Improved analytical description for non-isothermal solid-state transformation

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ABSTRACT

A generalized analytical description for non-isothermal solid-state transformation was developed, where a choice of both nucleation modes and approximations to the so-called "temperature integral" and "general temperature integral" is incorporated. The currently general description reduces to the originally analytical model, provided if coarse approximations adopted in [F. Liu, et al., Int. Mater. Rev. 52 (2007) 193] are chosen. Numerical calculations demonstrate that the accuracy of the general description is guaranteed by selecting an optimal combination of the approximations.

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1. Introduction

Solid-state phase transformations are important means for the adjustment of the microstructure and thus are the tuning of the properties of materials. To exploit this tool to its full extent, much effort is spent on the modeling of phase transformations [1–6]. Recently, an analytical phase-transformation model was proposed that incorporates a choice of nucleation and growth mechanisms, as well as impingement modes, and has been successfully applied to experimental results [7–9]. The model leads to equations for the degree of transformation that have the structure of the Johnson–Mehl–Avrami (JMA) equation but with variable kinetic parameters (n, the growth exponent, Q, the overall effective activation energy and K_0, the pre-exponential factor of rate constant), i.e. for a mixture of site saturation and continuous nucleation (or mixed nucleation). For isothermal transformation (i.e. the temperature holds constant upon transformation) and non-isothermal transformation (i.e. in this paper, the heating rate holds constant upon transformation), these kinetic parameters are, according to the analytical model, time-dependent and temperature-dependent, respectively. In the original treatment [7,8], to derive the analytical model, the so-called "general temperature integral" [10] cannot be

solved analytically and has to be approximated.[1]

$$\int_{T_0}^{T} T^M \exp\left(-\frac{Q'}{RT}\right) dT = \frac{RT^{M+2} \exp(-(Q'/RT))}{Q'} \tag{1}$$

where Q' as the constant activation energy of an Arrhenius equation, R the universal gas constant, T the temperature, T_0 the starting temperature, M a constant (for $M = 0$, the left-hand side of Eq. (1) becomes the so-called "temperature integral" [12,13]). Application of Eq. (1) is essential for deriving the analytical model, which, however, is too coarse to give a sufficiently precise description for non-isothermal transformation, particularly with low activation energy and/or high transformation temperature (i.e. $Q'/RT < 25$), e.g. the austenite–ferrite phase transformation of Fe–Mn alloys [14].

Within the last 50 years, a lot of approximations to the "temperature integral" and the "general temperature integral" have been proposed [10,12,15–26]. Generally, the more accurate the approximation is, the more complex the formula becomes (e.g. a recently proposed quasi-exact solution [27,28]). It is worth to do so, as Flynn [13] said that, in this age of vast computational capabilities, there is no valid reason not to use precise values for the temperature integral when calculating kinetics parameters.

On this basis, a question arises, i.e. is it possible to generalize the originally analytical model, by incorporating the above treatment

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[1] To avoid unnecessary complications, the effect of T_0 terms is not taken into account in the current treatment for the approximations. However, Starink [11] has realized that in a limited number of cases, the effect due to T_0 terms cannot be neglected. If this happens, the current model can also take the T_0 terms into consideration.

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Nomenclature

C_c	variable defined by d, m, Q_N, Q_G, $p_M(x)$ and $q(x)$
C_s	variable defined by d, m, Q_G and $q(x)$
D_0	pre-exponential factor of diffusion coefficient ($m^2\,s^{-1}$)
d	dimensionality of the growth
f	transformed fraction
f_a	model-predicted transformed fraction
f_n	numerical-calculated transformed fraction
g	particle-geometry factor
K_0	pre-exponential factor of rate constant
M	constant in general temperature integral
m	growth mode parameter
N_1^*	number of pre-exist nuclei per unit volume in mode of site saturation (m^{-3})
N_{01}	pre-exponential factor of nucleation rate in mode of continuous nucleation ($m^{-3}\,s^{-1}$)
n	growth exponent
Q	overall effective activation energy ($J\,mol^{-1}$)
Q_D	activation energy for diffusion ($J\,mol^{-1}$)
Q_G	activation energy for growth ($J\,mol^{-1}$)
Q_N	activation energy for nucleation ($J\,mol^{-1}$)
Q'	activation energy ($J\,mol^{-1}$)
R	universal gas constant ($J\,mol^{-1}\,K^{-1}$)
T	absolute temperature (K)
T_0	starting absolute temperature (K)
t	time for transformation (s)
V	real volume (m^3)
V^e	extended volume (m^3)
v	interface velocity ($m\,s^{-1}$)
v_0	pre-exponential factor of interface velocity ($m\,s^{-1}$)
x	variable defined by Q'/RT
x_e	extended transformed fraction
x_G	variable defined by Q_G/RT
x_N	variable defined by Q_N/RT
x_{N+G}	variable defined by $(Q_N+Q_G)/RT$
x_{N+2G}	variable defined by $(Q_N+2Q_G)/RT$
x_{N+3G}	variable defined by $(Q_N+3Q_G)/RT$
Y	volume at time t of a particle nucleated at time τ (m^3)
ε_r	relative error of the model-predicted transformed fraction (%)
τ	time for nucleation (s)
Φ	constant heating rate ($K\,s^{-1}$)

Table 1
Expressions of $q(x)$ considered in this work.

Authors	$q(x)$
Balarin [15]	$\sqrt{\dfrac{x}{x+4}}$
Cai et al. [16]	$\dfrac{x+0.66691}{x+2.64943}$
Urbanovici and Segal [17]	$\dfrac{x^2+3.5x}{x^2+5.5x+5}$
Chen and Liu [18]	$\dfrac{x^2+(16/3)x+(4/3)}{x^2+(22/3)x+10}$
Senum and Yang I [19]	$\dfrac{x^3+10x^2+18x}{x^3+12x^2+36x+24}$
Zsakó [20]	$\dfrac{x^4-4x^3+84x^2}{x^4-2x^3+76x^2+152x-32}$
Senum and Yang II [19]	$\dfrac{x^4+18x^3+86x^2+96x}{x^4+20x^3+120x^2+240x+120}$
Órfão [12]	$\dfrac{0.9999936x^4+7.5739391x^3+12.4648922x^2+3.6907232x}{x^4+9.5733223x^3+25.6329561x^2+21.0996531x+3.9584969}$

implies for the nucleation rate at time τ [7,8],

$$\dot{N}(T(\tau)) = N_1^*\delta\left(\frac{T(\tau)-T_0}{\Phi}\right) \tag{2}$$

with $\delta\{[T(\tau)-T_0]/\Phi\}$ denoting Dirac functions, N_1^* as the number of nuclei per unit volume, and Φ ($=dT/d\tau=dT/dt$) as the constant heating rate with $T(\tau)=T_0+\Phi\tau$.

The *continuous nucleation* rate per unit volume (i.e. the rate of formation of particles (nuclei) of supercritical size) is at large undercooling only determined by the rate of the jumping of atoms through the interface between the nucleus of critical size and the parent phase, which can be given by an Arrhenius term,

$$\dot{N}(T(\tau)) = N_{01}\exp\left(-\frac{Q_N}{RT(\tau)}\right) \tag{3}$$

where N_{01} is a temperature-independent pre-exponential factor, and Q_N is the temperature-independent activation energy for nucleation.

Here, a short introduction is given for (more general) mixed nucleation in non-isothermal transformation. "*Mixed nucleation*" represents a combination of site saturation and continuous nucleation modes: the nucleation rate is equal to some weighted sum of the nucleation rates according to continuous nucleation and site saturation [7,8]. Hence,

$$\dot{N}(T(\tau)) = N_1^*\delta\left(\frac{T(\tau)-T_0}{\Phi}\right) + N_{01}\exp\left(-\frac{Q_N}{RT(\tau)}\right) \tag{4}$$

where N_1^* and N_{01} include the relative contributions of the two modes of nucleation.

2.1.2. Modes of growth

The *diffusion-controlled* and the *interface-controlled growth* modes can be given in a compact form. At time t (i.e. temperature $T(t)=T_0+\Phi t$) the volume Y of a particle nucleated at time τ (i.e. temperature $T(\tau)$) is given by [7,8],

$$Y(T(t)) = g\left[\int_{T(\tau)}^{T(t)} v\,d\frac{T}{\Phi}\right]^{d/m} \tag{5}$$

where g is a particle-geometry factor, v the growth velocity, m the growth mode parameter ($m=1$ for interface-controlled growth; $m=2$ for volume diffusion controlled growth) and d is the dimensionality of the growth ($d=1, 2, 3$) [7,8].

For large undercooling, $v=v_0\exp(-Q_G/RT(t))$ with Q_G as the temperature-independent activation energy for growth. For interface-controlled growth, v_0 is a temperature-independent pre-exponential factor and Q_G represents the energy barrier at the interface. For volume diffusion-controlled growth, v_0 equals the pre-exponential factor for diffusion D_0 and Q_G represents the activation energy for diffusion, Q_D [8].

for the "temperature integral" and the "general temperature integral"? Here, a generally analytical description for non-isothermal solid-state transformation, which considers not only a choice of nucleation mechanisms, but also a choice of approximations to the "temperature integral" and the "general temperature integral", will be shown.

2. Theoretical

2.1. Theoretical background

In the following, a brief description for applied modes of nucleation and growth is given (i.e. solely for non-isothermal transformation).

2.1.1. Modes of nucleation

The term *site saturation* is used here for the case of initial nucleation site saturation where all nuclei are present at T_0 already. This

Table 2
Expressions of $p_M(x)$ considered in this work.

Authors	$p_M(x)$
Wanjun et al. [21]	$\frac{x}{x+(M+2)(0.00099441x+0.93695599)}$
Cai et al. I [22]	$\frac{x-0.054182M+0.65061}{x+0.93544M+2.62993}$
Cai et al. II [23]	$\frac{0.99954x+(0.044967M+0.58058)}{x+(0.94057M+2.5400)}$
Cai et al. III [10]	$\frac{1.0002486x+0.2228027\ln x-0.05241956M+0.2975711}{x+0.2333376\ln x+0.9496628M+2.2781591}$
Chen and Liu I [24]	$\left(1+\frac{M+2}{x}\right)/\left[1+2\frac{M+2}{x}+\frac{(M+1)(M+2)}{x^2}\right]$
Chen and Liu II [25]	$\frac{x}{(1.00141+0.00060M)x+(1.89376+0.95276M)}$
Chen and Liu III [25]	$\frac{x+(0.74981-0.0639M)}{(1.00017+0.00013M)x+(2.73166+0.92246M)}$
Capela et al. [26]	$\begin{bmatrix} 0.7110930099291700\left(\dfrac{x}{x+0.41577455678348}\right)^{M+2} \\ +0.2785177335692400\left(\dfrac{x}{x+2.294280360279042}\right)^{M+2} \\ +0.010389256501586\left(\dfrac{x}{x+6.289945082937479}\right)^{M+2} \end{bmatrix}$

2.1.3. Impingement

The number of supercritical nuclei formed in a unit volume, at time τ during a time lapse, $dT(\tau)/\Phi$, is calculated by Eqs. (2)–(4) for different modes. The volume of each of these nuclei grows from τ (i.e. $T(\tau)$) to t (i.e. $T(t)$) according to Eq. (5) where it is supposed that every particle grows into an infinitely large parent phase, in absence of other growing nuclei. In this hypothetical case, the volume of all particles at temperature T, called the extended transformed volume, V^e, can be described as,

$$V^e = \int_{T_0}^{T} V\dot{N}(T(\tau))Y(T)d\frac{T(\tau)}{\Phi} \tag{6}$$

with V as the sample volume, which is supposed to be constant throughout the transformation. Accordingly, the extended transformed fraction, x_e, is defined as $x_e = V^e/V$.

In reality, the particles do not grow individually into an infinitely large parent phase. A relationship between the real transformed fraction, f, and the extended transformed fraction, x_e, is required. Several equations for different types of hard impingement are summarized in Ref. [8]. In this study only the mode of random dispersed nuclei is taken into consideration [2–6],

$$\frac{df}{dx_e} = 1 - f \quad \text{and} \quad f = 1 - \exp(-x_e) \tag{7}$$

2.2. New derivation

Assuming mixed nucleation (i.e. Eq. (4)) and interface-controlled growth (i.e. Eq. (5)), the extended transformed fraction, x_e follows from Eq. (6) as,

$$x_e = \frac{V^e}{V} = \int_{T_0}^{T} \left[N_1^*\delta\left(\frac{T(\tau)-T_0}{\Phi}\right)\right.$$
$$\left.+N_{01}\exp\left(-\frac{Q_N}{RT(\tau)}\right)\right]g\left[\int_{T(\tau)}^{T} v_0\exp\left(-\frac{Q_G}{RT(t)}\right)d\frac{T(t)}{\Phi}\right]^{d/m}d\frac{T(\tau)}{\Phi} \tag{8}$$

Table 3
Expressions for C_s and C_c used in the currently analytical model.

d/m	$C_{s(d/m)}$	$C_{c(d/m)}$
1	$\frac{q(x_G)}{Q_G}$	$2\frac{q(x_G)}{Q_G}\left[\frac{q(x_N)}{Q_N}-\frac{p_2(x_{N+G})}{Q_N+Q_G}\right]$
2	$\left(\frac{q(x_G)}{Q_G}\right)^2$	$3\frac{q(x_G)^2}{Q_G{}^2}\left[\frac{q(x_N)}{Q_N}-2\frac{p_2(x_{N+G})}{Q_N+Q_G}+\frac{p_4(x_{N+2G})}{Q_N+2Q_G}\right]$
3	$\left(\frac{q(x_G)}{Q_G}\right)^3$	$4\frac{q(x_G)^3}{Q_G{}^3}\left[\frac{q(x_N)}{Q_N}-3\frac{p_2(x_{N+G})}{Q_N+Q_G}+3\frac{p_4(x_{N+2G})}{Q_N+2Q_G}-\frac{p_6(x_{N+3G})}{Q_N+3Q_G}\right]$

By defining $x = Q'/RT$, the "temperature integral" is expressed as [12,15–20],

$$\int_0^T \exp\left(-\frac{Q'}{RT}\right)dT = \frac{RT^2\exp(-(Q'/RT))}{Q'}q(x) \tag{9}$$

where $q(x)$ represents the rational functions of x derived using different methods. From Ref. [12], the expressions of the most accurate formula for $q(x)$ corresponding to different complexity-levels are gathered in Table 1. Assuming $x_G(T) = Q_G/RT$, $x_N(T) = Q_N/RT$, $x_{N+G}(T) = (Q_N+Q_G)/RT$, $x_{N+2G}(T) = (Q_N+2Q_G)/RT$, $x_{N+3G}(T) = (Q_N+3Q_G)/RT$, consequently, for $d/m = 1$, Eq. (8) can be rewritten as,

$$x_e = \frac{gv_0N_1^*}{\Phi}\left[\exp\left(-\frac{Q_G}{RT}\right)\frac{RT^2}{Q_G}q(x_G(T))-\exp\left(-\frac{Q_G}{RT_0}\right)\frac{RT_0{}^2}{Q_G}q(x_G(T_0))\right]$$
$$+\frac{gv_0N_{01}}{\Phi^2}\exp\left(-\frac{Q_G}{RT}\right)\frac{RT^2}{Q_G}q(x_G(T))\int_{T_0}^{T}\exp\left(-\frac{Q_N}{RT(\tau)}\right)dT(\tau)$$
$$-\frac{gv_0N_{01}}{\Phi^2}\int_{T_0}^{T}\exp\left(-\frac{Q_N+Q_G}{RT(\tau)}\right)\frac{RT(\tau)^2}{Q_G}q(x_G(T(\tau)))dT(\tau) \tag{10}$$

With reference to Table 1, the value of $q(x)$, close to unit, is insensitive to T, and thus the integral of the last term at the right-hand side of Eq. (10) can be approximated as $q(x_G(T))\int_{T_0}^{T}\exp(-((Q_N+Q_G))/RT(\tau))(RT(\tau)^2/Q_G)dT(\tau)$.

Corresponding to Eq. (9), the "general temperature integral" is expressed as [10,21–26],

$$\int_0^T T^M\exp\left(-\frac{Q'}{RT}\right)dT = \frac{RT^{M+2}\exp(-(Q'/RT))}{Q'}p_M(x) \tag{11}$$

where, $p_M(x)$ represents the functions of x and M (see Table 2) derived using different methods.

Neglecting the terms including T_0 (cf. Eq. (1)), Eq. (10) leads to,

$$x_e = gv_0N_1^*\exp\left(-\frac{Q_G}{RT}\right)\frac{RT^2}{\Phi}\frac{q(x_G)}{Q_G}+gv_0N_{01}\exp\left(-\frac{Q_N+Q_G}{RT}\right)$$
$$\times\left(\frac{RT^2}{\Phi}\right)^2\left(\frac{q(x_G)q(x_N)}{Q_GQ_N}-\frac{q(x_G)p_2(x_{N+G})}{Q_G(Q_N+Q_G)}\right) \tag{12}$$

Table 4
Expressions for the growth exponent, n, the overall effective activation energy, Q, and the pre-exponential factor of rate constant, K_0, to be insert in Eq. (14). For C_s and C_c, see Table 3.

Kinetic parameter	Mixed nucleation
n	$\frac{d}{m} + \frac{1}{1+(r_2/r_1)^{-1}}$
Q	$\frac{(d/m)Q_G+(n-(d/m))Q_N}{n}$
K_0^n	$\frac{gv_0^{d/m}}{((d/m)+1)^{1/(1+(r_2/r_1)^{-1})}}\left[\left(C_S N_1^*\left(1+\frac{r_2}{r_1}\right)\right)^{1/(1+(r_2/r_1))}\left(C_c N_{01}\left(1+\left(\frac{r_2}{r_1}\right)^{-1}\right)\right)^{1/(1+(r_2/r_1)^{-1})}\right]$
$\frac{r_2}{r_1}$	$\frac{C_c N_{01}\exp(-(Q_N/RT))}{((d/m)+1)C_S N_1^*}\left(\frac{RT^2}{\Phi}\right)$

Analogously, for $d/m = 2$ and 3,[2] a compact form results as,

$$x_e = gv_0^{d/m}N_1^*C_{s(d/m)}\exp\left(-\frac{(d/m)Q_G}{RT}\right)\left(\frac{RT^2}{\Phi}\right)^{d/m}$$
$$+\frac{1}{(d/m)+1}gv_0^{d/m}N_{01}C_{c(d/m)}\exp\left(-\frac{Q_N+(d/m)Q_G}{RT}\right)$$
$$\times\left(\frac{RT^2}{\Phi}\right)^{(d/m)+1} \tag{13}$$

where $C_{s(d/m)}$ and $C_{c(d/m)}$ are listed in Table 3. A detailed derivation is available in Appendix A. Assuming the impingement mode due to random nuclei dispersion (i.e. Eq. (7)), the transformed fraction can be represented by,

$$f = 1-\exp\left(-K_0^n\left(\frac{RT^2}{\Phi}\right)^n\exp\left(-\frac{nQ}{RT}\right)\right) \tag{14}$$

where n, Q, and K_0 are listed in Table 4.

Clearly, the currently analytical model has the same form as the originally analytical model (see Table I and Eq. (36) in Ref. [7]). The only difference between the two models is the expressions for C_s and C_c (see also r_2/r_1 in Table 4), which, due to the different approximations to "temperature integral" and "general temperature integral", affect the precision of the currently analytical description (see Tables 1–4).

Actually, if the condition of $q(x) = 1$ and $p_M(x) = 1$ is adopted, both Eqs. (9) and (11) reduce to Eq. (1), so that the currently analytical model reduces to the originally analytical model. Thus, the current model, as a generalized one of the original model, not only considers a choice of nucleation modes, but also incorporates a choice of approximations to the "temperature integral" and the "general temperature integral".

3. Comparative study for the model

A comparison of kinetic parameters (n, Q and K_0) deduced from the originally analytical model (i.e. $q(x) = 1$ and $p_M(x) = 1$) and from the currently analytical one (e.g. Chen and Liu formula as $q(x)$ and Cai et al. I formular as $p_M(x)$ in combination with Tables 3 and 4) has been performed for a series of non-isothermal transformations (i.e. $\Phi = 5$, 10, 20 and 40 K/min) assuming mixed nucleation, interface-controlled growth and impingement mode due to random nuclei dispersion (Fig. 1(a–c)). On this basis, a comparison between the model-predicted transformed fraction, f (i.e. using Eq. (14)) and the exact one (i.e. numerically calculated using Eqs. (6) and (8)) has also been performed; see Fig. 1(d). Values of model parameters are given in Table 5.

Table 5
Values for parameters used for model calculations.

	Model parameters					
	d/m	N_1^* (m^{-3})	N_{01} (m^{-3} s^{-1})	Q_N (J mol^{-1})	Q_G (J mol^{-1})	v_0 (m s^{-1})
Value	3	1×10^{15}	1×10^{25}	1×10^5	1.5×10^5	1×10^{10}

As shown in Fig. 1(a–c), insignificant deviations occur between the kinetic parameters (n, Q and K_0) predicted from the originally and those from the currently analytical model.[3] However, the relative small deviation causes a substantially magnified deviation (i.e. due to the originally and the currently analytical model) from the numerically calculated f data (Fig. 1(d)).[4] So, the influence of the temperature integral is strengthened through modeling the transformed fraction. This also implies that the kinetic parameters due to the currently analytical model should be more precise.

4. Accuracy evaluation for the model

As shown in Refs. [10,12,15–26], the accuracy of different approximations to the "temperature integral" and the "general temperature integral", i.e. the formulas for $q(x)$ and $p_M(x)$, depends principally on the specific value of x. Given a real phase transformation, the mechanism (e.g. activation energy and transformation temperature range) must be fixed, so that a specific formula of $q(x)$ and $p_M(x)$ should be preferred. So, by the model fits with different combinations of $q(x)$ and $p_M(x)$ to a real transformation, the currently analytical model allows to find the optimal combination.

Defining f_a and f_n as, respectively, the solution obtained from the model prediction (i.e. Eq. (14) with Tables 3 and 4) and the numerical calculation (i.e. Eqs. (6) and (8)), the relative deviation (in percentage) for the model-predicted f data can be expressed as,

$$\varepsilon_r(\%) = 100\left(\frac{f_a}{f_n}-1\right) \tag{15}$$

Eq. (15) is applied for a series of non-isothermal transformations assuming continuous nucleation,[5] interface-controlled growth and impingement mode due to random nuclei dispersion, for a range of x (i.e. $Q/RT = 5$–50). Each pair of $q(x)$ (Table 1) and $p_M(x)$ (Table 2) is adopted in the calculations. The deviations of the model-predicted f data from the numerical one are shown in Table 6.

Applying the originally analytical model, even at large x value, sufficiently precise model-predicted f data cannot be obtained (see Table 6). Whereas, using the currently analytical model, sufficiently precise model-predicted f data result for both high and low x values,

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[2] Whether the approach is applicable to transformations assuming volume diffusion controlled growth (i.e. $d/m = 1/2$ and 3/2) needs further investigation.

[3] The relative deviation for n, Q and K_0 between the two models are 0.49%, 0.15% and 0.42%, respectively.

[4] The relative deviation for f between the two models is 5.7%.

[5] Applying continuous nucleation is aiming to facilitate the calculation. As for continuous nucleation, Q holds constant in the whole process of transformation [8], which is convenient for a fixed x value. The treatment can also be applied to transformation with mixed nucleation, i.e. varying value of Q [8].

Table 6
Deviations (in percentage) of the model-predicted transformed fraction from the numerical one at selected x values.

Combination of the approximations		ε_r (%)							
$p_M(x)$	$q(x)$	5	7.5	10	15	20	30	40	50
1	1	_[a]	_[a]	_[a]	_[a]	_[a]	_[a]	4.3	6.6×10^{-1}
Wanjun et al.	Balarin	_[a]	3.3	1.7	6.0×10^{-1}	2.7×10^{-1}	1.5×10^{-1}	1.7×10^{-1}	2.2×10^{-1}
	Cai et al.	4.7	1.6	6.1×10^{-1}	1.1×10^{-1}	5.1×10^{-2}	1.2×10^{-1}	2.0×10^{-1}	2.7×10^{-1}
	Urbanovici and segal	3.5	1.7	8.9×10^{-1}	3.0×10^{-1}	1.4×10^{-1}	1.0×10^{-1}	1.5×10^{-1}	2.1×10^{-1}
	Chen and Liu	3.8	1.7	8.2×10^{-1}	2.6×10^{-1}	1.1×10^{-1}	9.2×10^{-2}	1.4×10^{-1}	2.0×10^{-1}
	Senum and Yang I	3.6	1.7	8.3×10^{-1}	2.6×10^{-1}	1.1×10^{-1}	9.3×10^{-2}	1.5×10^{-1}	2.0×10^{-1}
	Zsakó	4.7	1.8	2.8×10^{-1}	-7.5×10^{-1}	-8.2×10^{-1}	-5.4×10^{-1}	-2.9×10^{-1}	-1.1×10^{-1}
	Senum and Yang II	3.7	1.7	8.4×10^{-1}	2.6×10^{-1}	1.1×10^{-1}	9.3×10^{-2}	1.5×10^{-1}	2.0×10^{-1}
	Órfão	3.8	1.7	8.4×10^{-1}	2.6×10^{-1}	1.1×10^{-1}	9.3×10^{-2}	1.5×10^{-1}	2.0×10^{-1}
Cai et al. I	Balarin	_[a]	3.1	1.8	8.1×10^{-1}	4.3×10^{-1}	1.6×10^{-1}	6.7×10^{-2}	3.0×10^{-2}
	Cai et al.	3.3	1.4	7.3×10^{-1}	3.3×10^{-1}	2.1×10^{-1}	1.3×10^{-1}	9.7×10^{-2}	8.3×10^{-2}
	Urbanovici and segal	2.2	1.5	1.0	5.1×10^{-1}	2.9×10^{-1}	1.1×10^{-1}	4.6×10^{-2}	1.9×10^{-2}
	Chen and Liu	2.4	1.5	9.4×10^{-1}	4.7×10^{-1}	2.6×10^{-1}	1.0×10^{-1}	4.1×10^{-2}	1.6×10^{-2}
	Senum and Yang I	2.2	1.4	9.5×10^{-1}	4.8×10^{-1}	2.7×10^{-1}	1.0×10^{-1}	4.2×10^{-2}	1.6×10^{-2}
	Zsakó	3.3	1.6	3.9×10^{-1}	-5.3×10^{-1}	-6.7×10^{-1}	-5.4×10^{-1}	-3.9×10^{-1}	-3.0×10^{-1}
	Senum and Yang II	2.3	1.5	9.6×10^{-1}	4.8×10^{-1}	2.7×10^{-1}	1.0×10^{-1}	4.2×10^{-2}	1.6×10^{-2}
	Órfão	2.4	1.5	9.6×10^{-1}	4.8×10^{-1}	2.7×10^{-1}	1.0×10^{-1}	4.2×10^{-2}	1.6×10^{-2}
Cai et al. II	Balarin	3.8	1.4	4.7×10^{-1}	-1.3×10^{-1}	-2.8×10^{-1}	-3.1×10^{-1}	-2.7×10^{-1}	-2.2×10^{-1}
	Cai et al.	8.5×10^{-1}	-3.9×10^{-1}	-6.3×10^{-1}	-6.1×10^{-1}	-5.0×10^{-1}	-3.4×10^{-1}	-2.4×10^{-1}	-1.7×10^{-1}
	Urbanovici and segal	2.7×10^{-1}	-2.6×10^{-1}	-3.5×10^{-1}	-4.3×10^{-1}	-4.2×10^{-1}	-3.5×10^{-1}	-2.9×10^{-1}	-2.4×10^{-1}
	Chen and Liu	-2.9×10^{-3}	-3.0×10^{-1}	-4.2×10^{-1}	-4.7×10^{-1}	-4.4×10^{-1}	-3.6×10^{-1}	-2.9×10^{-1}	-2.4×10^{-1}
	Senum and Yang I	-1.8×10^{-1}	-3.1×10^{-1}	-4.1×10^{-1}	-4.6×10^{-1}	-4.4×10^{-1}	-3.6×10^{-1}	-2.9×10^{-1}	-2.4×10^{-1}
	Zsakó	9.2×10^{-1}	-1.6×10^{-1}	-9.7×10^{-1}	-1.5	-1.4	-1.0	-7.3×10^{-1}	-5.5×10^{-1}
	Senum and Yang II	-7.7×10^{-2}	-2.9×10^{-1}	-4.0×10^{-1}	-4.6×10^{-1}	-4.4×10^{-1}	-3.6×10^{-1}	-2.9×10^{-1}	-2.4×10^{-1}
	Órfão	-6.2×10^{-2}	-2.9×10^{-1}	-4.0×10^{-1}	-4.6×10^{-1}	-4.4×10^{-1}	-3.6×10^{-1}	-2.9×10^{-1}	-2.4×10^{-1}
Cai et al. III	Balarin	_[a]	2.9	1.7	7.8×10^{-1}	4.4×10^{-1}	2.0×10^{-1}	1.2×10^{-1}	7.7×10^{-2}
	Cai et al.	3.1	1.2	6.0×10^{-1}	3.0×10^{-1}	2.2×10^{-1}	1.7×10^{-1}	1.5×10^{-1}	1.3×10^{-1}
	Urbanovici and segal	2.0	1.3	8.8×10^{-1}	4.8×10^{-1}	3.0×10^{-1}	1.5×10^{-1}	9.6×10^{-2}	6.5×10^{-2}
	Chen and Liu	2.3	1.3	8.1×10^{-1}	4.4×10^{-1}	2.8×10^{-1}	1.4×10^{-1}	9.0×10^{-2}	6.2×10^{-2}
	Senum and Yang I	2.1	1.3	8.2×10^{-1}	4.4×10^{-1}	2.8×10^{-1}	1.5×10^{-1}	9.1×10^{-2}	6.3×10^{-2}
	Zsakó	3.2	1.4	2.7×10^{-1}	-5.6×10^{-1}	-6.6×10^{-1}	-4.9×10^{-1}	-3.4×10^{-1}	-2.5×10^{-1}
	Senum and Yang II	2.2	1.3	8.3×10^{-1}	4.4×10^{-1}	2.8×10^{-1}	1.5×10^{-1}	9.1×10^{-2}	6.3×10^{-2}
	Órfão	2.2	1.3	8.3×10^{-1}	4.4×10^{-1}	2.8×10^{-1}	1.5×10^{-1}	9.1×10^{-2}	6.3×10^{-2}
Chen and Liu I	Balarin	_[a]	2.7	1.6	7.4×10^{-1}	4.2×10^{-1}	1.9×10^{-1}	1.1×10^{-1}	7.9×10^{-2}
	Cai et al.	2.6	9.5×10^{-1}	4.9×10^{-1}	2.6×10^{-1}	2.0×10^{-1}	1.6×10^{-1}	1.4×10^{-1}	1.3×10^{-1}
	Urbanovici and segal	1.5	1.1	7.7×10^{-1}	4.4×10^{-1}	2.8×10^{-1}	1.5×10^{-1}	9.4×10^{-2}	6.7×10^{-2}
	Chen and Liu	1.8	1.0	7.0×10^{-1}	4.0×10^{-1}	2.6×10^{-1}	1.4×10^{-1}	8.8×10^{-2}	6.4×10^{-2}
	Senum and Yang I	1.6	1.0	7.1×10^{-1}	4.0×10^{-1}	2.6×10^{-1}	1.4×10^{-1}	8.9×10^{-2}	6.4×10^{-2}
	Zsakó	2.7	1.2	1.6×10^{-1}	-6.0×10^{-1}	-6.7×10^{-1}	-5.0×10^{-1}	-3.5×10^{-1}	-2.5×10^{-1}
	Senum and Yang II	1.7	1.1	7.2×10^{-1}	4.1×10^{-1}	2.6×10^{-1}	1.4×10^{-1}	8.9×10^{-2}	6.4×10^{-2}
	Órfão	1.7	1.1	7.2×10^{-1}	4.1×10^{-1}	2.6×10^{-1}	1.4×10^{-1}	8.9×10^{-2}	6.4×10^{-2}
Chen and Liu II	Balarin	_[a]	3.7	2.0	7.4×10^{-1}	3.5×10^{-1}	1.4×10^{-1}	1.2×10^{-1}	1.4×10^{-1}
	Cai et al.	_[a]	2.0	8.9×10^{-1}	2.6×10^{-1}	1.2×10^{-1}	1.1×10^{-1}	1.5×10^{-1}	1.9×10^{-1}
	Urbanovici and segal	4.1	2.1	1.2	4.4×10^{-1}	2.1×10^{-1}	9.4×10^{-2}	9.8×10^{-2}	1.3×10^{-1}
	Chen and Liu	4.4	2.0	1.1	4.0×10^{-1}	1.8×10^{-1}	8.4×10^{-2}	9.3×10^{-2}	1.2×10^{-1}
	Senum and Yang I	4.2	2.0	1.1	4.1×10^{-1}	1.8×10^{-1}	8.5×10^{-2}	9.4×10^{-2}	1.2×10^{-1}
	Zsakó	_[a]	2.2	5.5×10^{-1}	-6.0×10^{-1}	-7.5×10^{-1}	-5.5×10^{-1}	-3.4×10^{-1}	-1.9×10^{-1}
	Senum and Yang II	4.3	2.1	1.1	4.1×10^{-1}	1.9×10^{-1}	8.5×10^{-2}	9.3×10^{-2}	1.2×10^{-1}
	Órfão	4.3	2.1	1.1	4.1×10^{-1}	1.9×10^{-1}	8.5×10^{-2}	9.4×10^{-2}	1.2×10^{-1}
Chen and Liu III	Balarin	_[a]	2.9	1.7	7.6×10^{-1}	4.2×10^{-1}	1.8×10^{-1}	1.0×10^{-1}	7.3×10^{-2}
	Cai et al.	2.7	1.1	5.8×10^{-1}	2.8×10^{-1}	1.9×10^{-1}	1.5×10^{-1}	1.3×10^{-1}	1.3×10^{-1}
	Urbanovici and segal	1.6	1.2	8.6×10^{-1}	4.6×10^{-1}	2.8×10^{-1}	1.3×10^{-1}	8.2×10^{-2}	6.2×10^{-2}
	Chen and Liu	1.9	1.2	7.9×10^{-1}	4.2×10^{-1}	2.5×10^{-1}	1.2×10^{-1}	7.7×10^{-2}	5.9×10^{-2}
	Senum and Yang I	1.7	1.2	8.0×10^{-1}	4.3×10^{-1}	2.6×10^{-1}	1.2×10^{-1}	7.7×10^{-2}	5.9×10^{-2}
	Zsakó	2.8	1.3	2.4×10^{-1}	-5.8×10^{-1}	-6.8×10^{-1}	-5.1×10^{-1}	-3.6×10^{-1}	-2.5×10^{-1}
	Senum and Yang II	1.8	1.2	8.1×10^{-1}	4.3×10^{-1}	2.6×10^{-1}	1.2×10^{-1}	7.7×10^{-2}	5.9×10^{-2}
	Órfão	1.8	1.2	8.1×10^{-1}	4.3×10^{-1}	2.6×10^{-1}	1.2×10^{-1}	7.8×10^{-2}	5.9×10^{-2}
Capela et al.	Balarin	_[a]	3.0	1.7	7.9×10^{-1}	4.5×10^{-1}	2.0×10^{-1}	1.2×10^{-1}	8.1×10^{-2}
	Cai et al.	3.3	1.2	6.3×10^{-1}	3.1×10^{-1}	2.2×10^{-1}	1.7×10^{-1}	1.5×10^{-1}	1.3×10^{-1}
	Urbanovici and segal	2.4	1.4	9.1×10^{-1}	4.9×10^{-1}	3.1×10^{-1}	1.6×10^{-1}	9.7×10^{-2}	7.0×10^{-2}
	Chen and Liu	2.4	1.3	8.5×10^{-1}	4.5×10^{-1}	2.8×10^{-1}	1.5×10^{-1}	9.2×10^{-2}	6.7×10^{-2}
	Senum and Yang I	2.2	1.3	8.6×10^{-1}	4.6×10^{-1}	2.9×10^{-1}	1.5×10^{-1}	9.3×10^{-2}	6.7×10^{-2}
	Zsakó	2.2	1.5	3.0×10^{-1}	-5.5×10^{-1}	-6.5×10^{-1}	-4.9×10^{-1}	-3.4×10^{-1}	-2.4×10^{-1}
	Senum and Yang II	2.3	1.3	8.6×10^{-1}	4.6×10^{-1}	2.9×10^{-1}	1.5×10^{-1}	9.3×10^{-2}	6.7×10^{-2}
	Órfão	2.4	1.3	8.6×10^{-1}	4.6×10^{-1}	2.9×10^{-1}	1.5×10^{-1}	9.3×10^{-2}	6.7×10^{-2}

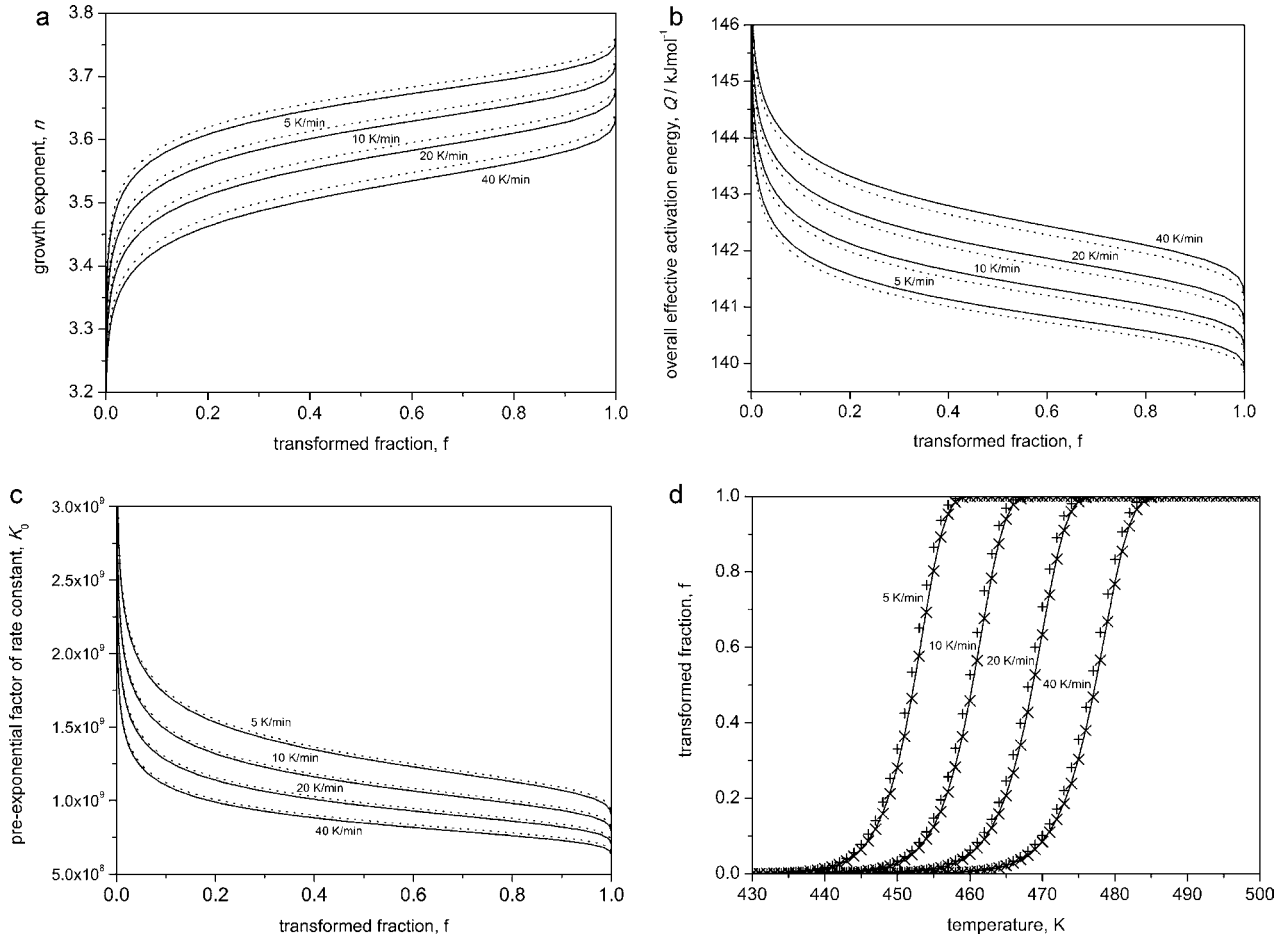[a] The relative error is large than 5%.

Fig. 1. Evolution of (a) growth exponent, n, (b) overall effective activation energy, Q, and (c) pre-exponential factor of the rate constant, K_0, with transformed fraction, as calculated by the originally analytical model (dotted line) and the currently analytical model (solid line); evolution of transformed fraction with temperature (d), as calculated by the numerical approach (solid line) and by Eq. (14) in combination with kinetic parameters by the originally analytical model (+) and by the currently analytical model (×); for non-isothermal phase transformations assuming mixed nucleation, interface-controlled growth and impingement due to random dispersed nuclei.

i.e. the deviations due to model predictions (i.e. except for the models with Balarin and Zsakó formulas as $q(x)$) are smaller than 0.5% for $x \geq 15$; the deviations due to model predictions (i.e. the combinations of Cai et al. II as $p_M(x)$ and Urbanovici and segal, Chen and Liu, Senum and Yang I, Senum and Yang II, and Órfão as $q(x)$) are smaller than 0.5% for $x < 15$ (see Table 6). So, the accuracy of the currently generalized analytical description can be guaranteed by selecting the optimal combination of the approximations in consideration.

Furthermore, the accuracy of the currently analytical model is affected by the approximation made below Eq. (10), so that increasing the accuracy of $q(x)$ does not necessarily improve the accuracy of the currently analytical model. As shown in Table 6, for specific $p_M(x)$ and x value, the minimum deviation is always obtained for the model predictions with Urbanovici and segal or Chen and Liu formula as $q(x)$, which does not correspond to the most precise formula for $q(x)$ (i.e. from Ref. [12], the Órfão formula).

5. Conclusions

A generalized analytical description for non-isothermal solid-state transformation was developed, where a choice of both nucleation modes and approximations to the so-called "temperature integral" and "general temperature integral" is incorporated. Numerical calculations have demonstrated that the currently analytical model, by selecting the optimal combination of the above approximations, is sufficiently precise to describe the transformation, corresponding to different values of x.

Acknowledgements

Appendix A.

For $d/m = 2$, Eq. (8), in combination with Eq. (9), can be rewritten as,

$$
x_e = g v_0^2 \frac{R^2}{\Phi^2 Q_G^2} \int_{T_0}^{T} \left[N_1^* \delta \left(\frac{T(\tau) - T_0}{\Phi} \right) + N_{01} \exp \left(-\frac{Q_N}{RT(\tau)} \right) \right]
$$

$$
\times \left[T^2 \exp \left(-\frac{Q_G}{RT} \right) q(x_G(T)) - T(\tau)^2 \exp \left(-\frac{Q_G}{RT(\tau)} \right) q(x_G(T(\tau))) \right]^2
$$

$$
\times d\frac{T(\tau)}{\Phi} \tag{A.1}
$$

Rearrangement of Eq. (A.1) gives,

$$x_e = g\upsilon_0^2 N_1^* \frac{R^2}{\Phi^2 Q_G^2} \int_{T_0}^{T} \delta(T(\tau) - T_0) \left[\begin{array}{l} T^2 \exp\left(-\frac{Q_G}{RT}\right) q(x_G(T)) \\ -T(\tau)^2 \exp\left(-\frac{Q_G}{RT(\tau)}\right) q(x_G(T(\tau))) \end{array} \right]^2 dT(\tau)$$

$$+ g\upsilon_0^2 N_0^1 \frac{R^2}{\Phi^3 Q_G^2} \left[\begin{array}{l} T^4 \exp\left(-\frac{2Q_G}{RT}\right) q^2(x_G(T)) \int_{T_0}^{T} \exp\left(-\frac{Q_N}{RT(\tau)}\right) dT(\tau) \\ -2T^2 \exp\left(-\frac{Q_G}{RT}\right) q(x_G(T)) \\ \times \int_{T_0}^{T} T(\tau)^2 \exp\left(-\frac{Q_N + Q_G}{RT(\tau)}\right) q(x_G(T(\tau))) \, dT(\tau) \\ + \int_{T_0}^{T} T(\tau)^4 \exp\left(-\frac{Q_N + 2Q_G}{RT(\tau)}\right) q^2(x_G(T(\tau))) \, dT(\tau) \end{array} \right] \quad \text{(A.2)}$$

By doing the approximation under Eq. (10), employing Eq. (11) and neglecting T_0 terms, Eq. (A.2) can be rewritten as,

$$x_e = g\upsilon_0^2 N_1^* \frac{R^2}{\Phi^2 Q_G^2} \left[T^4 \exp\left(-\frac{2Q_G}{RT}\right) q^2(x_G(T)) \right]$$

$$+ g\upsilon_0^2 N_0^1 \frac{R^2}{\Phi^3 Q_G^2} \left[\begin{array}{l} T^4 \exp\left(-\frac{2Q_G}{RT}\right) q^2(x_G(T)) \frac{R}{Q_N} \left(T^2 \exp\left(-\frac{Q_N}{RT}\right) q(x_N(T)) \right) \\ -2T^2 \exp\left(-\frac{Q_G}{RT}\right) q^2(x_G(T)) \frac{R}{Q_N + Q_G} \left(T^4 \exp\left(-\frac{Q_N + Q_G}{RT}\right) p_2(x_{N+G}(T)) \right) \\ + q^2(x_G(T)) \frac{R}{Q_N + 2Q_G} \left(T^6 \exp\left(-\frac{Q_N + 2Q_G}{RT}\right) p_4(x_{N+2G}(T)) \right) \end{array} \right] \quad \text{(A.3)}$$

Rearrangement of Eq. (A.3) leads to,

$$x_e = g\upsilon_0^2 N_1^* \left(\frac{q(x_G)}{Q_G} \right)^2 \exp\left(-\frac{2Q_G}{RT}\right) \left(\frac{RT^2}{\Phi} \right)^2 + \frac{1}{3} g\upsilon_0^2 N_{01} \left(3 \frac{q^2(x_G)}{Q_G^2} \right) \left(\frac{q(x_N)}{Q_N} - 2 \frac{p_2(x_{N+G})}{Q_N + Q_G} + \frac{p_4(x_{N+2G})}{Q_N + 2Q_G} \right) \times \exp\left(-\frac{Q_N + 2Q_G}{RT}\right) \left(\frac{RT^2}{\Phi} \right)^3 \quad \text{(A.4)}$$

Following an analogous treatment, for $d/m = 3$, Eq. (A.5) analogous to Eq. (A.3) results as,

$$x_e = g\upsilon_0^3 N_1^* \frac{R^3}{\Phi^3 Q_G^3} \left[T^6 \exp\left(-\frac{3Q_G}{RT}\right) q^3(x_G(T)) \right]$$

$$+ g\upsilon_0^3 N_{01} \frac{R^3}{\Phi^4 Q_G^3} \left[\begin{array}{l} T^6 \exp\left(-\frac{3Q_G}{RT}\right) q^3(x_G(T)) \frac{R}{Q_N} \left(T^2 \exp\left(-\frac{Q_N}{RT}\right) q(x_N(T)) \right) \\ -3T^4 \exp\left(-\frac{2Q_G}{RT}\right) q^3(x_G(T)) \frac{R}{Q_N + Q_G} \left(T^4 \exp\left(-\frac{Q_N + Q_G}{RT}\right) p_2(x_{N+G}(T)) \right) \\ +3T^2 \exp\left(-\frac{Q_G}{RT}\right) q^3(x_G(T)) \frac{R}{Q_N + 2Q_G} \left(T^6 \exp\left(-\frac{Q_N + 2Q_G}{RT}\right) p_4(x_{N+2G}(T)) \right) \\ - q^3(x_G(T)) \frac{R}{Q_N + 3Q_G} \left(T^8 \exp\left(-\frac{Q_N + 3Q_G}{RT}\right) p_6(x_{N+3G}(T)) \right) \end{array} \right] \quad \text{(A.5)}$$

Rearrangement of Eq. (A.5) gives,

$$x_e = g\upsilon_0^3 N_1^* \left(\frac{q(x_G)}{Q_G} \right)^3 \exp\left(-\frac{3Q_G}{RT}\right) \left(\frac{RT^2}{\Phi} \right)^3 + \frac{1}{4} g\upsilon_0^3 N_{01} \left(4 \frac{q^3(x_G)}{Q_G^3} \right) \left(\frac{q(x_N)}{Q_N} - 3 \frac{p_2(x_{N+G})}{Q_N + Q_G} + 3 \frac{p_4(x_{N+2G})}{Q_N + 2Q_G} - \frac{p_6(x_{N+3G})}{Q_N + 3Q_G} \right)$$

$$\times \exp\left(-\frac{Q_N + 3Q_G}{RT}\right) \left(\frac{RT^2}{\Phi} \right)^4 \quad \text{(A.6)}$$

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