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Parameter determination of an evolution model for phase transformations in steel

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Abstract

The paper is concerned with a general ansatz of a phenomenological evolution model for solid-solid phase transformation kinetics in steel. To model the phase transition of austenite-ferrite, -pearlite or -bainite, a first order nonlinear ordinary differential equation (ODE) is considered. The main goal of this paper is to derive certain conditions for parameters which are based on data obtained from transformation diagrams. This leads to a set of independent parameters for which the inverse problem has an unique solution.

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1 Introduction and goal

Steels can exhibit a wide variety of properties depending on composition as well as the phases and microconstituents present, which in turn depend on the heat treatment. One can conveniently describe what is happening during transformation with transformation diagrams. Isothermal transformation diagrams shows what happens when a steel is held at a constant temperature for a prolonged period. Isothermal transformation (IT) diagrams, also referred to as time-temperature-transformation (TTT) diagrams, describing the decomposition of austenite. The procedure starts at a high temperature, normally in the austenitic range after holding there long enough to obtain homogeneous austenite, followed by rapid cooling to the desired hold temperature [1]. An example of an IT diagram is given in Fig. 1. This is the way the diagram itself was developed. Therefore the IT diagram may be read only along the isotherms.

In an isothermal reaction most experimental transformation curves are sigmoidal in shape, see Fig. 2. The kinetics of isothermal phase transformations have been described by the Johnson-Mehl-Avrami-Kolmogorov

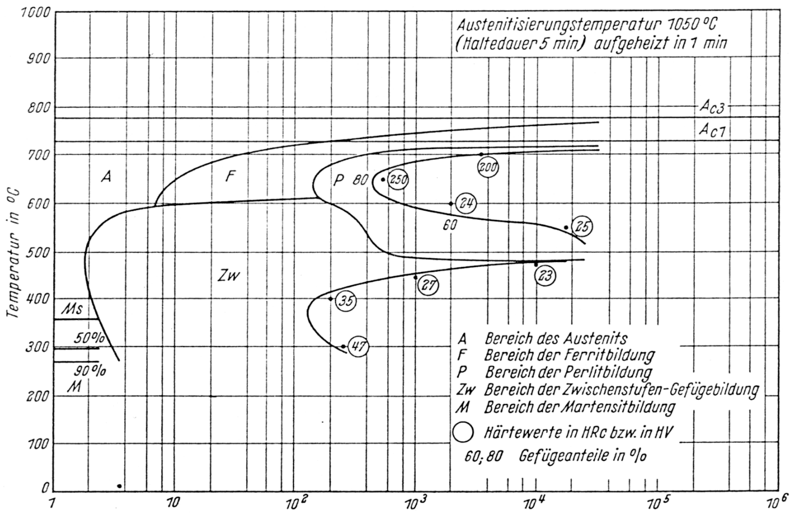


Fig. 1: Isothermal transformation diagram for the steel 42CrMo4 from [2].

(JMAK) phenomenological model since the 40's, see for example the standard textbook [3, p. 18] or [4]. We also refer to the work [5], which discusses extensions of the range of transformations based on submodels for the mechanisms: nucleation, growth and impingement. Furthermore, various classification schemes, based on thermodynamics, microstructure or mechanism are discussed and criticized from a practical as well as a more fundamental point of view in [6]. Various phase transition models and generalisations to get more practicable tools for simulations based on ODEs are discussed in [7]. The parameter determination therein uses a least-square approximation to fit a model against a transformation curve obtained from dilatometer experiments. For modelling, simulation and process control of a heat treatment we refer to [8].

We consider the following growth model for the phases ferrite, pearlite or bainite.

$$y'(t) = (a + y(t))^r (y_{eq} - y(t))^s g\,, \quad y(0) = y_0$$

The parameter a was introduced in the mentioned work [7] and the parameters r and s for $a = 0$ were established in [9]. A frequently used ansatz with $a = 0$, $g = 1$ and $s = 1 - r$ was used in [10]. In the case $r = 0$ and $s = 1$ we recover the model of Leblond and Devaux [11]. However, all these generalisations are more or less formally with the aim to extend the range of applications and these are not motivated by thermodynamics, microstructure or mechanism considerations. Therefore, at this stage in practical simulations it amonts to a data fitting problem to determine the model parameters, which

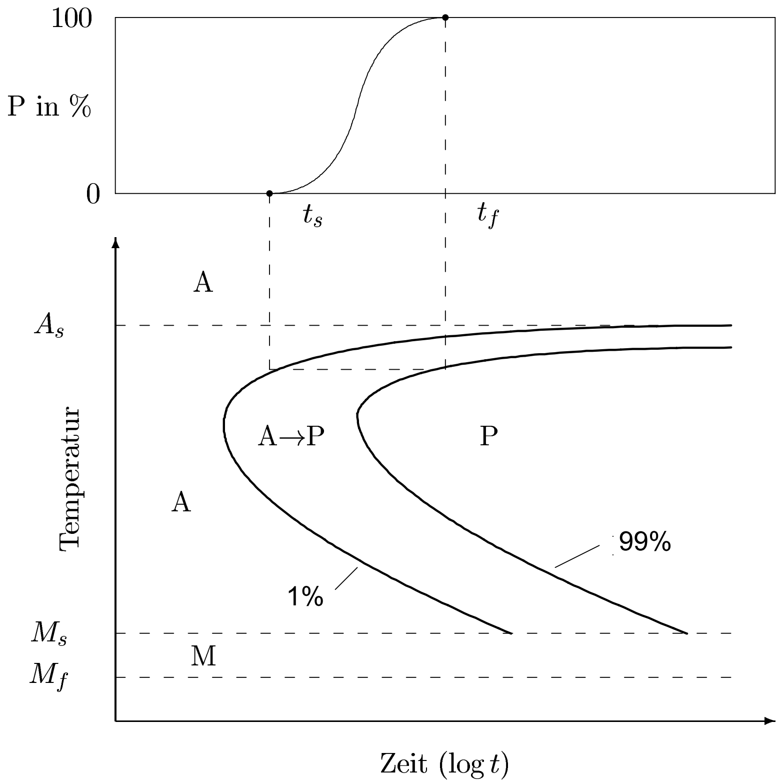


Fig. 2: Relationship of an isothermal reaction curve for pearlite formation to the IT diagram. Source [9].

are only be valid in a small range of heat treatment simulations. In this paper, only data obtained from IT diagrams will be considered to determine the unknown parameters. In other words, the begin and end time of a transformation obtained from an IT diagram should be matched exactly by the model.

The following questions are still open and will be answered in this work.

- Is the model ansatz possibly suitable for all isothermal transformation curves?
- Is the transformation curve unique for given data?

In Section 2 we first formulate the inverse problem with appropriate data condition. Some mathematical properties of a more general ODE $y' = f(y)g$ will be analyzed in Section 3 and Section 4 deals with properties of a certain function H, which are tools for further sections. A central point of this work, discussed at the beginning of Section 5, is to consider an additional control point (the inflection point), which characterizes the sigmoidal shape mathematically. And this leads to a classification into: data, independent parameters and dependent parameters. Moreover, the independent parameters have clear geometrical meaning. The Theorems 6.6 and 6.12 mark the top end and offers the possibility to choose the set of independent parameters for given data, which then leads to an unique transformation curve.

It should be mentioned, that growth models also play an important role in mathematical biology and if $r = s = 1$ and $a = 0$, we obtain the Verhulst-Pearl logistic growth equation [12]. An analysis of the Verhulst-Pearl logistic growth equation including its point of inflection, was given in the early work [13].

2 The inverse problem

Basically, the phase transformation should fulfill the following data conditions

$$\begin{array}{rcll} y(t_1) & = & y_1 & \text{start fraction} \\ y(t_2) & = & y_2 & \text{end fraction} \\ & & y_{eq} & \text{equilibrium fraction} \end{array} \tag{1}$$

and without loss of generality let $y_{eq} \leq 1$. The proposal considers the following inverse problem

Problem. Find parameters $r, s, g, a, y_0 \in \mathbb{R}_{\geq 0}$ such that data condition (1) holds for a solution y of the initial value problem

$$\begin{array}{rcl} y'(t) & = & (a + y(t))^r (y_{eq} - y(t))^s g \,, \quad t > 0 \\ y(0) & = & y_0 \end{array} \tag{2}$$

3 Some properties of $y' = f(y)g$

In this section we consider

$$\begin{array}{rcl} y' & = & f(y)g \,, \quad t > 0 \\ y(0) & = & y_0 \end{array} \tag{3}$$

with the assumption

(A1) Let $f : [0, \infty) \to (0, \infty)$ Lipschitz continuous, $g \neq 0$ and $y_0 \geq 0$.

It is well known that the problem (3) has an unique solution if (A1) holds. This is a consequence of the Picard-Lindelöf theorem. Next, we state two transformation results for the initial value problem (3).

Proposition 3.1. *Let $p_0 \in \mathbb{R}$ and*

$$p' = f(p)g\ , \quad p(0) = p_0 \tag{4}$$

$$q' = f(q)g\ , \quad q(0) = q_0 \tag{5}$$

Then it holds $q(t+a) = p(t)$ for all $t \geq 0$ and $a \in \mathbb{R}$ iff the following condition for q_0 holds

$$g = \frac{1}{a}\int\limits_{q_0}^{p_0} \frac{1}{f(y)}\,\mathrm{d}y$$

Proof. First we identify the equations (4,5)

$$\frac{p'}{f(p)} = \frac{q'}{f(q)} = g$$

After integration with respect to time this is equivalent to

$$\int\limits_{t}^{t+a} \frac{p'}{f(p)}\,\mathrm{d}t = \int\limits_{t}^{t+a} \frac{q'}{f(q)}\,\mathrm{d}t = ag$$

and after integration by substitution and use of $q(t+a) = p(t)$ we result in

$$\frac{1}{a}\int\limits_{q(t+a)}^{p(t+a)} \frac{1}{f(y)}\,\mathrm{d}y = \frac{1}{a}\int\limits_{q(t)}^{p(t)} \frac{1}{f(y)}\,\mathrm{d}y = g$$

for arbitrary t. The proof is shown for $t = 0$. □

Proposition 3.2. *Let $p_0 \in \mathbb{R}$. Iff*

$$p' = f(p)g\ , \quad p(0) = p_0 \tag{6}$$

$$q' = f(q)\frac{g}{a}\ , \quad q(0) = p_0 \tag{7}$$

then it holds $q(at) = p(t)$ for all $t \geq 0$.

Proof. We integrate the equations (6,7) as follows

$$q(at) = q(0) + \frac{g}{a} \int\limits_0^{at} f(q)\,\mathrm{d}t$$

$$p(t) = p(0) + g \int\limits_0^{t} f(p)\,\mathrm{d}t$$

Both initial values are equal and if $q(at) = p(t)$ is true, then the following expression must also be valid

$$\frac{1}{a} \int\limits_0^{at} f(q)\,\mathrm{d}t = \int\limits_0^{t} f(p)\,\mathrm{d}t$$

If we insert the equations (6,7), then the last equation is equivalent to

$$\frac{1}{a} \int\limits_0^{at} q' \frac{a}{g}\,\mathrm{d}t = \int\limits_0^{t} p' \frac{1}{g}\,\mathrm{d}t$$

But this is nothing else then

$$q(at) - q(0) = p(t) - p(0) \;\Leftrightarrow\; q(at) = p(t)$$

□

The next statement contains a particular scaling which ensures the duration $t_2 - t_1$ of the essential time evolution.

Proposition 3.3. *Let $p_0 \in \mathbb{R}$. Iff*

$$g = \frac{1}{t_2 - t_1} \int_{p_1}^{p_2} \frac{1}{f(y)}\,\mathrm{d}y$$

in the initial value problem

$$p' = f(p)g\,, \quad p(0) = p_0 \tag{8}$$

then it holds

$$p^{-1}(p_2) - p^{-1}(p_1) = t_2 - t_1$$

Proof. Without loss of generality we consider the case $p(0) = p_1$. This case is a simple shift realized by translation Proposition 3.1. With $\tau = t_2 - t_1$ we have to show: $p(\tau) = p_f$. Integration of equation (8) leads to

$$p(\tau) = p_s + g \int_0^\tau f(p)\,\mathrm{d}t \stackrel{!}{=} p_f$$

and after inserting g we obtain

$$\left(\int_{p_1}^{p_2} \frac{1}{f(p)}\,\mathrm{d}p \right) \left(\int_0^\tau f(p)\,\mathrm{d}t \right) \stackrel{!}{=} (p_2 - p_1)\tau$$

The integrals of the factorable function $(p, t) \mapsto 1/f(p) \cdot f(p(t))$ can be written as

$$\int_{p_1}^{p_2} \int_0^\tau \frac{1}{f(p)} \cdot f(p(t))\,\mathrm{d}t\,\mathrm{d}p \stackrel{!}{=} (p_2 - p_1)\tau$$

and after substitution this leads to

$$\int_0^\tau \int_0^\tau \frac{p'(t)}{f(p(t))} \cdot h(p(t))\,\mathrm{d}t\,\mathrm{d}t \stackrel{!}{=} (p_2 - p_1)\tau$$

which is equivalent to

$$(p(\tau) - p(0)) \int_0^\tau \mathrm{d}t \stackrel{!}{=} (p_2 - p_1)\tau$$

After use of $p(0) = p_1$ we have concluded the proof. □

4 Some properties of the function H

In the following sections we need some properties of a function which will occur as integrand. We first define

$$\hat{H}(m, r, s, a, y) := \left(\frac{a + m}{a + y} \right)^r \left(\frac{eq - m}{eq - y} \right)^s \tag{9}$$

and a special representation of the first exponent

$$r(s, a) := \frac{a + m}{eq - m} s \tag{10}$$

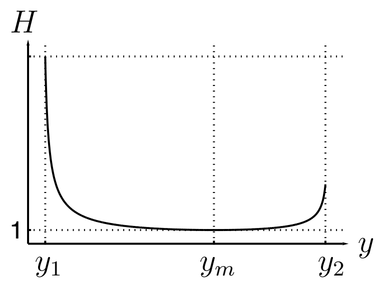


Fig. 3: Example plot of $H(s, a, .)$ with $a = 0$.

with the assumption

(A2) Let $s \geq 0$. Furthermore, let $0 < eq$, $0 \leq a$, $m < eq$ and $0 < a + m$.

And if the last definition is inserted in $\hat{H}$ with fix parameter m , the following definition will be used for the sake of simplicity

$$H(s, a, y) := \hat{H}(m, r(s, a), s, a, y) \tag{11}$$

An example plot of y dependency is shown in Fig. 3. Some properties of H will be discussed now.

Lemma 4.1. *Suppose that (A2) is satisfied and $y, z \in (0, eq)$. Then it holds*

$$\begin{aligned} \hat{H}(m, r, s, a, m) &= 1 && (12) \\ \hat{H}(y, r, s, a, z) &= \hat{H}(m, r, s, a, z)/\hat{H}(m, r, s, a, y) && (13) \\ H(1, a, y) &> 1\,,\; y \neq m && (14) \\ H(s, a, y) &= H(1, a, y)^s && (15) \\ H(s, a, y) &> 1\,,\; y \neq m && (16) \end{aligned}$$

And for the derivatives with respect to s it holds

$$\begin{aligned} \partial_s H(s, a, y) &= H(s, a, y) \log(H(1, a, y)) && (17) \\ \partial_s H(s, a, m) &= 0 && (18) \\ \partial_s H(s, a, y) &> 0\,,\; y \neq m && (19) \end{aligned}$$

And for the derivatives with respect to y it holds

$$\begin{aligned}
\partial_y \hat{H}(m,r,s,a,y) &= \hat{H}(m,r,s,a,y)\left(\frac{s}{eq-y} - \frac{r}{a+y}\right) && (20)\\
\partial_{yy} \hat{H}(m,r,s,a,y) &= \hat{H}\cdot\left(\frac{s}{eq-y} - \frac{r}{a+y}\right)^2 + \\
&+ \hat{H}\cdot\left(\frac{s}{(eq-y)^2} + \frac{r}{(a+y)^2}\right) && (21)\\
\partial_{yy} H(s,a,y) &> 1\,,\ s>0 && (22)
\end{aligned}$$

And for the derivatives with respect to a it holds

$$\begin{aligned}
\partial_a H(s,a,y) &= H(s,a,y)\frac{s}{eq-m}\cdot \\
&\cdot\left(1 - \frac{a+m}{a+y} + \log\left(\frac{a+m}{a+y}\right)\right) && (23)\\
\partial_a H(s,a,m) &= 0 && (24)\\
\partial_a H(s,a,y) &< 0\,,\ y\neq m\,,\ s>0 && (25)
\end{aligned}$$

Proof. The equations (12,13) and (15) are clear. And the inequality (16) is a consequence of the inequality (14) and (15). The first derivatives (17,20) and (23) with respect to s, y and a follow directly from basic calculus rules. The second derivative (21) ditto. The identity (18) is a consequence of (17) and (12). Obviously, the first order derivative inequality (19) holds with (17) and (16). The second order one (22) is shown by (21) and (16). Finally, the inequality (14) can be shown with Bernoulli's inequality $(1+x)^r \geq 1+rx$ for $x>-1$. We set $x=(a+m)/(a+y)-1$ and obtain

$$\begin{aligned}
H(1,a,y) &= \left(\frac{a+m}{a+y}\right)^{r(1,a)}\left(\frac{eq-m}{eq-y}\right) \geq \\
&\geq \left(1 + r(1,a)\left(\frac{a+m}{a+y} - 1\right)\right)\left(\frac{eq-m}{eq-y}\right) = \\
&= \frac{(eq-y)a + (m-y)^2 - y^2 + eq\cdot y}{(a+y)(eq-y)} \overset{!}{>} 1\,,\ y\neq m
\end{aligned}$$

and this is fulfilled iff

$$m^2 + a\cdot eq - a\cdot y + eq\cdot y - 2my \overset{!}{>} (eq-y)(a+y)\,,\ y\neq m$$

But this is nothing else than $(m-y)^2 \stackrel{!}{>} 1$ which is true for $y \neq m$ and therefore (14) holds. Figure 3 shows a sample plot of H with varying y. The identity (24) holds, because the term in brackets of (23) is zero in this case. And in the inequality (25), the $H > 0$ because of the inequality (16). Only the term in brackets is less than zero, because for $x > 0$ and $x \neq 1$ it holds $1 + \log(x) < x$. □

Lemma 4.2. *Suppose that (A2) is satisfied and $y \in (0, eq)$. The map $y \mapsto H(s, a, y)$ is strictly monotonically increasing if $m < y$. And strictly monotonically decreasing if $y < m$.*

Proof. With regard to the inequality (16) the derivative $\partial_y H$, mentioned in (20), is greater than zero iff

$$\begin{aligned} \frac{s}{eq-y} - \frac{r(s,a)}{a+y} > 0 \quad &\Leftrightarrow \quad (a+y)s > r(s,a)(eq-m) \\ &\Leftrightarrow \quad (a+eq)y > (a+eq)m \\ &\Leftrightarrow \quad y > m \end{aligned}$$

For this case the map is strictly monotonically increasing. The decreasing case is shown for '<'. □

Lemma 4.3. *Suppose that (A2) is satisfied and $y \in (0, eq)$. The map $y \mapsto H(s, a, y)$ is strict convex.*

Proof. Strictly convexity is equivalent to $\partial_{yy} H(s, a, y) > 1$ which was shown in Lemma 4.1. □

Lemma 4.4. *Suppose that (A2) is satisfied and $0 < y_1 < y_2 < eq$. Then it holds*

$$\int_{y_1}^{y_2} \partial_s H(s,a,y)\,\mathrm{d}y \quad > \quad 0 \tag{26}$$

$$\int_{y_1}^{y_2} \partial_a H(s,a,y)\,\mathrm{d}y \quad < \quad 0 \tag{27}$$

Proof. From the properties (18) and (19) of Lemma 4.1 it is known that the map $\partial_s H(., a, y)$ is positive for all $y \neq y_m$ and otherwise zero. And therefore the inequality (26) holds for $s > 0$. And from the properties (24) and (25) of Lemma 4.1 it is known that the map $\partial_a H(., a, y)$ is negative for all $y \neq y_m$ and otherwise zero. And therefore the inequality (27) holds for $s > 0$. □

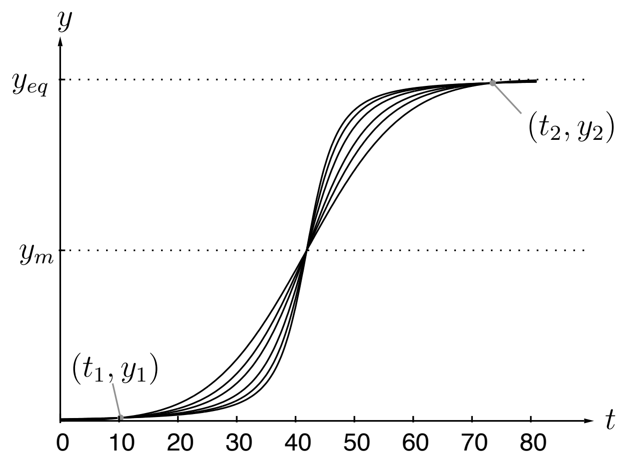


Fig. 4: Several solutions of the ODE (2) which all fulfill the condition (1). The independent parameters are $y_m = 0.5y_{eq}$ and $y_{tm} \in \{2.0, 2.5, 3.0, 4.0, 5.0, 6.0\}$ for the case $y_0 > 0$.

5 Parameter conditions

This section introduces an additional control point, which defines the desired characteristic growth behaviour of ODE (2). An obvious one is the inflection point $(t_m, y(t_m))$ of the solution y. In order to obtain $y' > 0$ in the initial value problem (2) the following assumption is necessary.

(A3) Let $0 \le y_0 < y_{eq}$ and $0 \le a$. Furthermore, let exclusive $y_0 > 0$ or $a > 0$.

In the further text, we will denote the case $y_0 > 0$, $a = 0$ shortly with case $y_0 > 0$ and the case $a > 0$, $y_0 = 0$ with the case $a > 0$. The inflection point is defined as a solution of the

Problem 5.1. Suppose that (A3) is satisfied and y fulfills the differential equation (2). Find a $t_m > 0$ such that

$$y'(t_m) = \max_{t \in (0,\infty)} y'(t) = f_{r,s}(y)g \tag{28}$$

where $f_{r,s}(y) := (a + y)^r (y_{eq} - y)^s$.

Notice, that $f_{r,s}(.)$ is Lipschitz continuous and therefore it is well known that the initial value problem has an unique solution.

Proposition 5.2. *(necessary condition) If t_m is the global maximum of Problem 5.1, then it holds*

$$(y_{eq} - y(t_m))r = (a + y(t_m))s \tag{29}$$

Proof. The necessary condition $y''(t_m) = 0$ must be true. After short calculation it ends up with

$$y''(t_m)/g = rf_{r-1,s}(y(t_m)) - sf_{r,s-1}(y(t_m))$$

and after dividing this equation by $f_{r-1,s-1}(y(t_m))$ we obtain the necessary condition (29). □

Proposition 5.3. *(sufficient condition) If equation (29) and the condition*

$$s > 0 \tag{30}$$

holds, then t_m maximizes the Problem 5.1.

Proof. We show $y'''(t_m) < 0$. This is equivalent to

$$\begin{aligned} y'''/g &= (y')^2\left[(r-1)rf_{r-2,s} - 2rsf_{r-2,s-1} + (s-1)sf_{r,s-2}\right] \\ &\quad + y''\left[rf_{r-1,s} - sf_{r,s-1}\right] < 0 \end{aligned}$$

and after inserting the necessary condition $y'' = 0$ and its equivalent equation (29) into this inequality, and furthermore dividing by $f_{r-2,s-2}(y(t_m)) \cdot (y')^2$ we obtain the condition $-(a + y(t_m))s < 0$. The assumption (A3) is satisfied and therefore it holds $a + y(t) > 0$ for all $t \geq 0$. So, $s > 0$ and this implies that $y'''(t_m) < 0$. □

To point out the data character of the values at the maximum of (28) we define $y_{tm} = y'(t_m)$ and $y_m = y(t_m)$. And this leads to the following classification

data	t_1, t_2, y_1, y_2, y_{eq}
independent parameters	y_m, y_{tm}
dependent parameters	a, y_0, g, r, s

Choosing the transformation characteristic by independent parameters is demonstrated in Fig. 4. We are now able to determine the dependent parameters of the ODE (2) by the data and by the independent parameters which will be shown below.

If $y_m < y_{eq}$ then the definition of $r(s, a)$ from (10) is equivalent to the condition (29) and determines r directly. At the maximum it holds (28) which leads to

$$g_m(s,a) := \frac{y_{tm}}{(a+y_m)^{r(s,a)}(y_{eq}-y_m)^s} \tag{31}$$

Furthermore, we obtain from the scaling Proposition 3.3

$$g_{sc}(s,a) := \frac{1}{t_2-t_1}\int_{y_1}^{y_2} \frac{1}{(a+y)^{r(s,a)}(y_{eq}-y)^s}\,\mathrm{d}y$$

and from the translation Proposition 3.1

$$g_{tr}(s,a,y_0) := \frac{1}{t_1}\int_{y_0}^{y_1} \frac{1}{(a+y)^{r(s,a)}(y_{eq}-y)^s}\,\mathrm{d}y$$

After identifying the last three equations we obtain

$$y_{tm} = F_{sc}(s,a) = F_{tr}(s,a,y_0) \tag{32}$$

with the definitions

$$F_{sc}(s,a) := \frac{1}{t_2-t_1}\int_{y_1}^{y_2} H\,\mathrm{d}y \tag{33}$$

$$F_{tr}(s,a,y_0) := \frac{1}{t_1}\int_{y_0}^{y_1} H\,\mathrm{d}y \tag{34}$$

and the function H from definition (11). The next statement shows that this construction really satisfies the desired data condition

Lemma 5.4. *Suppose that (A3) is satisfied. Let $y_m < y_{eq}$ and $a + y_m > 0$. If a $s > 0$ exists with $g_{sc}(s,a) = g_{tr}(s,a,y_0) =: g$ then the ODE (2) fulfills $y(t_1) = y_1$ and $y(t_2) = y_2$.*

Proof. With Proposition 3.3 the equality $g_{sc}(s,a) = g$ implies $y^{-1}(y_2) - y^{-1}(y_1) = t_2 - t_1$. And with Proposition 3.1 the equality $g_{tr}(s,a,y_0) = g$ implies $y(t_1) = y_1$. In detail: consider $p' = p^r(y_{eq}-p)^s g$, $p(0) = y_1$. This leads to $p^{-1}(y_2) - p^{-1}(y_1) = t_2 - t_1$; cf. Proposition 3.3. And the ODE (2) is $y' = y^r(y_{eq}-y)^s g$, $y(0) = y_0$ with the same parameters. But this precisely identifies the t_1 in Proposition 3.1 with $y(t+t_1) = p(t)$. Especially it holds $y(0+t_1) = p(0) = y_1$ and $y(t_2 - t_1 + t_1) = p(t_2 - t_1) = y_2$, because $p^{-1}(y_1) = 0$. □

Before we show that the equation (32) has a solution, we analyse the growth behaviour of (33) and (34).

Lemma 5.5. *The functions F_{sc} and F_{tr} are strictly monotonically increasing in the first argument, and moreover both are strictly monotonically decreasing in the second argument.*

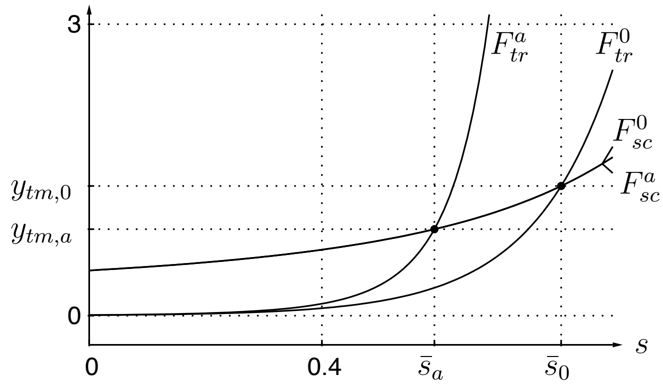


Fig. 5: Shows two solutions $\bar{s}_a$ and $\bar{s}_0$ of the second equation in (37); cf. Theorem 5.6. First with $a = 10^{-7}, y_0 = 0$ and second with $a = 0, y_0 = 0.000916118$ and for both $y_m = 0.6$. The values of F_{sc} are nearly identical. Pearlie data are taken from steel C100W1 at isothermal temperature 451°C; cf. Fig. 10.

Proof. We consider

$$F_{sc}(s,a) = \frac{1}{t_2 - t_1} \int_{y_1}^{y_2} H(s,a,y)\,\mathrm{d}y$$

and its derivative

$$\partial_s F_{sc}(s,a) = \frac{1}{t_2 - t_1} \int_{y_1}^{y_2} \partial_s H(s,a,y)\,\mathrm{d}y$$

From Lemma 4.4 follows that $\partial_s F_{sc}(s,a)$ is positive for $s > 0$. Hence, $F_{sc}(.,a)$ is strictly monotonically increasing, because of the monotonicity of the Riemann integral. The same arguments are true for $F_{tr}(.,a,y_0)$. And the decreasing cases follow from the negativity of $\partial_a H(s,.,y)$ for $y \neq y_m$; s. property (25). $\square$

The following theorem ensures that the second equation of (32) has an unique solution under certain conditions. An example is shown in Fig. 5.

Theorem 5.6. *Suppose that (A3) is satisfied with*

$$\frac{y_2 - y_1}{t_2 - t_1} > \frac{y_1 - y_0}{t_1} \tag{35}$$

and

$$\hat{H}(y, (a + y_m)/(y_{eq} - y_m), 1, a, y_0) > 1 \ , \ \forall y \in \{y_1, y_2\} \tag{36}$$

Then it exists an unique $\bar{s} > 0$ *with*

$$F_{tr}(\bar{s}, a, y_0) = F_{sc}(\bar{s}, a) \tag{37}$$

Moreover

$$\partial_s F_{tr}(\bar{s}, a, y_0) > \partial_s F_{sc}(\bar{s}, a) \tag{38}$$

Proof. The functions F_{tr} and F_{sc} are strictly monotonically increasing in the first argument; cf. Lemma 5.5. The idea is to find two values s_0 and s_1 for which holds

$$F_{tr}(s_0, a, y_0) < F_{sc}(s_0, a) \tag{39}$$

$$F_{tr}(s_1, a, y_0) > F_{sc}(s_1, a) \tag{40}$$

Then the continuity implies the existence of an $\bar{s} \in (s_0, s_1)$ that satisfies (37) and the strict monotonicity implies the uniqueness of a solution. The value $s_0 = 0$ together with the assumption (35) ensures the inequality (39). Now we show the existence of s_1 which fulfills the property (40). From the upper sum we get the following estimation

$$F_{sc}(s, a) \leq \frac{y_2 - y_1}{t_2 - t_1} H^{max}(s, a) \tag{41}$$

with

$$\begin{aligned} H^{max}(s, a) &= \max_{y \in [y_1, y_2]} H(s, a, y) \\ &= \max\{H(s, a, y_1), H(s, a, y_2)\} \end{aligned} \tag{42}$$

A maxima lies at the boundary, because $y \mapsto H(s, a, y)$ is strict convex (s. Lemma 4.3). We consider the first case $H_{max}(s, a) = H(s, a, y_1)$; cf. Fig. 3. From the strict monotonicity of H concerning y follows that if $y_0 < y_1$ then $H(s, a, y_0) > H^{max}(s, a)$. And considering with regard to the other case $H_{max}(s, a) = H(s, a, y_2)$. By applying the inequality (16) of Lemma 4.1, the mentioned condition (36) is equivalent to $H(s, a, y_0) > H^{max}(s, a)$.

Let $\hat{s} > 0$. The mean value theorem ensures the existence of a $\bar{y} \in (y_0, y_1)$ with

$$\frac{y_1 - y_0}{t_1} H(\hat{s}, a, \bar{y}) = F_{tr}(\hat{s}, a, y_0)$$

and the strictly monotonically decreasing of H concerning y implies

$$\frac{y_1 - y_0}{t_1} H(\hat{s}, a, \hat{y}) < F_{tr}(\hat{s}, a, y_0) \ , \ \hat{y} = \frac{y_1 + \bar{y}}{2}$$

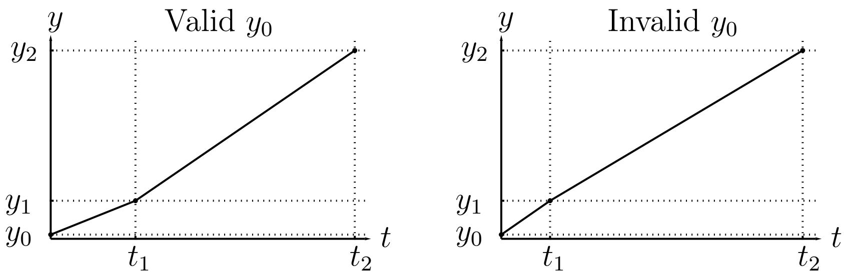


Fig. 6: Example of valid and invalid y_0; see condition (35) in Lemma 5.6.

Furthermore, from property (19) of Lemma 4.1 it is know that $s \mapsto H(s, a, y)$ is strictly monotonically increasing for $y_m \neq y$ and therefore the last inequality holds for all $s \geq \hat{s}$

$$\frac{y_1 - y_0}{t_1} H(s, a, \hat{y}) < F_{tr}(s, a, y_0) \tag{43}$$

The strict monotonicity of $y \mapsto H(s, a, y)$ ensures that if $\hat{y} < y_1$ then it holds

$$H^{max}(s, a) < H(s, a, \hat{y}) \tag{44}$$

Again, the monotonicity of $s \mapsto H(s, a, y)$ together with (44) ensures the existence of a value $s_1 > 0$ for which

$$\frac{y_2 - y_1}{t_2 - t_1} H^{max}(s_1, a) < \frac{y_1 - y_0}{t_1} H(s_1, a, \hat{y})$$

Connecting the inequalities (41) and (43) to the left and to the right completes the proof of existence.

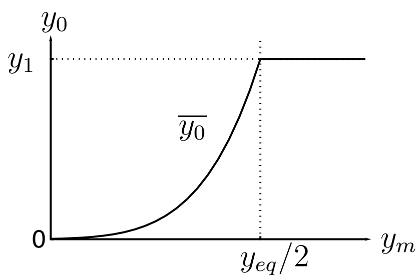
In order to show the inequality (38), we add the inequalities (39,40) and obtain

$$\frac{F_{sc}(\bar{s} + \varepsilon, a) - F_{sc}(\bar{s}, a)}{\varepsilon} < \frac{F_{tr}(\bar{s} + \varepsilon, a, y_0) - F_{tr}(\bar{s}, a, y_0)}{\varepsilon} \tag{45}$$

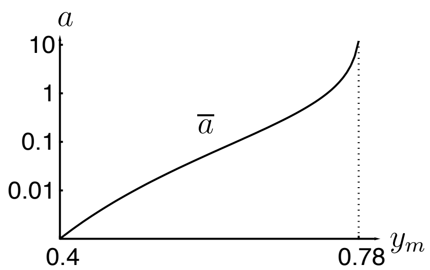
where $\varepsilon > 0$ such that $\bar{s} + \varepsilon \in (s_1, s_2)$. Because of the strict monotonicity, the inequalities (39,40) are true for all $s \in (s_1, s_2)$. Passing to the limit in (45) ends the proof. $\square$

6 Parameter existence

This section considers the two cases of interest from assumption (A3) separately. The parameter conditions of Theorem 5.6 at hand leads to admissible parameter ranges.



Case $y_0 > 0$: The upper bound $\overline{y_0}$ is only a restriction for $y_m < y_{eq}/2$.



Case $a > 0$: Here, the upper bound $\overline{a}$ is only a restriction for $y_m < 0.78$.

Fig. 7: Example plot of upper bounds for y_0 and a; s. Subsection 6.1 and Subsection 6.2.

6.1 The case $y_0 > 0$

In order to obtain unique bounds for y_0, the following assumption is required

(A4) Let $y_1 < y_m$.

The condition (35) is a restriction for y_0; see Fig. 6. The explicit lower bound must also be greater than zero, therefore

$$\underline{y_0} := \max\left\{0, y_1 - \frac{y_2 - y_1}{t_2 - t_1} t_1\right\}$$

For this case it is always possible to find a valid y_0 with $\underline{y_0} < y_0 < y_1$ if $y_m \geq y_{eq}/2$; in this case y_1 maximizes (42) and condition (36) is not required. But if $y_m < y_{eq}/2$, the condition (36) becomes to an upper bound $\overline{y_0}$ of y_0.

$$\overline{y_0} := \begin{cases} y_1 & , y_m \geq y_{eq}/2 \\ y < y_1 : \left(\frac{y_2}{y}\right)^{r(1,0)} \frac{y_{eq}-y_2}{y_{eq}-y} = 1 & , \text{else} \end{cases}$$

Roughly speaking, the set of valid start values $(\underline{y_0}, \overline{y_0})$ shrinks for smaller t_1 and smaller $y_m (< y_{eq}/2)$. Note that the solution of the equation which defines the upper bound $\overline{y_0}$ is unique, because of Lemma 4.2 and (A4); see for example Fig. 7 on the left-hand side. In detail the upper bound $\overline{y_0}$ for $y_m < y_{eq}/2$ is defined by $H(1, 0, \overline{y_0}) = H(1, 0, y_2)$ with $\overline{y_0} < y_1$.

This preliminary consideration based on the Theorem 5.6 will be resumed in the following corollary.

Corollary 6.1. *If* $y_0 \in (\underline{y_0}, \overline{y_0})$ *then the equation* $F_{tr}(s, 0, y_0) = F_{sc}(s, 0)$ *has an unique solution* $s > 0$.

Lemma 6.2. *Let the assumptions of Theorem 5.6 be true. Then the implicit function* $\lambda_0 : (\underline{y_0}, \overline{y_0}) \to \mathbb{R}_{>0}$*, defined by the graph*

$$G_{\lambda_0} = \{(y_0, s) : F_{tr}(s, 0, y_0) = F_{sc}(s, 0)\,,\ y_0 \in (\underline{y_0}, \overline{y_0})\}$$

is strictly monotonically increasing.

Proof. The graph $G_{\lambda_0} \neq \emptyset$, because the Corollary 6.1 holds, which ensures that for all $y_0 \in (\underline{y_0}, \overline{y_0})$ it exists an unique solution $\bar{s} > 0$. Formally

$$\lambda_0'(y_0) = \frac{\partial_{y_0} F_{tr}(\lambda_0(y_0), 0, y_0)}{\partial_s F_{sc}(\lambda_0(y_0), 0) - \partial_s F_{tr}(\lambda_0(y_0), 0, y_0)}$$

The partial derivative of F_{tr} and F_{sc} concerning s are existing (s. property (17)) and $\partial_{y_0} F_{tr}(s, 0, y_0) = -\frac{1}{t_1} H(s, 0, y_0)$. It follows, that the numerator is negative, because $H(s, 0, y_0) > 1$; s. (16). Obviously, the denominator is also negative, which is a consequence of inequality (38) in Theorem 5.6; cf. Fig. 5. Therefore, the implicit function theorem implies that the implicit function λ_0 exists with λ_0' as above. Hence, it holds $\lambda_0'(y_0) > 0$ for $y_0 \in (\underline{y_0}, \overline{y_0})$ and therefore the implicit function λ_0 is strictly monotonically increasing. ☐

Lemma 6.3. *The function* $y_0 \mapsto F_{sc}(\lambda_0(y_0), 0)$ *with* $y_0 \in (\underline{y_0}, \overline{y_0})$ *is strictly monotonically increasing.*

Proof. Both functions, λ_0 and $s \mapsto F_{sc}(s, 0)$, are strictly monotonically increasing, which was shown in the last lemma and Lemma 5.5. The concatenation of these functions results once more in a strictly monotonically increasing function. ☐

The last two lemmas allows the definition of the following parameter ranges

Definition 6.4. The co-domain of the implicit function λ_0 is denoted by $(\underline{s_0}, \overline{s_0})$ with

$$\underline{s_0} := \lim_{y_0 \to \underline{y_0}} \lambda_0(y_0)$$

$$\overline{s_0} := \lim_{y_0 \to \overline{y_0}} \lambda_0(y_0)$$

And the slope range is denoted by $(\underline{y_{tm0}}, \overline{y_{tm0}})$ with

$$\underline{y_{tm0}} := \lim_{y_0 \to \underline{y_0}} F_{sc}(\lambda_0(y_0), 0)$$

$$\overline{y_{tm0}} := \lim_{y_0 \to \overline{y_0}} F_{sc}(\lambda_0(y_0), 0)$$

Remark 6.5. If $y_m \geq y_{eq}/2$ and $y_0 \to y_1$ then $\overline{s_0} \to +\infty$ and $\overline{y_{tm0}} \to +\infty$. From Lemma 6.2 it is known that λ_0 and $s \mapsto F_{sc}(s,0)$ are strictly monotonically increasing. On the other hand, for a given s_0 the function $F_{tr}(s_0,0,y_0) \to 0$ if $y_0 \to y_1$. But it is also holds $F_{tr}(s,0,y_0) = F_{sc}(s,0)$ which can only be true if $s \to +\infty$.

With this results at hand, we state the

Theorem 6.6. *If $y_m \in (y_1, y_{eq})$ and $y_{tm} \in (\underline{y_{tm0}}, \overline{y_{tm0}})$ then the inverse Problem (2) has an unique solution which fulfills the necessary and sufficient condition (5.2,5.3).*

Proof. To show is that the given independent parameters leads to unique dependent parameters y_0, g, r and s of the ODE (2), which fulfills the data condition (1).

The map $y_0 \mapsto y_{tm} = F_{sc}(\lambda_0(y_0), 0)$ is one-to-one and $y_0 \mapsto s = \lambda_0(y_0)$ too; cf. Lemma 6.3 and Lemma 6.2. Then clearly, $r = r(s,0)$ and $g = g_m(s,0)$ with equations (10,31).

The equality $\lambda_0(y_0) = s$ is equivalent to $g_{sc}(s,0) = g_{tr}(s,0,y_0)$ and therefore it implies with Lemma 5.4, that the data condition (1) holds. From Lemma 6.2 it is known that $s > 0$, which is the sufficient condition. And the necessary condition holds, because of $r = r(s,0)$. ☐

For the sake of clarity we resume the strategy to determine the dependent parameters of the initial value problem (2) in the Algorithm 1.

Algorithm 1 Dependent parameter determination in case of $y_0 > 0$

1. Set (t_1, y_1), (t_2, y_2) and y_{eq} taken from TTT diagram
2. Set the height of the inflection point $y_m \in (y_1, y_{eq})$
3. Set the slope at the inflection point $y_{tm} \in (\underline{y_{tm0}}, \overline{y_{tm0}})$
4. Calculate $\tilde{s}$ by solving:
$$y_{tm} = F_{sc}(s,0)\ ,\ s \in (\underline{s_0}, \overline{s_0})$$
5. Calculate $\tilde{y}_0$ by solving:
$$y_{tm} = F_{tr}(\tilde{s},0,y_0)\ ,\ y_0 \in (\underline{y_0}, \overline{y_0})$$
6. Calculate $g = g(\tilde{s},0)$ with (31) and $r = r(\tilde{s},0)$ with (10)

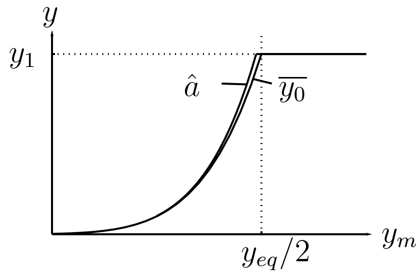


Fig. 8: Comparison of the upper bounds $\overline{y_0}$ and $\hat{a}$; see Subsection 6.1 and Lemma 6.8.

6.2 The case $a > 0$

The condition (35) becomes to a restriction on the data

$$\frac{y_2 - y_1}{t_2 - t_1} > \frac{y_1}{t_1} \tag{46}$$

So, if this condition is not fulfilled, then there is no possibility to compensate these invalidation with any independent parameter. And the condition (36) leads to the following upper bound $\overline{a}$ of a

$$\overline{a} = \begin{cases} a > 0 : \left(\frac{a+y_2}{a}\right)^{r(1,a)} \frac{y_{eq}-y_2}{y_{eq}} = 1 & \text{if exists} \\ +\infty & \text{else} \end{cases} \tag{47}$$

because of $\hat{H}(y, r(1,a), 1, a, 0) > 1$, with $y = y_2$, is the sharper case. This can be shown with Bernoulli's inequality and a short calculation, which ends up with $y_{eq} - y > 1/r(a,a)$ for all $y \in \{y_1, y_2\}$. For example see Fig. 7 on the right-hand side. The upper bound $\overline{a}$ is only a restriction until the equation (47) has a solution, which can be easily checked, because $a \mapsto \hat{H}(y_2, r(1,a), 1, a, 0)$ is a strictly monotone increasing mapping. Hence, this justifies the following corollary of Theorem 5.6

Corollary 6.7. *If $a \in (0, \overline{a})$ then the equation $F_{tr}(s, a, 0) = F_{sc}(s, a)$ has an unique solution $s > 0$.*

Lemma 6.8. *Let the assumptions of Theorem 5.6 be true. Then the implicit function $\lambda_1 : (0, \overline{a}) \to \mathbb{R}$, defined by the graph*

$$G_{\lambda_1} = \{(a, s) : F_{tr}(s, a, 0) = F_{sc}(s, a)\,,\ a \in (0, \overline{a})\}$$

has the derivative

$$\lambda_1'(a) = -\frac{\partial_a F_{sc}(\lambda_1(a), a) - \partial_a F_{tr}(\lambda_1(a), a, 0)}{\partial_s F_{sc}(\lambda_1(a), a) - \partial_s F_{tr}(\lambda_1(a), a, 0)} \tag{48}$$

and moreover if $a \in (0, \hat{a})$ with $\hat{a} = \min\{\overline{a}, 1 - y_2\}$ then it holds $\lambda_1' > 0$.

Proof. The graph $G_{\lambda_1} \neq \emptyset$, because the Corollary 6.7 holds, which ensures that for $0 < a < \overline{a}$ it exists an unique solution s. The partial derivative of F_{tr} and F_{sc} concerning s are existing (s. property (17)). Obviously, the inequality (38) in Theorem 5.6 implies, that the denominator is negative. Therefore, the implicit function theorem implies that the existing implicit function λ_1 is differentiable by (48).

It follows an analysis of the numerator. Let $(s,a) \in G_{\lambda_1}$. It is clear that $F_{tr}(s,a,0) = F_{sc}(s,a) =: Y$ with $s := \lambda_1(a)$. The derivative with equation (23) leads to

$$\begin{aligned} \partial_a F_{tr}(s,a,0) &= \frac{1}{t_1}\int_0^{y_1} \partial_a H \,\mathrm{d}y \\ &= \frac{s}{y_{eq}-y_m}(1-(a+y_m)+\log(a+y_m))Y \\ &\quad -\frac{s}{y_{eq}-y_m}\frac{1}{t_1}\int_0^{y_1} \underbrace{(\frac{1}{a+y}+\log(a+y))}_{=:k(y)} H \,\mathrm{d}y \end{aligned}$$

This calculation can also be done for $\partial_a F_{sc}$ which then only differs in the factor $1/t_1$ and in the integration bounds. Then the difference of the partial derivatives becomes to

$$\partial_a F_{sc} - \partial_a F_{tr} = \underbrace{\frac{s}{y_{eq}-y_m}}_{>0}\left\{\frac{1}{t_1}\int_0^{y_1} Hk - \frac{1}{t_2-t_1}\int_{y_1}^{y_2} Hk\right\} \tag{49}$$

Obviously, the function k has the following properties: for y with $0 \leq y < 1-a$ the values are bounded $1 < k(y) < +\infty$ and furthermore k is strictly monotone decreasing. Together with the monotonicity of the Riemann integral it implies that the mentioned difference is positive if $y_2 < 1-a$, because then the monotonicity of k does not change in the integrals. In details it holds as seen above

$$\begin{aligned} F_{tr}(s,a,0) &= F_{tr}(s,a,0) \\ \Leftrightarrow \frac{1}{t_1}\int_0^{y_1} H &= \frac{1}{t_2-t_1}\int_{y_1}^{y_2} H \\ \Rightarrow \frac{1}{t_1}\int_0^{y_1} Hk &> \frac{1}{t_2-t_1}\int_{y_1}^{y_2} Hk \end{aligned}$$

Hence, it holds $\lambda_1'(a) > 0$ for $a \in (0,\hat{a})$. □

Remark 6.9. If $a > 1-y$ for $0 < y < y_2$ it follows that $\lambda_1'(a) < 0$. Hence, it exists a $a_0 \in (\hat{a},1)$ for which $\lambda_1'(a_0) = 0$.

In Lemma 5.5 was shown that the function $(s,a) \mapsto F_{sc}(s,a)$ is strictly monotonically increasing in the first and strictly monotonically decreasing in the second argument. Inserting the function λ_1 from the last lemma leads not directly to a monotonicity statement of the function $a \mapsto F_{sc}(\lambda_1(a), a, 0)$ as in Subsection 6.1. The next statements clarify this issue

Lemma 6.10. *The function $a \mapsto F_{sc}(\lambda_1(a), a)$ with $a \in (0, \hat{a})$ is strictly monotonically increasing. Even it holds $F_{sc}(\lambda_1(.), .)' > 0$.*

Proof. The derivative of the function is $F_{sc}(\lambda_1(.), .)' = \lambda_1' \partial_s F_{sc} + \partial_a F_{sc}$ which is after inserting of λ_1' from (48) equivalent to

$$F_{sc}(\lambda_1(.), .)' = -\frac{(\partial_a F_{sc} - \partial_a F_{tr})\partial_s F_{sc} + (\partial_s F_{sc} - \partial_s F_{tr})\partial_a F_{sc}}{\partial_s F_{sc} - \partial_s F_{tr}}$$

Obviously, the denominator is negative, which is a consequence of inequality (38). It is left to show that the numerator is positive. After expanding them and collecting $\partial_s F_{sc}$ it must hold

$$(2\partial_a F_{sc} - \partial_a F_{tr})\underbrace{\partial_s F_{sc}}_{>0} - \underbrace{\partial_a F_{sc} \partial_s F_{tr}}_{<0} \overset{!}{>} 0$$

Furthermore, Lemma 4.4 ensures that $\partial_s F_{sc}$ and $\partial_s F_{tr}$ are positive. And $\partial_a F_{sc}$ is negative, because of the inequality (25). Therefore, it is only left to show that

$$2\partial_a F_{sc} \overset{!}{>} \partial_a F_{tr} \tag{50}$$

But this is true, because $\lambda_1'(a) > 0$ which was shown in Lemma 6.8 and therefore it even holds $\partial_a F_{sc} > \partial_a F_{tr}$. $\square$

The result of the last lemmata justifies the definition of the following co-domains.

Definition 6.11. The co domain of the implicit function λ_1 is denoted by $(\underline{s_1}, \overline{s_1})$ with

$$\underline{s_1} := \lim_{a \to 0} \lambda_1(a)$$

$$\overline{s_1} := \lim_{a \to \hat{a}} \lambda_1(a)$$

And the slope range is denoted by $(\underline{y_{tm1}}, \overline{y_{tm1}})$ with

$$\underline{y_{tm1}} := \lim_{a \to 0} F_{sc}(\lambda_1(a), a)$$

$$\overline{y_{tm1}} := \lim_{a \to \hat{a}} F_{sc}(\lambda_1(a), a)$$

Theorem 6.12. *If $y_m \in (0, y_{eq})$ and $y_{tm} \in (\underline{y_{tm1}}, \overline{y_{tm1}})$ then the inverse Problem (2) has an unique solution which fulfills the necessary and sufficient condition (5.2,5.3).*

Proof. To show is that the given independent parameters leads to unique dependent parameters a, g, r and s of the ODE (2), which fulfills the data condition (1).

The map $a \mapsto y_{tm} = F_{sc}(\lambda_1(a), a)$ is one-to-one and $a \mapsto s = \lambda_1(a)$ too; cf. Lemma 6.10 and Lemma 6.8. Then clearly, $r = r(s, a)$ and $g = g_m(s, a)$ with equations (10,31).

The equality $\lambda_1(a) = s$ is equivalent to $g_{sc}(s, a) = g_{tr}(s, a, 0)$ and therefore it implies with Lemma 5.4, that the data condition (1) holds. From Lemma 6.8 it is known that $s > 0$, which is the sufficient condition. And the necessary condition holds, because of $r = r(s, a)$. □

For the sake of clarity we resume the strategy to determine the dependent parameters of the initial value problem (2) in the Algorithm 2.

Algorithm 2 Dependent parameter determination in case of $a > 0$

1. Set (t_1, y_1), (t_2, y_2) and y_{eq} taken from TTT diagram which holds the data condition
$$\frac{y_2 - y_1}{t_2 - t_1} > \frac{y_1}{t_1}$$
2. Set the height of the inflection point $y_m \in (y_1, y_2)$
3. Set the slope at the inflection point $y_{tm} \in (\underline{y_{tm1}}, \overline{y_{tm1}})$
4. Calculate $(\tilde{s}, \tilde{a})$ by solving the system:
$$\begin{aligned} y_{tm} &= F_{tr}(s, a, 0) \\ y_{tm} &= F_{sc}(s, a) \\ & \quad (s, a) \in (\underline{s_1}, \overline{s_1}) \times (0, \hat{a}) \end{aligned}$$
5. Calculate $g = g(\tilde{s}, \tilde{a})$ with (31) and $r = r(\tilde{s}, \tilde{a})$ with (10)

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7 Discussion and examples

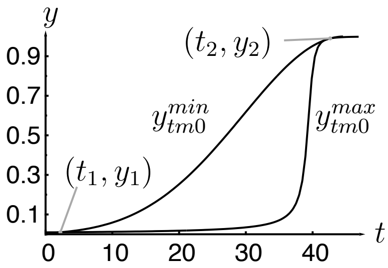
In order to use Algorithm 1 and Algorithm 2 for calculations it is reasonable to define closed sets as subsets of the defined co-domains from Definition

Case $y_0 > 0$: Maximal ranges

	min	max
y_0	0.005	0.0095
s_0	0.506	1.447
y_{tm0}	0.040	0.465

Case $a > 0$: Maximal ranges

	min	max
a	0.007	0.063
s_1	0.403	0.835
y_{tm1}	0.034	0.049



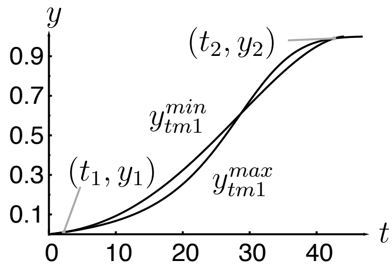


Fig. 9: Possible range of bainite phase transition of steel Ck45 at isothermal temperature 402°C with $y_m = 0.6$.

6.4 and Definition 6.11, especially consider Remark 6.5. The open domain mappings are: for the case $y_0 > 0$

$$(\underline{y_0}, \overline{y_0}) \underset{\lambda_0}{\longrightarrow} (\underline{s_0}, \overline{s_0}) \underset{F_{sc}}{\longrightarrow} (\underline{y_{tm0}}, \overline{y_{tm0}})$$

and for the case $a > 0$

$$(0, \hat{a}) \underset{\lambda_1}{\longrightarrow} (\underline{s_1}, \overline{s_1})\,,\ \overset{\circ}{G}_{\lambda_1} \underset{F_{sc}}{\longrightarrow} (\underline{y_{tm1}}, \overline{y_{tm1}})$$

with $\overset{\circ}{G}_{\lambda_1} = G_{\lambda_1} \cap ((\underline{s_1}, \overline{s_1}) \times (0, \hat{a}))$. And the suitable closed subsets should be denoted by $[y_0^{min}, y_0^{max}] \subset (\underline{y_0}, \overline{y_0})$ and $[a^{min}, a^{max}] \subset (0, \hat{a})$. Thus, the mapped co-domains are also closed. Hence, it ends with

$$[y_0^{min}, y_0^{max}] \underset{\lambda_0}{\longrightarrow} [s_0^{min}, s_0^{max}] \underset{F_{sc}}{\longrightarrow} [y_{tm0}^{min}, y_{tm0}^{max}] \tag{51}$$

and

$$[a^{min}, a^{max}] \underset{\lambda_1}{\longrightarrow} [s_1^{min}, s_1^{max}]\,,\ \bar{G}_{\lambda_1} \underset{F_{sc}}{\longrightarrow} [y_{tm1}^{min}, y_{tm1}^{max}] \tag{52}$$

with $\bar{G}_{\lambda_1} = G_{\lambda_1} \cap ([s_1^{min}, s_1^{max}] \times [a^{min}, a^{max}])$. Remember, that the parameter r in the initial value problem (2) is defined by (10).

Maximal parameter ranges

Now, consider Fig. 9 for instance. This shows the possible range of bainite phase transition of the steel Ck45 at an isothermal temperature reachable

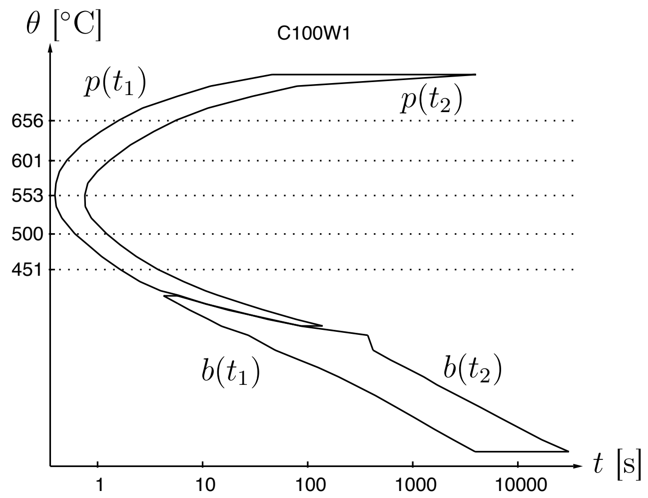


Fig. 10: Digitized isothermal TTT diagram of the steel C100W1 (austenitization temperature 860°C) with the phases pearlite and bainite; [2].

with the model ansatz (2). From the numerical point of view neither the lower bounds nor the upper one are easy to treat. If the lower bounds are to small, then the factor $(y_{eq}-y)^s$ of the right-hand side of the ode (2) affords problems for the ode solver. On the other hand, the upper bounds are problematic for the numerical integration in the Algorithm 1 and Algorithm 2, because the integrands becomes singular at the integration bounds. The closed subset in the example shown on the right-hand side of Fig. 9 was defined from a larger open set $[a^{min}, a^{max}] \subset (0, \overline{a})$. If we look at the details of Lemma 6.8, we find out that the upper bound $\hat{a}$ is conservative. An alternative is to check that $\overline{a}$, the largest possible value, fulfills $\partial_a F_{sc} \geq \partial_a F_{tr}$, which can be calculated by (49). Moreover, it is even sufficient to show that $2\partial_a F_{sc} \geq \partial_a F_{tr}$; cf. (50). In both cases, the ranges are chosen as large as possible until either the ode solver or the numerical integration are limiting. To the mentioned drawback of the case $y_0 > 0$ opposes the benefit that the available range of the independent parameters seems to be always larger than for the case $a > 0$.

Variation of the inflection point

The following example illustrates the variation of y_{tm0}^{min} with respect to y_m for a given $y_0^{min} = 10^{-7}$. This is shown in Fig. 11 for several isothermal

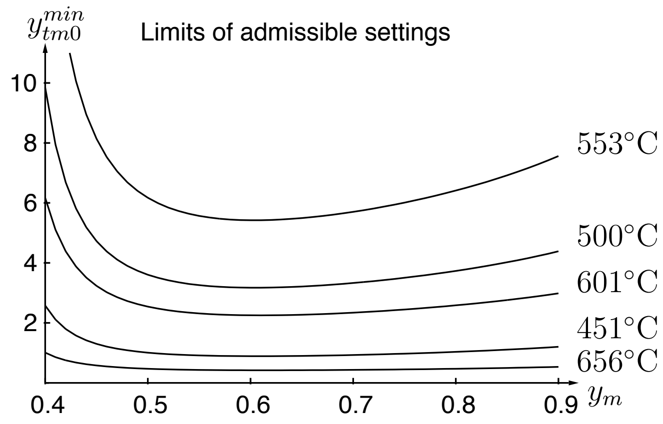


Fig. 11: Each line $y_{tm0}^{min}(.)$ marks the lower bound of admissible choices of (y_m, y_{tm}) with $y_0^{min} = 10^{-7}$ for an isothermal cooling process. The data of the isothermals are taken from Fig. 10.

temperatures. The data at the temperatures are taken from TTT diagram of the steel C100W1, which is shown in Fig. 10; [2]. In this case the upper bounds y_{tm0}^{max} are far from practical relevance. In fact, the upper bound $y_0^{max} < \overline{y_0}$ is not independent from y_m as shown at the beginning of Subsection 6.1, but this leads not to significant decreasing of the upper bounds. Notice, that the minima of each curve are all near by $y_m = 0.6$.

Compare of cases $y_0 > 0$ and $a > 0$

A drawback of the model (2) with $a = 0$ is the required start value $y(0) > 0$ for applications in a thermomechanic model. This would generate undesirable initial thermal expansion (cf. [14]). Generally, from the numerical point of view the model case $a > 0$ needs more care. Furthermore, the allowed ranges of the independent parameters are significantly smaller than for the case $y_0 > 0$. Another bottleneck is the violation of the pure data condition (46) for some isothermal temperatures. The following table contains a list of the checked steel grades:

steel	phase	temperature in °C	data cond. (46)
42CrMo4	ferrite	750	invalid
	bainite	425-590	invalid
C1080	pearlite	220, 685	invalid
C100W1	all	all	valid
Ck45	all	all	valid

8 Conclusions

We have investigated a mathematical model for phase transition kinetics in steel. In contrast to an approximation of the model against a given measured transformation curve, we enforced that the begin and end points stated as data from an IT diagram should be matched exactly. The introduction of the point of inflection characterized the desired sigmoidal shape mathematically and led to a classification into: data, independent parameters and dependent parameters. Moreover, the independent parameters have clear geometrical meaning and its range was also specified within the existence of an unique solution is ensured.

As seen in the examples of the previous section, the historical earlier model case $y_0 > 0$, see at the beginning of Section 5, has a significantly wider range of variation of the inflection point than the case $a > 0$, cf. Fig. 9, and sometimes it is even impossible to fulfill the data condition (46) in that case. Nevertheless, the case $a > 0$ may be preferable in a simulation with thermochemical coupling as mentioned above. With regard to non isothermal heat treatment simulations, a wide range of variation of the independent parameters may offer the possibility to obtain an agreement with an IT diagram *and* a corresponding continuous cooling transformation (CCT) diagram.

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