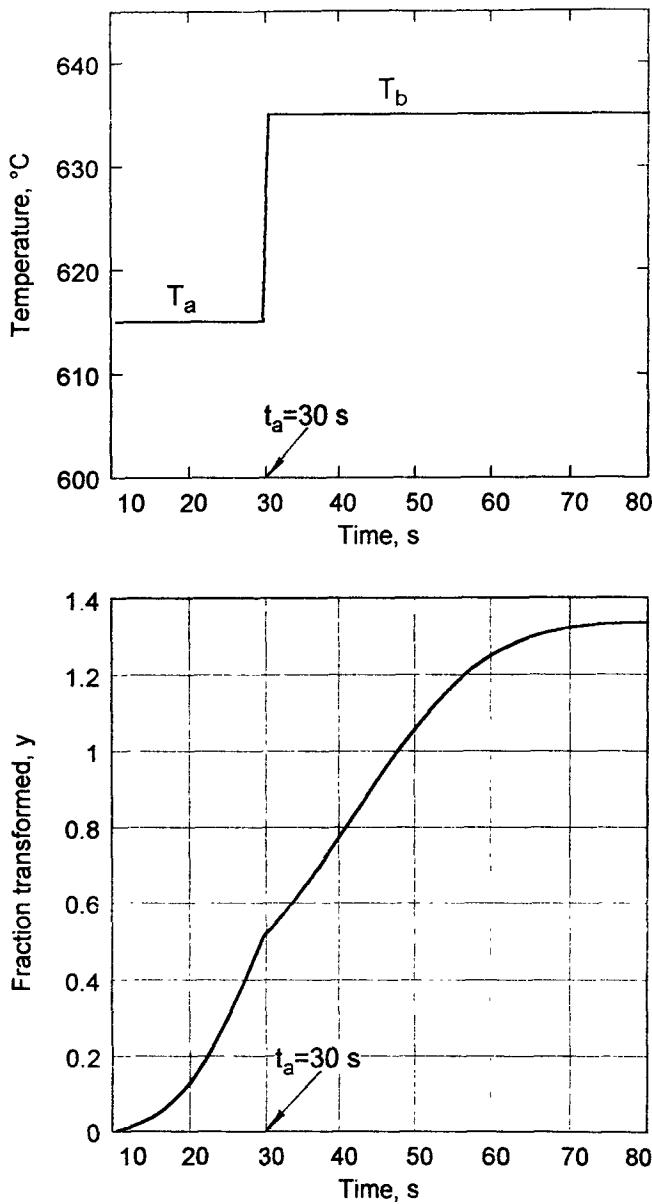


Fig. 7 Kinetic curve predicted from Eq A2 and A3

The main conclusions can be summarized as follows:

- After analyzing the austenite/pearlite transformation in a low alloy eutectoid steel during continuous cooling, the authors found that the pearlite fractions predicted by the kinetic differential equation (Eq 39) and the additivity rule are in agreement with experimental results obtained by dilatometric measurements. The semi additive differential equation (Eq 39) and the use of the additivity rule lead to similar results. This is explained by the “structure” of the differential Eq 30 generated on the basis of the additivity rule. Differential Eq 39 is a similar type. Theoretically, Eq 30 and 39 can be identical only if the Avrami exponent is constant, and the weighting function $f_2(t, y, T, \bar{T}) \equiv 1$. In this case, Eq 39 is additive.

- Comparing the methods based on the application of the additivity rule and differential Eq 39, the application of the latter is advantageous due to simpler numerical computations. If differential Eq 39 is not able to meet the requirements related to the prediction accuracy, then the use of the generalized Avrami type kinetic differential equation defined as shown below is recommended. In this case, however, parameter q and the weighting function f_2 should be estimated by performing preliminary nonisothermal experiments.

$$\frac{dy}{dt} = \frac{nK^{1/q}}{f_2(t, T, \bar{T})} t^{(n-q)/q} [Y_e - y] \left\{ \ln \left(\frac{Y_e}{Y_e - y} \right) \right\}^{(q-1)/q}$$

- Pearlite amounts predicted by applying Eq 36 and 38 differ considerably from those obtained by dilatometric measurements. It was found that Eq 38 overestimates, while Eq 36 underestimates the measured amount of pearlite. Finally, it was proven mathematically that kinetic differential Eq 37 is inapplicable to the prediction of nonisothermal transformations.

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References

- T. Réti, M. Gergely, and P. Tardy, *Mater. Sci. Technol.*, Vol 3, 1987, p 365-371
- J.W. Cahn, *Acta Metall.*, Vol 4, 1956, p 572-575
- J.W. Christian, *The Theory of Transformations in Metals and Alloys*, Pergamon Press, Oxford, 1975
- J.B. Leblond, G. Mottet, J. Devaux, and J.C. Devaux, *Mater. Sci. Technol.*, Vol 1, 1985, p 818-821
- M. Gergely, S. Somogyi, T. Réti, and T. Konkoly, Computerized Properties Prediction and Technology Planning in Heat Treatment of Steels, *Heat Treating*, Vol 4, *ASM Handbook*, ASM International, 1991, p 638-656
- M. Gergely, T. Réti, P. Tardy, and G. Buza, Prediction of Transformation Characteristics and Microstructure of Case Hardened Engineering Components, *Proc. of the International Conference Heat Treatment 1984*, The Metals Society, 1984, p 20.1-20.7
- M. Umemoto, N. Nishioka, and I. Tamura, Kinetics of Proeutectoid Ferrite Reaction During Isothermal Holding and Continuous Cooling in Plain Carbon Steel, *Proc. of the Third International Congress on Heat Treatment of Materials*, 1983 (Shanghai, China), The Metals Society, 1984, p 5.35-5.43
- E.B. Hawbolt, R. Kamat, B. Chau, and J.K. Brimacombe, Application of Isothermal Phase Transformation Kinetics to Predict Continuous Cooling Behaviour, *Proc. of the Conference Phase Transformation '87*, The Institute of Metals, 1988, p 522-525
- J.B. Austin and R.L. Rickett, *Trans. AIME*, Vol 135, 1939, p 396-415
- J. Burke, *The Kinetics of Phase Transformations in Metals*, Pergamon Press, Oxford, 1965
- M. Gergely and T. Réti, *J. Heat Treat.*, Vol 5 (No. 2), 1988, p 125-140

12. M. Avrami, *J. Chem. Phys.*, Vol 7, 1939, p 1103-1112; Vol 8, 1940, p 212-224; Vol 9, 1941, p 177-184
13. E. Woldt, *J. Phys. Chem. Solids*, Vol 53 (No. 4), 1992, p 521-527
14. A.J. Fletcher, *Thermal Stress and Strain Generation in Heat Treatment*, Elsevier Applied Science, London, 1989, p 50-52
15. E. Scheil, *Arch. Eisenhüttenwes.*, Vol 9 (No. 12), 1936, p 619-622
16. M. Umemoto, K. Horiuchi, and I. Tamura, *Trans. ISIJ*, Vol 23, 1983, p 690-695
17. G. Buza, H.P. Hougardy, and M. Gergely, *Steel Res.*, Vol 57, 1986, p 650-653
18. C. Verdi and A. Visentin, *Acta Metall.*, Vol 35, 1987, p 2711-2717
19. T. Réti, T. Bell, Y. Sun, and A. Bloyce, *Mater. Sci. Forum*, Vol 163-165, 1994, p 673-680
20. F. Wever and O. Krisement, *Arch. Eisenhüttenwes.*, Vol 23 (No. 5-6), 1952, p 229-237
21. J.S. Kirkaldy and R.C. Sharma, *Scr. Metall.*, Vol 16, 1982, p 1193-1198
22. I.A. Wierszylowski, *Metall. Trans. A*, Vol 22, 1991, p 993-999
23. T.T. Pham, E.B. Hawbolt, and J.K. Brimacombe, *Metall. Trans. A*, Vol 26, 1995, p 1987-1992
24. P.K. Agarwal and J.K. Brimacombe, *Metall. Trans. B*, Vol 12, 1981, p 121-133
25. M. Gergely, T. Réti, and S. Somogyi, Computer Programs in the Service of Heat Treatment Technologists and Steel Selectors, *Proc. of the 5th Int. Congress on Heat Treatment of Materials*, Vol I, 1985, p 186-195
26. E.J. Mittermejer, *J. Mater. Sci.*, Vol 27, 1992, p 3977-3987
27. T. Réti, "Computer Simulation of Transformation Processes Occurring During Heat Treating," Doctoral thesis, Hungarian Academy of Sciences, 1994
28. J.B. Leblond and J. Devaux, *Acta Metall.*, Vol 32, 1984, p 137-146
29. T. Inoue, S. Nagaki, T. Kishino, and M. Monkawa, *Ing. Arch.*, Vol 50, 1981, p 315-327
30. T. Inoue and Z. Wang, *Mater. Sci. Technol.*, Vol 1, 1985, p 845-850
31. M. Umemoto, Z.H. Guo, and I. Tamura, *Mater. Sci. Technol.*, Vol 3, 1987, p 249-255
32. R.C. Reed and H.K.D.H. Bahadesia, *Mater. Sci. Technol.*, Vol 8, 1992, p 421-435
33. T. Kemény and J. Sestak, *Thermochim. Acta*, Vol 110, 1987, p 113-129
34. D.W. Henderson, *J. Therm. Anal.*, Vol 15, 1979, p 325-331
35. T.J.W. De Bruijn, W.A. De Jong, and P.J. Van der Berg, *Thermochim. Acta*, Vol 45, 1981, p 315-325