On the possible generalization of JMAK-type kinetic functions

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Abstract. The Johnson-Mehl-Avrami-Kolmogorov (JMAK) kinetic equation is generally used for describing the progress of solid state diffusion-controlled transformations. The traditional JMAK model is applicable for modeling only monophase decomposition (precipitation) processes. This paper deals with possible generalizations of the classical JMAK kinetic model by taking into consideration the simultaneous occurrence of more parallel transformations. It is revealed that the Jones-Bhadeshia kinetic model belonging to the family of the strongly coupled multiphase models has only a limited practical application because it contains only few fitting parameters. Moreover, it has been shown and demonstrated that for predicting decomposition processes it is more advantageous to use a multiphase kinetic model including a finite set of ordinary autonomous differential equations.

1. Introduction, preliminary considerations

For the phenomenological description of diffusion-based transformation processes occurring in alloys various kinetic equations have been suggested in the literature [1-7]. The most popular, widely used kinetic model was established in the late 1930s, independently by Johnson and Mehl, Avrami and Kolmogorov [1]. It is referred to as the Johnson-Mehl-Avrami-Kolmogorov (JMAK) transformation model, and the corresponding kinetic equation is represented by

\[ X(t) = 1 - \exp\left(-Kt^n\right) \]  

where \( X = X(t) \) is the transformed fraction at time \( t \), \( K \) is the reaction rate constant, and \( n \) is the Avrami exponent. In Eq.(1) the reaction rate constant \( K \) is given by

\[ K = K(T, E) = A \exp\left(-\frac{E}{RT}\right) \]  

where \( T \) is the absolute temperature in Kelvin, \( E \) is the activation energy, \( A \) is the frequency factor and \( R \) is the universal gas constant. For constant temperature, the transformation rate can be derived by differentiating Eq.(1) with respect to time

\[ \frac{dX}{dt} = K^n (1 - X) nt^{n-1}. \]  

Several attempts have been made to generalize equations (1) and/or (3) to treat two or more transformation processes (phase decomposition processes) occurring simultaneously [8-14]. A detailed comparative analysis of various decomposition models devoted to the extension of the traditional JMAK kinetic equation to the prediction of simultaneous transformations is given in [7].
2. A possible extension of the Jones-Bhadeshia multiphase kinetic model

In what follows starting with the concept outlined in Refs. [9-12], we investigate some possible extensions of the isothermal kinetic model represented by Eq.(3). Let us assume that there exists a parent phase \( \gamma \) which decomposes simultaneously into \( J \) distinct phases \((\alpha_1, \alpha_2, \ldots, \alpha_J)\) during isothermal transformation and this precipitation process is described by an ordinary differential equation system

\[
\frac{dX_j}{dt} = f(X_1, X_2, \ldots, X_J)g_j(t).
\]

(4)

The transformed fractions are denoted by \( X_j \) and \( f(X_1, X_2, \ldots, X_J) \) and \( g(t) \) are appropriately selected non-negative real functions. To generate the solution of the above differential equation system, we have introduced some simplifying hypotheses. It is assumed that in Eq.(4)

\[ f(X_1, X_2, \ldots, X_J) = \left[ 1 - \sum_{j=1}^{J} X_j \right]^p \quad \text{and} \quad g_j(t) = K_j g(t) \]

by definition, where \( p \) and \( K_j \) are positive numbers, \( g(t) \) is a positive function of time if \( t > 0 \).

As a result of a simple transformation, we obtain a system of non-linear ordinary differential equations defined as

\[
\frac{dX_j}{dt} = K_j \left[ 1 - \sum_{j=1}^{J} X_j \right]^p g(t).
\]

(5)

The set of ordinary differential equations (5) represents a strongly coupled multiphase kinetic model (SCMK model) because

\[
\frac{dX_j}{dt} = \frac{K_j}{K_i} \frac{dX_i}{dt} \quad \text{for any } i, j > 1.
\]

This implies that functions \( X_j(t) \) can be directly calculated by

\[
X_j(t) = \frac{K_j}{K_i} X_i(t) \quad \text{for } j > 1.
\]

(6)

Assuming that parameters \( p, K_i \) and function \( g(t) \) are appropriately defined, the differential equations (5) can be rewritten in the following alternative form:

\[
\frac{dX_j}{dt} = K_j \left[ 1 - \frac{X_j}{\sum_{i=1}^{J} K_i} \right]^p g(t).
\]

(7)

Based on the concept outlined previously it is assumed that the solutions \( X_j(t) \) of the differential equation system satisfy the following conditions:

i) \( X_j(0) = 0, \lim_{t \to \infty} X_j(t) = Y_j > 0 \) if \( t \to \infty \) and \( \sum_{j=1}^{J} Y_j = 1 \),

ii) \( \frac{dX_j}{dt} = \frac{K_j}{K_i} \frac{dX_i}{dt} \) and \( X_j(t) = \frac{K_j}{K_i} X_i(t) = \frac{Y_j}{Y_i} X_i(t) \) for \( 1 \leq i, j \leq J \),

iii) \( \sum_{j=1}^{J} X_j(t) = Y_1(t) \sum_{j=1}^{J} Y_j = X_i(t) \frac{Y_j}{Y_i} \),

iv) \( \sum_{j=1}^{J} K_j(t) = K_{i1} Y_1 = K_2 Y_2, \ldots, = K_{iJ} Y_J \),

where \( Y_j \) stands for the maximum transformed fractions for which \( \sum Y_j = 1 \) holds.

If the above restrictions are fulfilled, the differential equations (7) can be transformed into a simplified form. As a particular case, the transformation rate for the phase \( \alpha_i \) can be calculated as
\[
\frac{dX_i}{dt} = K_i \left\{1 - \frac{X_i}{K_i} \sum_{j=1}^{i} K_j \right\} g(t) = K_i \left\{1 - \frac{X_i}{Y_i} \right\} g(t)
\]  

(8)

It is important to emphasize that if \(X_1(t)\) is known, then \(X_j(t)\) for \(1 < j \leq J\) can be simply generated by
\[X_j(t) = \frac{Y_j}{Y_1} X_1(t).
\]

(9)

3. Investigation of the SCMK models

In what follows, starting with Eq. (8), we determine the solutions of differential equations included in the SCMK model for some particular cases.

\textit{a) The case of } p=1. \textit{One obtains that}
\[
\frac{dX_i}{dt} = K_i \left\{1 - \frac{X_i}{Y_1} \right\} g(t)
\]
\[
(10)
\]

where
\[
g(t) = nt^{n-1}
\]
\[
(11)
\]

and \(n \geq 1\) is a positive number. Then we have
\[
\int_{0}^{X} \frac{du}{1-u/Y_1} = Y_1 \int_{0}^{X} \frac{du}{Y_1-u} = K_i \int_{0}^{1} g(\tau)d\tau = K_i t^n.
\]

It follows that
\[
X_1(t) = Y_1 \left[1 - \exp \left\{- \frac{K_i}{Y_1} \int_{0}^{1} g(\tau)d\tau \right\}\right] = Y_1 \left[1 - \exp \left\{- \frac{K_i}{Y_1} t^n \right\}\right]
\]
and
\[
X_j(t) = \frac{Y_j}{Y_1} X_1(t) = Y_j \left[1 - \exp \left\{- \frac{K_i}{Y_1} t^n \right\}\right].
\]

\textit{b) The case of } p=2 \textit{In this case we get}
\[
\frac{dX_i}{dt} = K_i \left\{1 - \frac{X_i}{Y_1} \right\}^2 g(t) = K_i \left\{1 - \frac{X_i}{Y_1} \right\}^2 nt^{n-1}
\]
\[
(12)
\]

and
\[
\int_{0}^{X} \frac{du}{(1-u/Y_1)^2} = Y_1 \int_{0}^{X} \frac{du}{(Y_1-u)^2} = K_i \int_{0}^{1} g(\tau)d\tau = K_i t^n.
\]

Because
\[
Y_1 \int_{0}^{X} \frac{du}{(Y_1-u)^2} = Y_1 \left\{\frac{Y_1}{Y_1-x_1} - 1\right\}
\]
\[
(13)
\]

this implies that
\[
\frac{Y_1 - X_1}{Y_1} = \left\{1 + \frac{K_i}{Y_1} \int_{0}^{1} g(\tau)d\tau \right\}^{-1} = \left\{1 + \frac{K_i}{Y_1} t^n \right\}^{-1}.
\]

Consequently,
\[ X_i(t) = Y_i \left[ 1 - \frac{Y_i}{Y_i + K_i t^n} \right]. \]

It is easy to check that
\[ X_j(t) = \frac{Y_j}{Y_i} X_i(t) = Y_j \left[ 1 - \frac{Y_i}{Y_i + K_i t^n} \right], \]

and \( \lim X_i(t) = Y_j \) holds if \( t \to \infty \).

c) The case of \( p=1/2 \).

It is interesting to note that if \( p=1/2 \), then for \( X_1(t) \) the condition \( \lim X_1(t) = Y_1 \) is not fulfilled when \( t \) tends to infinity. Consider the kinetic differential equation given as
\[ \frac{dX_i}{dt} = K_i \left( 1 - \frac{X_i}{Y_i} \right) n t^{-1}. \]

If \( p=1/2 \), it follows that
\[ \frac{du}{\sqrt{1-u/Y_i}} = \frac{du}{\sqrt{Y_i - u}} = K_i \int_0^t n \tau^{n-1} d\tau = K_i t^n. \]

But
\[ \sqrt{Y_i} \int_0^{X_i} \frac{du}{\sqrt{Y_i - u}} = 2 \sqrt{Y_i} \left\{ \sqrt{Y_i} - \sqrt{Y_i - X_i} \right\} = K_i t^n \]

consequently,
\[ X_i(t) = Y_i \left\{ \sqrt{Y_i} - \frac{K_i t^n}{2 \sqrt{Y_i}} \right\}^2 = Y_i \left[ 1 - \left( 1 - \frac{K_i t^n}{2 Y_i} \right)^2 \right]. \]

By definition \( 0 \leq X_i \leq Y_i \). From Eq.(12) and Eq.(13) it follows that if \( X_1=Y_1 \) then \( 2 Y_1 = K_i t^n \) holds, consequently \( t_1 = (2 Y_1/K_i)^{1/n} \). This observation implies that if \( t \) tends to infinity, then \( \lim X_i(t) = -\infty \) holds.

4. Correspondence between the Jones-Bhadeshia model and the SCMK models

In what follows, the relations between the Jones-Bhadeshia kinetic model and the strongly coupled multiphase kinetic models are investigated. The Jones-Bhadeshia kinetic model describes the isothermal simultaneous precipitation of phases \( \alpha_1 \) and \( \alpha_2 \) from a parent phase [9]. The corresponding volume fractions of two product phases are denoted by \( X_1 \) and \( X_2 \). In the model the microstructural parameter \( \chi \) plays a decisive role. It is defined by
\[ \chi = \frac{G_2^3 I_2}{G_1^3 I_1}, \]

where \( G_1, G_2, I_1 \) and \( I_2 \) are growth and nucleation rate of precipitating phases \( \alpha_1 \) and \( \alpha_2 \), respectively. Moreover it is assumed that both precipitating phases are represented by spherical particles, their volume fractions \( V_i(t) \) and \( V_2(t) \) are given by
\[ V_i(t) = \frac{4\pi}{3} G_i^3 (t-\tau)^3 \]

for time \( t \) if \( t > \tau \). According to Jones and Bhadeshia the precipitated fractions of phases \( \alpha_1 \) and \( \alpha_2 \) can be calculated as
\[
X_i(t) = \left(\frac{1}{1+\chi}\right) \left[1 - \exp \left(-\frac{1}{3} (1+\chi)^2 \pi G_i I_i t^4 \right)\right]
\]
(15)

\[
X_j(t) = \left(\frac{\chi}{1+\chi}\right) \left[1 - \exp \left(-\frac{1}{3} \frac{1+\chi}{\chi} \pi G^*_i I_i t^4 \right)\right]
\]
(16)

Now, for comparison, consider the SCMK model represented by Eq.(8). Supposing that \(J=2\), \(p=1\) and \(n=4\), then in this particular case, the corresponding set of kinetic differential equations will be

\[
\frac{dX_1}{dt} = 4K_1 \left[1 - \frac{X_1}{Y_1}\right] t^4
\]
(17)

\[
\frac{dX_2}{dt} = 4K_2 \left[1 - \frac{X_2}{Y_2}\right] t^4
\]
(18)

By solving the above system of differential equations one obtains that

\[
X_i(t) = Y_i \left[1 - \exp \left(-\frac{K_i}{Y_i} t^4\right)\right]
\]
(19)

\[
X_j(t) = Y_j \left[1 - \exp \left(-\frac{K_j}{Y_j} t^4\right)\right] = Y_j \left[1 - \exp \left(-\frac{K_j}{Y_j} t^4\right)\right].
\]
(20)

Introduce the following parameters defined by

\[
Y_1 = \frac{1}{1+\chi}, \quad Y_2 = 1+Y_1 = \frac{\chi}{1+\chi},
\]

\[
K_1 = \frac{1}{3} (1+\chi)^2 \pi G_i I_i, \quad \text{and}
\]

\[
K_2 = \frac{1}{3} \frac{1+\chi}{\chi} \pi G^*_i I_2 = \frac{1}{3} (1+\chi)^2 \pi G^*_i I_1 = \frac{K_1}{Y_1}.
\]

Based on the above formulas it is easy to see that the two kinetic models represented by Eqs.(15-16) and Eqs.(19-20) are equivalent, consequently, the Jones-Bhadeshia multiphase model can be considered as a special type of SCMK models.

**Example 1** Consider the Jones-Bhadeshia kinetic model outlined in Ref. [9].

Let \(J=2\), \(p=1\), \(n=4\), \(\chi=8\),

\[
Y_1 = \frac{1}{1+\chi} = \frac{-1}{9}, \quad Y_2 = 1-Y_1 = \frac{\chi}{1+\chi} = \frac{8}{9},
\]

and \(C = K_1/Y_1 = K_2/Y_2 = 1/625\). For the transformed fractions of phases \(\alpha_1\) and \(\alpha_2\) we get

\[
X_i(t) = Y_i \left[1 - \exp \left(-\frac{K_i}{Y_i} t^4\right)\right] = \frac{1}{9} \left[1 - \exp \left(-\frac{1}{625} t^4\right)\right]
\]
and

\[
X_j(t) = Y_j X_i(t) = 8X_i(t)
\]

If the time is equal to \(t_x = (Y_i/K_i)^{1/4} = 1/C^{1/4} = 5\), in this particular case, one obtains that

\[
X_i(t_x) = Y_i \left[1 - \exp \left[-1\right]\right] = 0.63212(1/9) = 0.07024,
\]

\[
X_j(t_x) = Y_j \left[1 - \exp \left[-1\right]\right] = 0.63212(8/9) = 0.561885.
\]

**Example 2** Let \(J=3\), \(Y_1=Y_3=1/4\), \(Y_1 = 1/2\), \(p=1\), \(n=4\), \(K_j=CY_j\) and \(C=1/625\). Then the solutions relating to the corresponding SCMK model are:
The isothermal kinetic equations (22) represent a multiphase decomposition model where the simultaneous precipitation reactions are independent, and the progress of jth precipitation process does not depend on the degree of transformation of the others.

- In the particular case, if J=1 holds, the differential equation (21) is identical to the JMAK kinetic differential equation extended to the description of non-isothermal transformation processes [1,2].

- In the multiphase model represented by Eqs. (21 and 22) the independent parameters are: J ≥ 2, Y_1 >0, Y_2 >0,...,Y_{J-1} >0, n_1 >0, n_2 >0,..., n_{J-1} >0, B_1>0, B_2>0,..., B_{J-1}>0. Consequently, if J ≥2 is a fixed positive integer, then the number of freely selected model parameters is relatively large, i.e. J – 1 + 2J = 3J - 1.

Our preliminary tests have verified that the AMK model represented by Eq.(22) is successfully applicable for describing the isothermal austenite decomposition into ferrite and pearlite.


6. Using the AMK model for the prediction of isothermal austenite decomposition in a hypoeutectoid steel

Consider the isothermal decomposition of austenite in low alloy 34Cr4 steel [13]. The unknown model parameters \( Y_j, n_j \) and \( B_j \) of simultaneous ferrite and pearlite precipitations can be estimated from the measured isothermal transformation diagrams (IT diagrams), where times \( t_s \) and \( t_f \) characterize the start and finish of the isothermal austenite transformation as a function of temperature \( T \) plotted in a form of C-curves. According to the classical definition of C-curves, \( t_s \) and \( t_f \) stand for the times belonging to 1\% and 99\% of relative transformed fractions. For the computation of model parameters \( n_j \) and \( B_j \) characterizing the jth precipitation reaction, the following formulas are used [13]

\[
n_j(T) = \frac{6.1273}{\ln(t_f/t_s)}
\]

and

\[
B_j(T) = \frac{0.01005}{t_s^{n_j}}.
\]

If \( T = 650 \, ^\circ\text{C} \), then in this particular case the kinetic parameters of ferrite precipitation are \( Y_1 = 0.25, t_{s1} = 2 \, \text{sec}, t_{f1} = 35 \, \text{sec} \), and for the corresponding parameters of pearlite precipitation \( Y_2 = 0.75, t_{s2} = 15 \, \text{sec}, t_{f2} = 90 \, \text{sec} \) yield. From these data one obtains that \( n_1 = 2.1408, B_1 = 2.2789 \times 10^{-3}, n_2 = 3.4197 \) and \( B_2 = 9.5559 \times 10^{-7} \), respectively.

The computed results relating to the simultaneous ferrite and pearlite precipitations at 650 \, ^\circ\text{C} \) are demonstrated in Fig. 1.

![Figure 1 Predicted isothermal decomposition of austenite into ferrite and pearlite at 650 \, ^\circ\text{C}](image)

An important property of the autonomous decomposition model is that, disregarding the equality \( \sum Y_j = 1 \), the differential equations included in the kinetic model are considered to be independent. It should be noted that an advantage of using the autonomous decomposition model is that it can be applied to the prediction of isothermal and non-isothermal diffusion controlled transformation processes.
7. Conclusions
The multiphase SCMK kinetic model represented by Eq.(7) incorporates the classical JMAK kinetic model if equalities $J=1$, $p=1$ and $g(t)=nt^{n-1}$ are fulfilled. As a particular case, if $J=1$, $p=1$ and $g(t)=nt^{n-1}$ hold, the Austin-Rickett kinetic equation is obtained [4]. As it is known, the model parameter $p$ represents the so-called impingement exponent related to the fraction untransformed [2]. Comparing the SCMK and AMK kinetic models we can conclude that the practical application of AMK models seems to be more advantageous because they contain more free fitting parameters.

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