

# PARAMETER IDENTIFICATION IN NON-ISOTHERMAL NUCLEATION AND GROWTH PROCESSES

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ABSTRACT. We study non-isothermal nucleation and growth phase transformations, which are described by a generalized Avrami model for the phase transition coupled with an energy balance to account for recalescence effects. The main novelty of our work is the identification of temperature dependent nucleation rates. We prove that such rates can be uniquely identified from measurements in a subdomain and apply an optimal control approach to develop a numerical strategy for its computation.

## 1. INTRODUCTION

According to [6], nucleation and growth processes may occur in all metastable systems and the initial or final phase may be solid, liquid, or gaseous. The new phase grows at the expense of the old one by the migration of the interphase boundary. At a fixed temperature the reaction proceeds isothermally and will continue until it is complete. Hence the final amount of transformation is independent of temperature as long as the equilibrium phase fraction is so.

To become more specific let us consider a test volume  $V \subset \mathbb{R}^3$  in which a transformation from a phase  $A$  to a phase  $B$  happens. We call  $V^A(t)$  and  $V^B(t)$  the sub-volumes occupied by phases  $A$  and  $B$  at time  $t$ , respectively, i.e.

$$V = V^A(t) + V^B(t) \quad \text{for all } t \in [0, T].$$

Moreover, we define the phase volume fraction of the product phase,

$$P(t) = \frac{V^B(t)}{V}.$$

We introduce the growth rate  $\rho$ , which we assume to be a constant. In many cases such a linear isotropic growth is well justified. However, especially in solid-solid phase transitions with an underlying grain structure one would observe rather an anisotropic growth perpendicular to the grain boundary. When the composition of the matrix also changes during the transformation, a parabolic growth corresponding to  $\rho \sim t^{-1/2}$  can be expected.

Assuming spherical growth the volume of a phase  $B$  region originating from a nucleus born at time  $\tau$  is given by

$$(1.1) \quad v(t, \tau) = \frac{4\pi}{3} \rho^3 (t - \tau)^3.$$

In the sequel we use the abbreviation  $\gamma := 4\pi\rho^3$ . The way to derive the nucleation and growth model is to start with an *extended volume*  $V_{ext}^B$  of the new phase  $B$  disregarding impingement of different  $B$  sub-regions. To this end, multiplying the single grain volume

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(1.1) with the number of nuclei born at time  $\tau$ , i.e.,  $\alpha(\theta(\tau))V$ , we obtain the extended volume fraction

$$(1.2) \quad V_{ext}^B(t) = \frac{\gamma V}{3} \int_0^t \alpha(\theta(\tau))(t - \tau)^3 d\tau.$$

Here,  $\alpha$  is the temperature  $\theta$  dependent nucleation rate which denotes the number of stable nuclei formed per unit time and space. After some time the  $B$  sub-regions will first impinge and then grow into each other. Moreover, new nuclei will be born in already transformed regions. In reality, the new phase grows either until the growing process ceases locally due to impingement of sub-regions or until an equilibrium volume  $V_{eq}^B(\theta)$  is reached with corresponding equilibrium volume fraction

$$P_{eq}(\theta) = \frac{V_{eq}^B(\theta)}{V}.$$

Usually, the equilibrium value is temperature dependent and can be extracted from the respective equilibrium phase diagram. Then, we may assume only that fraction of an incremental extended volume fraction  $dV_{ext}^B$  contributes to the growth of the really transformed fraction  $dV^B$ , which previously has not been transformed. In other words we conjecture that

$$(1.3) \quad dV^B = \left(1 - \frac{V^B}{V_{eq}^B(\theta)}\right) dV_{ext}^B.$$

This so-called Avrami correction has been investigated independently by Avrami [1, 2, 3] and Kolmogorov [16], see also [14]. Tacitly assuming that  $\theta$  is a constant, we integrate (1.3) using (1.2) to obtain

$$(1.4) \quad -\ln\left(1 - \frac{P}{P_{eq}(\theta)}\right) = \frac{\gamma}{3} \frac{1}{P_{eq}(\theta)} \int_0^t \alpha(\theta(\tau))(t - \tau)^3 d\tau$$

from which we conclude

$$(1.5) \quad P(t) = P_{eq}(\theta) \left(1 - e^{-\frac{\gamma}{3} \frac{1}{P_{eq}(\theta)} \int_0^t \alpha(\theta(\tau))(t - \tau)^3 d\tau}\right).$$

In the case of a constant nucleation rate and  $P_{eq} \equiv 1$ , (1.5) boils down to the classical Johnson-Mehl-Avrami-Kolmogorov equation

$$(1.6) \quad P(t) = 1 - e^{-\frac{\pi}{3} \rho^3 \alpha t^4}.$$

Note that the latter is still often used to quantify phase transitions in steel, especially in the engineering sciences, see, e.g., [23]. Our interest is to identify the temperature dependent nucleation rate  $\alpha(\theta)$  in the generalized Avrami model (1.5). To simplify the exposition in the sequel we assume  $P_{eq} \equiv 1$ .

Phase transitions are known to be accompanied by the release or consumption of latent heat, which is usually assumed to be proportional to the phase growth rate  $P_t$ . To incorporate this effect it is convenient to take the derivative of (1.4) with respect to time (recall that we assume  $(P_{eq} \equiv 1)$  and replace (1.5) with the integro-differential

equation

$$(1.7a) \quad P_t(t) = \gamma(1 - P(t)) \int_0^t \alpha(\theta(\tau))(t - \tau)^2 d\tau$$

$$(1.7b) \quad P(0) = 0.$$

For numerical purposes and the derivation of optimality conditions it is more favorable to work with an ODE. To this end we define the new unknown variable

$$(1.8) \quad \eta(t) := \ln \left( \frac{1}{1 - P(t)} \right).$$

Taking now the fourth derivative in (1.4), we can rewrite (1.7) equivalently with the fourth order ODE

$$(1.9a) \quad \eta^{(4)}(t) = 2\gamma\alpha(\theta(t))$$

$$(1.9b) \quad \eta(0) = \eta'(0) = \eta''(0) = \eta'''(0) = 0.$$

To account for the release of latent heat during the phase change we couple the phase kinetics with the balance of internal energy, which reads

$$\rho \frac{\partial e}{\partial t} - \nabla \cdot (\kappa \nabla \theta) = 0,$$

where we have employed Fourier's law of heat conduction. Here,  $\rho$  is the mass density,  $e$  the specific internal energy and  $\kappa$  the heat conductivity. Now we proceed as in [24] and assume that there exists a differentiable material function  $\hat{e}$  such that the internal energy takes the form

$$e(x, t) = \hat{e}(\theta, P),$$

with the partial derivatives

$$(1.10) \quad \frac{\partial \hat{e}}{\partial \theta} = c, \quad \frac{\partial \hat{e}}{\partial P} = -L,$$

where  $L$  denotes the latent heat and  $c$  the specific one, respectively. Then the energy balance reads as

$$(1.11) \quad \rho c \theta_t - \nabla \cdot (\kappa \nabla \theta) = \rho L P_t.$$

Equivalently (cf. (1.8)), we will write the latent heat term as  $\rho L \eta_t e^{-\eta(t)}$ . The goal of this paper is to study the system (1.7) or (1.9) together with (1.11). We investigate the solvability of the state system and study the inverse problem of identifying the temperature dependent nucleation rate  $\alpha(\theta)$ . To this end we also establish a uniqueness result. We refer to Choulli, Ouhabaz and Yamamoto [5], DuChateau and Rundell [7], Egger, Engl and Klivanov [8], Isakov [13], Klivanov [15], Lorenzi [19], Pilant and Rundell [20]. Those papers discuss parabolic equations without integral term, and proved the uniqueness with boundary measurements and the key is the maximum principle. To the best of our knowledge we do not know the works on uniqueness in determination of nonlinear terms for integral-differential equation, e.g. nonlinear parameter identification in the nonlocal integral-differential equation.

Justified by the uniqueness result we employ an optimal control approach to the numerical identification of the nucleation rate. This is done in the spirit of [21], where the identification of a nonlinear heat transfer law is studied. In [10] a similar approach has been taken to identify a temperature dependent rate law for the coagulation of cancerous tissue. In addition we note that optimal control problems for nucleation and

growth models related to the crystallization of polymers have been studied in [4, 9]. In [18] a simplified version of the generalized Avrami model has been developed.

The paper is organized as follows. Section 2 contains the well-posedness of our coupled model with appropriate boundary and initial conditions. In Section 3 we show that indeed the nucleation rate  $\alpha$  can be uniquely determined from measurements in a subdomain. We will utilize an optimal control approach in Section 4 to identify the nucleation rate  $\alpha$  by minimizing a cost functional defined on a subdomain. In the last section we exploit the adjoint based approach for a numerical identification of nucleation rates.

## 2. WELL-POSEDNESS OF THE FORWARD MODEL

For sake of simplicity, we skip most of the physical-based constants and obtain the simplified forward problem in the following parabolic-ODE coupled system. We assume  $\Omega \subset \mathbb{R}^3$  to be a domain with  $C^{1,1}$  boundary. We consider a transition from phase  $A$  stable at high temperature to a low temperature phase  $B$ . Accordingly, we consider cooling processes assuming that the initial temperature  $\theta_0$  is greater than the coolant temperature  $\theta_w$ , assumed to be constant. Then the governing parabolic system for the temperature distribution  $\theta$  is

$$(2.1a) \quad \theta_t - \kappa \Delta \theta = L(\theta) P_t \quad \text{in } \Omega \times (0, T);$$

$$(2.1b) \quad \kappa \partial_\nu \theta + \sigma(\theta - \theta_w) = 0 \quad \text{on } \partial\Omega \times (0, T);$$

$$(2.1c) \quad \theta(x, 0) = \theta_0 \quad \text{in } \Omega$$

where  $\nu$  is the normal vector,  $\sigma > 0$  is the constant heat exchange coefficient and  $\kappa > 0$  the constant heat conductivity. The governing ODE system for the phase volume fraction  $P$  is

$$(2.2a) \quad P_t = \gamma(1 - P) \int_0^t \alpha(\theta)(t - \tau)^2 d\tau \quad \text{in } \Omega \times (0, T);$$

$$(2.2b) \quad P(0) = 0 \quad \text{in } \Omega.$$

As mentioned in the last section, changing of variables  $\eta = \ln\left(\frac{1}{1-P}\right)$  and taking additional initial conditions, we can reformulate an equivalent parabolic-ODE coupled system

$$(2.3a) \quad \theta_t - \kappa \Delta \theta = L(\theta) e^{-\eta} \eta_t \quad \text{in } \Omega \times (0, T);$$

$$(2.3b) \quad \kappa \partial_\nu \theta + \sigma(\theta - \theta_w) = 0 \quad \text{on } \partial\Omega \times (0, T);$$

$$(2.3c) \quad \theta(x, 0) = \theta_0 \quad \text{in } \Omega$$

and

$$(2.4a) \quad \frac{d^4 \eta}{dt^4} = 2\gamma \alpha(\theta) \quad \text{in } \Omega \times (0, T);$$

$$(2.4b) \quad \eta^{(i)}(0) = 0, \quad i = 0, \dots, 3, \quad \text{in } \Omega.$$

The following assumptions are important in the sequel:

(A1)  $\theta_0$  and  $\theta_w$  are positive constants satisfying  $\theta_0 > \theta_w$ .

(A2)  $L$  is in  $C^{1,1}(\mathbb{R})$ , and  $L(\theta) = 0$  if  $\theta \leq \theta_-$  or  $\theta \geq \theta_+$ , and  $L(\theta) \neq 0$  if  $\theta_- < \theta < \theta_+$ , where  $\theta_{\pm}$  are chosen such that  $\theta_w \leq \theta_- < \theta_+ = \theta_0$ .

(A3) The admissible set for  $\alpha(\theta)$  is

$$\mathcal{A}_{ad} := \left\{ \alpha \in C^{1,\gamma}(\mathbb{R}) : \|\alpha\|_{C^{1,\gamma}} \leq M_0, \text{supp}\alpha \subset (\theta_-, \theta_+), \alpha(s)|_{s \in \mathbb{R}} \geq 0 \right\}$$

(A4) The measurement data satisfies  $\theta_m \in L^p(0, T; L^p(\omega))$ , where  $\omega$  is an interior open domain satisfying  $\omega \subset \Omega$ .

*Remark 2.1.* According to (A1)–(A3) we consider a cooling process from high initial temperature to quenchant temperature. The phase transition happens in the subdomain  $[\theta_-, \theta_+] \subset [\theta_w, \theta_0]$ .

To proceed further, we recall a standard parabolic regularity result for linear parabolic equations in the space  $W_p^{2,1}(Q) := W^{1,p}(0, T; L^p(\Omega)) \cap L^p(0, T; W^{2,p}(\Omega))$  where  $Q := \Omega \times (0, T)$  is the space-time cylinder.

**Lemma 2.2.** ([17, Theorem 9.1]) *Assume that assumption (A1) holds. Then for any  $f \in L^p(\Omega)$  ( $p \in (1, \infty)$ ), there exists a unique solution in  $W_p^{2,1}(Q)$  for the parabolic system*

$$\begin{aligned} \theta_t - \kappa \Delta \theta &= f && \text{in } \Omega \times (0, T); \\ \kappa \partial_\nu \theta + \sigma(\theta - \theta_w) &= 0 && \text{on } \partial\Omega \times (0, T); \\ \theta(x, 0) &= \theta_0 && \text{in } \Omega \end{aligned}$$

and satisfies the following a priori estimate

$$\|\theta\|_{W_p^{2,1}(Q)} \leq C_1 + C_2 \|f\|_{L^p(Q)}.$$

with constants  $C_{1,2}$  and  $C_1 = 0$  if  $\theta_0 = \theta_w = 0$ . If in addition  $p > 5/2$ , then for  $\epsilon \in (0, 2 - 5/p)$  the solution  $\theta$  is in  $C^{0,\epsilon}(\bar{Q})$  and the same estimate holds for the  $C^{0,\epsilon}(\bar{Q})$ -norm.

Meanwhile, the a priori estimates for the ODE system are carried out by changing of variables  $\eta := \ln\left(\frac{1}{1-P}\right)$ .

**Lemma 2.3.** *Assume (A2), let  $\theta \in L^1(Q)$  and fix a finite final time  $T$ . Then there holds  $\eta(t) \in [0, \eta_{\max}]$  with  $t \in [0, T]$  and a constant  $\eta_{\max} < \infty$ . Moreover, there exists a constant  $M$  independent of  $\theta$  s.t.*

$$\|\eta\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \leq M.$$

At the same time, assume that there exist  $\theta_1, \theta_2 \in L^p(Q)$  with  $p \in [2, \infty)$  with solutions  $\eta_1, \eta_2$ , then the following estimate holds with a constant  $L > 0$

$$\|\eta_1 - \eta_2\|_{W^{1,p}(0,T;L^p(\Omega))} \leq L \|\theta_1 - \theta_2\|_{L^p(Q)}.$$

*Proof.* The proof follows by changing of variables  $\eta := \ln\left(\frac{1}{1-P}\right)$  from the original ODE system on  $P$  in (2.2). Notice

$$\begin{cases} \eta_t &= \gamma \int_0^t \alpha(\theta)(t - \tau)^2 d\tau; \\ \eta(0) &= 0. \end{cases}$$

Assuming  $\theta \in L^1(Q)$  and the initial condition, we conclude that  $\eta(t)$  is increasing and finite in the time interval  $[0, T]$  such that  $0 \leq \eta(t) \leq \eta_{\max} = \frac{\gamma}{12} M_0 T^4$ . Moreover,  $\eta_t$  satisfies  $0 \leq \eta_t \leq \frac{\gamma}{3} M_0 T^3$ . The rest of the proof follows by testing the difference of  $\eta_1, \eta_2$  by  $|\eta_1 - \eta_2|^{p-2}(\eta_1 - \eta_2)$  and applying the Gronwall's and Young's inequalities.  $\square$

*Remark 2.4.* We emphasize that by adding appropriate initial conditions, the original ODE system (2.2) is equivalent to the 4-th order ODE system (2.4). The *a priori* estimates in Lemma 2.3 are adjusted, respectively, in the following estimates

$$\begin{aligned} \|\eta\|_{W^{4,\infty}(0,T;L^\infty(\Omega))} &\leq M; \\ \|\eta_1 - \eta_2\|_{W^{4,p}(0,T;L^p(\Omega))} &\leq L\|\theta_1 - \theta_2\|_{L^p(Q)}. \end{aligned}$$

In the sequel, we denote by  $\eta$  the solution of the 4-th order ODE system (2.4) where the standard estimates in Lemma 2.3 are sufficient for the well-posedness of the forward model.

**Corollary 2.5.** *Let  $\theta \in L^1(Q)$  and fix a finite final time  $T$ , the term  $e^{-\eta}\eta_t$  is nonnegative and bounded with an a priori estimate*

$$\|e^{-\eta}\eta_t\|_{L^\infty(0,T;L^\infty(\Omega))} \leq M$$

where the constant  $M$  is independent of  $\eta$  and  $\theta$ .

Now, we are ready to present the main existence theorem for the parabolic-ODE coupled system (2.3)-(2.4).

**Theorem 2.6.** *Assume that assumptions (A1)-(A3) hold and let  $p > 5/2$ . Then the parabolic-ODE coupled system (2.3)-(2.4) admits a unique solution  $(\theta, \eta)$  such that  $\theta \in W_p^{2,1}(Q) \cap C^{0,\epsilon}(\bar{Q})$  for some  $\epsilon \in (0, 1)$  and  $\eta \in W^{1,\infty}(0, T; L^\infty(\Omega))$ .*

*Proof.* Fix a finite final time  $T > 0$ , we consider the following closed set

$$K_T := \{\theta \in W_p^{2,1}(Q) : \theta(x, 0) = \theta_0\}.$$

Choose  $\hat{\theta} \in K_T$ , and define  $\eta$  be the solution of (2.4) where the governing ODE has the form

$$(2.5) \quad \frac{d^4\eta}{dt^4} = 2\gamma\alpha(\hat{\theta}).$$

The solution  $\eta$  uniquely exists and satisfies the *a priori* estimates in Lemma 2.3.

Now define  $\theta$  as the solution to (2.3), where the right-hand side of the governing parabolic equation is replaced by the solution  $\eta$  to (2.5). Since the *a priori* estimates in Lemma 2.2 and Corollary 2.5 are independent of  $\hat{\theta}$ , we can infer that the operator  $S : \hat{\theta} \rightarrow \theta$  maps  $K_T$  onto itself.

At the same time, defining  $S(\hat{\theta}_i) = \theta_i$ ,  $i = 1, 2$  with  $\hat{\theta}_{1,2} \in K_T$ , we can obtain, for  $\theta = \theta_1 - \theta_2$  and  $\hat{f} := L(\hat{\theta}_1)e^{-\eta_1}\eta_{1,t} - L(\hat{\theta}_2)e^{-\eta_2}\eta_{2,t}$ , where  $\eta_i$  is the solution to (2.5) with respect to  $\hat{\theta}_i$  and  $\eta_{i,t}$  is the time derivative of each  $\eta_i$ ,

$$\begin{cases} \theta_t - \kappa\Delta\theta = \hat{f} & \text{in } (0, T) \times \Omega; \\ \kappa\partial_\nu\theta + \sigma\theta = 0 & \text{on } (0, T) \times \partial\Omega; \\ \theta(x, 0) = 0 & \text{in } \Omega. \end{cases}$$

Lemmas 2.2, 2.3, (A1), and Hölder's inequality then yield

$$\|\theta_1 - \theta_2\|_{W_p^{2,1}(Q)} \leq C\|\hat{f}\|_{L^p(Q)} \leq C\|\hat{\theta}_1 - \hat{\theta}_2\|_{L^p(Q)} \leq CT^{\frac{p-1}{p}}\|\hat{\theta}_1 - \hat{\theta}_2\|_{W_p^{2,1}(Q)}.$$

Thus,  $S$  is a contraction map if we choose  $T := T^+$  sufficient small. The existence of a unique local solution then follows from Banach's fixed point theorem. The global *a*

*a priori* estimates in Lemma 2.2 and Corollary 2.5 guarantee that such an estimate holds true on the whole interval  $[0, T]$ .  $\square$

Moreover, one can prove upper and lower bounds of  $\theta$ , which allow the choice of constant temperatures  $\theta_-$  and  $\theta_+$  in the admissible set  $\mathcal{A}_{ad}$ .

**Lemma 2.7.** *Assume  $\alpha \in \mathcal{A}_{ad}$  and  $(\theta, \eta)$  are the solutions of (2.3) and (2.4). Then we have*

$$\theta_w \leq \theta \leq \theta_0$$

for all  $(x, t) \in \Omega \times (0, T)$  and all  $\alpha \in \mathcal{A}_{ad}$ .

*Proof.* Consider the decomposition

$$\theta = \theta_w + [\theta - \theta_w]_+ - [\theta - \theta_w]_-$$

where  $[x]_+ = \max\{x, 0\}$  and  $[x]_- = -\min\{x, 0\}$  are the positive and negative part functions. Testing (2.3) with  $[\theta - \theta_w]_-$  and integrate in  $Q$ , we obtain

$$\begin{aligned} \frac{1}{2} \int_{\Omega} [\theta - \theta_w]_-^2 dx + \kappa \int_0^T \int_{\Omega} |\nabla [\theta - \theta_w]_-|^2 dx dt &= - \int_0^T \int_{\Omega} e^{-\eta} \eta_t [\theta - \theta_w]_- dx dt \\ &+ \int_0^T \int_{\partial\Omega} \sigma [\theta - \theta_w]_-^2 dx dt. \end{aligned}$$

By the trace theorem, we obtain that

$$\int_0^T \int_{\partial\Omega} \sigma [\theta - \theta_w]_-^2 dx dt \leq \sigma \int_0^T \|[\theta - \theta_w]_-\|_{H^{\frac{1}{2}}(\Omega)}^2 dt.$$

Implementing the interpolation inequality, we derive

$$\int_0^T \int_{\partial\Omega} \sigma [\theta - \theta_w]_-^2 dx dt \leq \sigma \int_0^T (\|[\theta - \theta_w]_-\|_{L^2(\Omega)}) (\|[\theta - \theta_w]_-\|_{H^1(\Omega)}) dt.$$

Young's inequality then yields

$$\begin{aligned} \int_0^T \int_{\partial\Omega} \sigma [\theta - \theta_w]_-^2 dx dt &\leq \frac{\kappa}{2} \int_0^T \int_{\Omega} |\nabla [\theta - \theta_w]_-|^2 dx dt \\ &+ c_1 \int_0^T \int_{\Omega} [\theta - \theta_w]_-^2 dx dt, \end{aligned}$$

with a constant  $c_1$  depending on  $\sigma$  and  $\kappa$ .

Noticing the non-positivity of the term  $-\int_0^T \int_{\Omega} e^{-\eta} \eta_t [\theta - \theta_w]_- dx dt$ , we can conclude that

$$\frac{1}{2} \int_{\Omega} [\theta - \theta_w]_-^2 dx \leq C \int_0^T \int_{\Omega} [\theta - \theta_w]_-^2 dx dt.$$

Gronwall's inequality then yields  $[\theta - \theta_w]_- = 0$ . Invoking (A1), a similar reasoning yields the upper bound for  $\theta$ .  $\square$

## 3. UNIQUENESS OF THE INVERSE PROBLEMS

In the preceding section we have seen that for any  $\alpha \in \mathcal{A}_{ad}$  there exists a unique solution  $\theta(\alpha), P(\alpha)$  to the the state system (2.1), (2.2). In this section, we consider the solution  $\theta(\alpha)(x, t)$  in the class  $W_2^{2,1}(Q)$ . Now, we consider the inverse problem and ask if we can identify  $\alpha$  from temperature measurements in an arbitrary subdomain  $\omega \subset \Omega$  with non-zero measure, i.e. we consider the problem

(IP) determine  $\alpha$  by  $\theta|_{\omega \times (0, T)}$ .

We are ready to state the main result on the inverse problem.

**Theorem 3.1.** (*uniqueness*) Assume (A1)-(A3). If  $\theta(\alpha^1)(x, t) = \theta(\alpha^2)(x, t)$  for  $x \in \omega$  and  $0 < t < T$ , then  $I := \{\theta(\alpha^1)(x, t) : x \in \omega, 0 < t < T\}$  is a non-empty open interval and  $\alpha^1(\eta) = \alpha^2(\eta)$  for  $\eta \in \bar{I}$ .

*Remark 3.2.* (1) For our inverse problem, we cannot expect any maximum principle or monotone property of  $\theta$  with respect to  $\alpha$ , and we use interior observation data in  $\omega \times (0, T)$ .

(2) This is a local uniqueness result, that is, we can prove the uniqueness only over an interval  $I$ .

(3) As is seen by the proof, the local uniqueness also follows, if we replace assumption (A2) by one of the following conditions:

- $\theta_0$  is not a constant function in  $\omega$ .
- $\theta_0$  is constant in  $\omega$  and  $\theta_w(x, t) \not\equiv \theta_0$  on  $\partial\Omega \times (0, T)$ .

**Corollary 3.3.** Under the same assumption of Theorem 3.1, if  $\alpha^k, k = 1, 2$  are real-analytic in  $\{\eta : \alpha^k(\eta) \neq 0\}$  and  $\theta(\alpha^1)(x, t) = \theta(\alpha^2)(x, t)$  for  $x \in \omega$  and  $0 < t < T$ , then  $\text{supp } \alpha^1 = \text{supp } \alpha^2$  and  $\alpha^1 = \alpha^2$  on  $\text{supp } \alpha^1$ .

*Remark 3.4.* By modifying the uniqueness proof, we can prove some conditional stability estimate for  $\|\alpha^1 - \alpha^2\|_{C(\bar{I})}$  by suitable norm provided that  $\alpha^1, \alpha^2$  are in some bounded set. Here we omit details.

For the proof we need the following

**Lemma 3.5.** Let  $z \in W_2^{2,1}(\Omega \times (0, T))$  satisfy

$$\begin{aligned} \partial_t z - \kappa \Delta z &= \int_0^t A(x, t, \tau) z(x, \tau) d\tau, \quad x \in \Omega, 0 < t < T \\ z(x, 0) &= 0, \quad x \in \Omega \end{aligned}$$

with  $A \in L^\infty(\Omega \times (0, T)^2)$ . If  $z = 0$  in  $\omega \times (0, T)$ , then  $z = 0$  in  $\Omega \times (0, T)$ .

The proof of Lemma 3.5 is done by a Carleman estimate and given in the Appendix.

*Proof of Theorem 3.1.* We set  $u = \theta(\alpha^1), v = \theta(\alpha^2), p = P(\alpha^1), q = P(\alpha^2)$  and

$$y = u - v, \quad r = p - q.$$

Then  $y = 0$  in  $\omega \times (0, T)$ . Then

$$(3.1) \quad \partial_t y = \kappa \Delta y + L(u) \partial_t r + (L(u) - L(v)) \partial_t q \quad \text{in } \Omega \times (0, T)$$



and

$$(3.2) \quad \partial_t r = \gamma(1-p) \int_0^t \alpha^1(u)(t-\tau)^2 d\tau - \gamma(1-q) \int_0^t \alpha^2(v)(t-\tau)^2 d\tau.$$

We set

$$\Sigma_1 = \{(x, t) \in \omega \times (0, T) : \theta_- < u(x, t) < \theta_0\}.$$

Then

$$(3.3) \quad \alpha^k(u(x, t)) = 0, \quad k = 1, 2, (x, t) \in \omega \times (0, T) \setminus \Sigma_1$$

by  $\text{supp } \alpha^k \subset (\theta_-, \theta_0)$  and

$$(3.4) \quad L(u(x, t)) \neq 0, \quad (x, t) \in \Sigma_1$$

by assumption (A2).

By  $y = 0$  in  $\omega \times (0, T)$ , (3.1) and (3.4), we have  $\partial_t r = 0$  in  $\Sigma_1$ . By  $r(x, 0) = 0$ ,  $x \in \Omega$ , we see that  $r = 0$  in  $\Sigma_1$ . Hence (3.2) and  $u = v$  in  $\omega \times (0, T)$  yield

$$(1-p(x, t)) \int_0^t (\alpha^1(u)(x, \tau) - \alpha^2(u)(x, \tau))(t-\tau)^2 d\tau = 0, \quad (x, t) \in \Sigma_1.$$

By (2.2) and  $\alpha \geq 0$ , we can verify that  $p(x, t) < 1$  for  $(x, t) \in \bar{\Omega} \times [0, T]$  and

$$\int_0^t (\alpha^1(u)(x, \tau) - \alpha^2(u)(x, \tau))(t-\tau)^2 d\tau = 0, \quad (x, t) \in \Sigma_1.$$

Hence

$$\alpha^1(u(x, t)) = \alpha^2(u(x, t)), \quad (x, t) \in \Sigma_1.$$

Therefore by (3.3) we have

$$(3.5) \quad \alpha^1(u(x, t)) = \alpha^2(u(x, t)), \quad (x, t) \in \omega \times (0, T).$$

It suffices that  $I = \{u(x, t) : x \in \omega, 0 \leq t \leq T\}$  contains at least two points. Then, the intermediate value theorem yields that  $I$  is a non-empty open interval. Assume that  $u(x, t) = \theta(\alpha^1)(x, t)$  is constant for  $x \in \omega$  and  $0 < t < T$ . Then  $u \equiv \theta_0$  in  $\omega \times (0, T)$  by (2.1). We set  $z = u - \theta_0$ . Therefore  $z = 0$  in  $\omega \times (0, T)$ . On the other hand, by (3.3) we obtain  $\alpha^1(\theta_0) = 0$ . The mean value theorem yields  $\alpha^1(u(x, \tau)) = \alpha^1(z + \theta_0) = \alpha^1(\theta_0) + (\alpha^1)'(\mu)z = (\alpha^1)'(\mu)z(x, \tau)$  for  $(x, \tau) \in \Omega \times (0, T)$ , where  $\mu$  is between  $\theta_0$  and  $u(x, \tau)$ . Hence with  $A \in L^\infty(\Omega \times (0, T)^2)$ , we can rewrite (2.1) as

$$(3.6) \quad \partial_t z - \kappa \Delta z = \int_0^t A(x, t, \tau) z(x, \tau) d\tau, \quad x \in \Omega, 0 < t < T$$

and

$$(3.7) \quad z(x, 0) = 0, \quad x \in \Omega.$$

In view of Lemma 3.5, we have  $u = \theta_0$  in  $\Omega \times (0, T)$ . Therefore the boundary condition of  $\theta^1$  yields  $\theta_0 = \theta_w$ . This contradicts  $\theta_0 > \theta_w$ . Thus the proof is completed.  $\square$

## 4. ANALYSIS OF THE OPTIMAL CONTROL PROBLEM

**4.1. Interior measurement.** The minimization approach is realized by the following cost functional

$$J(\theta, \eta) := \frac{1}{2} \int_0^T \int_{\omega} (\theta - \theta_m)^2 dx dt$$

with the measurement data  $\theta_m$  in a small interior domain  $\omega \subset \Omega$  satisfying (A4). Thus the optimal control problem in current work is to

$$(4.1) \quad \min_{\alpha \in \mathcal{A}_{ad}} J(\theta, \eta) \quad \text{subject to} \quad (2.3) - (2.4).$$

Taking a minimizing sequence and proceeding with similar arguments as in [10], we can prove the following existence theorem.

**Theorem 4.1.** *The optimal control problem (4.1) has a solution  $\bar{\alpha} \in \mathcal{A}_{ad}$ .*

**4.2. Differentiability of the solution operator.** In view of Section 2, we are ready to introduce the well-defined solution operator  $F$ , s.t.

$$F : \alpha \mapsto (\theta(\alpha), \eta(\alpha)), \quad \mathcal{A}_{ad} \rightarrow W_p^{2,1}(Q) \cap C^{0,\epsilon}(\bar{Q}) \times W^{1,p}(0, T; L^p(\Omega)).$$

To show the Gâteaux differentiability of  $F$ , we need the following stability estimate for two feasible solutions  $\alpha_{1,2} \in \mathcal{A}_{ad}$  which follows easily from Lemma 2.2 and Theorem 2.6:

**Lemma 4.2.** *Let  $(\theta_{1,2}, \eta_{1,2})$  be the solutions of (2.3)-(2.4) corresponding to  $\alpha_{1,2} \in \mathcal{A}_{ad}$ . Then there is a constant  $C$  such that*

$$\|\theta_1 - \theta_2\|_{W_p^{2,1}(Q)} + \|\theta_1 - \theta_2\|_{C^{0,\epsilon}(\bar{Q})} + \|\eta_1 - \eta_2\|_{W^{1,p}(0,T;L^p(\Omega))} \leq C \|\alpha_1 - \alpha_2\|_{C[\theta_-, \theta_+]}$$

Next, we choose a second coefficient function  $\tilde{\alpha} \in \mathcal{A}_{ad}$  and define the admissible perturbation  $\alpha^\epsilon = \alpha + \epsilon(\tilde{\alpha} - \alpha)$  with a small constant  $\epsilon$ . Denote  $(\theta^\epsilon, \eta^\epsilon)$  and  $(\theta, \eta)$  the solutions of (2.3)-(2.4) corresponding to  $\alpha$  and  $\alpha^\epsilon$ , respectively, we define  $u = \lim_{\epsilon \rightarrow 0} \frac{\theta^\epsilon - \theta}{\epsilon}$  and  $v = \lim_{\epsilon \rightarrow 0} \frac{\eta^\epsilon - \eta}{\epsilon}$ . In view of the definition of  $\alpha^\epsilon$ , we can conclude

$$\lim_{\epsilon \rightarrow 0} \frac{\alpha^\epsilon(\theta^\epsilon) - \alpha(\theta)}{\epsilon} = \alpha'(\theta)u + \tilde{\alpha}(\theta) - \alpha(\theta)$$

and

$$\lim_{\epsilon \rightarrow 0} \frac{L(\theta^\epsilon)e^{-\eta^\epsilon} \eta_t^\epsilon - L(\theta)e^{-\eta} \eta_t}{\epsilon} = L'(\theta)e^{-\eta} \eta_t - L(\theta)e^{-\eta} \eta_t v + L(\theta)e^{-\eta} v_t.$$

Hence, we formally can derive the following linearized system for  $(u, v)$ :

$$(4.2a) \quad u_t - \kappa \Delta u = L'(\theta)u e^{-\eta} \eta_t - L(\theta)e^{-\eta} \eta_t v + L(\theta)e^{-\eta} v_t, \quad \text{in } \Omega \times (0, T);$$

$$(4.2b) \quad \partial_\nu u + \sigma u = 0, \quad \text{on } \partial\Omega \times (0, T);$$

$$(4.2c) \quad u|_{t=0} = 0, \quad \text{in } \Omega,$$

and

$$(4.3a) \quad \frac{d^4 v}{dt^4} = 2\gamma(\tilde{\alpha}(\theta) - \alpha(\theta) + \alpha'(\theta)u);$$

$$(4.3b) \quad v^{(i)}(0) = 0, \quad (i = 0, \dots, 3).$$

Regarding (A1), it is easy to see that the linearized system (4.2), (4.3) admits a unique solution with the same regularity as the state system. Now, we define

$$u^\varepsilon = \theta^\varepsilon - \theta - \varepsilon u; \quad v^\varepsilon = \eta^\varepsilon - \eta - \varepsilon v.$$

To verify that  $(u, v)$  is indeed the Gâteaux derivative of  $(\theta, \eta)$ , it remains to show

$$\|u^\varepsilon\|_{W_p^{2,1}(Q)} + \|u^\varepsilon\|_{C^{0,\varepsilon}(\bar{Q})} + \|v^\varepsilon\|_{W^{1,p}(0,T;L^p(\Omega))} = o(\varepsilon)$$

However, this can be done using a first order Taylor expansion and the *a priori* estimates of Theorem 2.6 and Lemma 4.2. All in all, we can infer

**Theorem 4.3.** *The solution operator*

$$F : \alpha \in \mathcal{A}_{ad} \rightarrow W_p^{2,1}(Q) \cap C^{0,\varepsilon}(\bar{Q}) \times W^{1,p}(0, T; L^p(\Omega))$$

subject to (2.3)-(2.4) is Gâteaux differentiable. The directional derivative  $(u, v)$  in direction  $\tilde{\alpha} - \alpha$  is defined as the solution to (4.2)-(4.3).

Following the standard techniques (see, e.g., [22]), we introduce the Lagrange multiplier  $(\vartheta, \zeta)$  and the Lagrangean

$$\begin{aligned} \mathcal{L}(\theta, \eta, \vartheta, \zeta) := & \frac{1}{2} \int_0^T \int_\omega (\theta - \theta_m)^2 dx dt - \int_0^T \int_\Omega (\theta_t - \kappa \Delta \theta - L(\theta) e^{-\eta} \eta_t) \vartheta dx dt \\ & - \int_0^T \int_{\partial\Omega} (\kappa \partial_\nu \theta + \sigma(\theta - \theta_w)) \vartheta dx dt - \int_0^T \int_\Omega \left( \frac{d^4 \eta}{dt^4} - 2\gamma \alpha(\theta) \right) \zeta dx dt. \end{aligned}$$

Taking the derivative with respect to  $\theta$  we derive

$$\begin{aligned} \mathcal{L}_\theta(\theta, \eta, \vartheta, \zeta)h = & \int_0^T \int_\omega (\theta - \theta_m) h dx dt + \int_0^T \int_\Omega \vartheta_t h dx dt - \int_\Omega \vartheta h \Big|_0^T dx + \int_0^T \int_\Omega L'(\theta) h e^{-\eta} \eta_t \vartheta dx \\ & + \int_0^T \int_\Omega h \kappa \Delta \vartheta dx dt - \int_0^T \int_{\partial\Omega} \kappa \partial_\nu \vartheta h dx dt + \int_0^T \int_{\partial\Omega} \kappa \partial_\nu h \vartheta dx dt \\ & - \int_0^T \int_{\partial\Omega} \kappa \partial_\nu h \vartheta dx dt - \int_0^T \int_{\partial\Omega} \sigma h \vartheta + \int_0^T \int_\Omega 2\gamma \alpha'(\theta) \zeta h dx dt. \end{aligned}$$

Thus the adjoint  $\vartheta$  satisfies the parabolic system

$$(4.4a) \quad -\vartheta_t - \kappa \Delta \vartheta = L'(\theta) e^{-\eta} \eta_t \vartheta + 2\gamma \alpha'(\theta) \zeta + \chi_\omega (\theta - \theta_m) \quad \text{in } \Omega \times (0, T);$$

$$(4.4b) \quad \kappa \partial_\nu \vartheta + \sigma \vartheta = 0 \quad \text{on } \partial\Omega \times (0, T);$$

$$(4.4c) \quad \vartheta(T) = 0 \quad \text{in } \Omega$$

where  $\chi_\omega$  is the characteristic function on  $\omega$ .

The adjoint equation for  $\eta$  is derived by taking the  $\eta$  derivative with respect to the Lagrangean, i.e.

$$\begin{aligned} \mathcal{L}_\eta(\theta, \eta, \vartheta, \zeta)k = & - \int_0^T \int_\Omega L'(\theta) \theta_t e^{-\eta} \vartheta k dx - \int_0^T \int_\Omega L(\theta) e^{-\eta} \vartheta_t k dx dt + \int_\Omega L(\theta) e^{-\eta} p k \Big|_0^T dx \\ & - \int_0^T \int_\Omega \frac{d^4 \zeta}{dt^4} k dx dt + \left( \int_\Omega \frac{d^3 \zeta}{dt^3} k dx - \int_\Omega \frac{d^2 \zeta}{dt^2} \frac{dk}{dt} dx + \int_\Omega \frac{d\zeta}{dt} \frac{d^2 k}{dt^2} dx - \int_\Omega \zeta \frac{d^3 k}{dt^3} dx \right) \Big|_0^T \end{aligned}$$

or equivalently

$$(4.5a) \quad -\frac{d^4\zeta}{dt^4} = L'(\theta)\theta_t e^{-\eta\vartheta} + L(\theta)e^{-\eta}\vartheta_t \quad \text{in } \Omega \times (0, T);$$

$$(4.5b) \quad \zeta^{(i)}(T) = 0, \quad i = 0, \dots, 3, \quad \text{in } \Omega.$$

To obtain an *a priori* estimate for the adjoint system we can proceed in a standard manner. First, we integrate (4.5) three times and obtain

$$\zeta_t(t) = \frac{1}{2} \int_t^T (t-s)^2 \left( L'(\theta)\theta_s e^{-\eta\vartheta} + L(\theta)e^{-\eta}\vartheta_s \right) ds$$

We test this equation with  $|\zeta|^{p-2}\zeta$ , use the inequalities of Gronwall and Young, and the regularity of data and state variables to conclude

$$\int_{\Omega} |\zeta(t)|^p dx \leq c_1 + c_2 \|\vartheta\|_{W_p^{2,1}(\Omega \times (t, T))}^p.$$

Using this estimate and writing  $\vartheta(t) = -\int_t^T \vartheta_s ds$  we obtain for the right-hand side of (4.4a)

$$\|L'(\theta)e^{-\eta}\eta_t\vartheta + 2\gamma\alpha'(\theta)\zeta + \chi_{\omega}(\theta - \theta_m)\|_{L^p(\Omega \times (T, t))}^p \leq c_3 + c_4 \int_t^T \|\vartheta\|_{W_p^{2,1}(\Omega \times (s, T))}^p ds.$$

Hence, using Gronwall's Lemma and Lemma 2.2, we obtain an *a priori* estimate for  $\vartheta$  in  $W_p^{2,1}(Q)$ . In the same way one can use a contraction argument to show that the adjoint system admits a unique solution

Finally, we will formulate the first order necessary optimality condition. To this end, we employ the linearized and adjoint system and integrate by parts with respect to time to obtain

$$\begin{aligned} 0 &\leq \int_0^T \int_{\omega} (\theta - \theta_m) u dx dt \\ &\stackrel{(4.4)}{=} \int_0^T \int_{\Omega} \vartheta u_t dx dt + \int_0^T \int_{\Omega} \kappa \nabla \vartheta \nabla u dx dt - \int_0^T \int_{\Omega} L'(\theta) e^{-\eta} \eta_t \vartheta u dx dt \\ &\quad + \int_0^T \int_{\partial\Omega} \sigma \vartheta u dx dt - 2 \int_0^T \int_{\Omega} \gamma \alpha'(\theta) \zeta u dx dt \\ &\stackrel{(4.2)}{=} -2 \int_0^T \int_{\Omega} \gamma \alpha'(\theta) \zeta u dx dt - \int_0^T \int_{\Omega} L(\theta) e^{-\eta} \eta_t v \vartheta dx dt + \int_0^T \int_{\Omega} L(\theta) e^{-\eta} v_t \vartheta dx dt \\ &= -2 \int_0^T \int_{\Omega} \gamma \alpha'(\theta) \zeta u dx dt - \int_0^T \int_{\Omega} L'(\theta) \theta_t e^{-\eta} \vartheta v dx dt - \int_0^T \int_{\Omega} L(\theta) e^{-\eta} \vartheta_t v dx dt \\ &\stackrel{(4.5)}{=} -2 \int_0^T \int_{\Omega} \gamma \alpha'(\theta) \zeta u dx dt + \int_0^T \int_{\Omega} \frac{d^4\zeta}{dt^4} v dx dt \\ &\stackrel{(4.3)}{=} 2\gamma \int_0^T \int_{\Omega} (\tilde{\alpha}(\theta) - \alpha(\theta)) \zeta dx dt. \end{aligned}$$

We summarize the first order necessary optimality condition in the following theorem:

**Theorem 4.4.** *Assume (A1)–(A4), then there exists an optimal control  $\bar{\alpha} \in \mathcal{A}_{ad}$ , an optimal state set  $(\bar{\theta}, \bar{\eta})$  satisfying (2.3)–(2.4), and the adjoint state  $(\vartheta, \zeta)$  satisfying (4.4)–(4.5). Moreover, the following variational inequality holds true s.t.*

$$\int_0^T \int_{\Omega} (\alpha(\bar{\theta}) - \bar{\alpha}(\bar{\theta})) \zeta \geq 0, \quad \text{for all } \alpha \in \mathcal{A}_{ad}$$

where  $\mathcal{A}_{ad}$  is the admissible set.

**4.3. Interior & boundary measurement.** We also admit that the cost functional can be established as

$$J(\theta, \eta) := \frac{1}{2} \int_0^T \int_{\omega} (\theta - \theta_{m,1})^2 dx dt + \frac{1}{2} \int_0^T \int_{\partial\Omega} (\theta - \theta_{m,2})^2 dx dt.$$

Then the corresponding adjoint system for the temperature satisfies

$$(4.6) \quad \begin{cases} \vartheta_t + \kappa \Delta \vartheta &= -2\gamma \alpha'(\theta) \zeta - \chi_{\omega}(\theta - \theta_{m,1}) & \text{in } \Omega \times (0, T); \\ \partial_{\nu} \vartheta + \sigma \vartheta &= \theta_{m,2} - \theta & \text{on } \partial\Omega \times (0, T); \\ \vartheta(T) &= 0, \end{cases}$$

where  $\chi_{\omega}$  is the characteristic function on  $\omega$ . Other adjoint for the phase fraction and the first order necessary optimality condition are the same as previous subsection.

## 5. NUMERICAL SIMULATION

In this section we present a numerical example by implementing the optimal control problem (4.1) to a 2D problem as an illustration. For simplicity's sake the following parabolic-ODE coupled system will be considered with a constant latent heat  $L := L(\theta)$ ,

$$(5.7) \quad \begin{cases} \theta_t - \kappa \Delta \theta &= LP_t & \text{in } \Omega \times (0, T); \\ \kappa \partial_{\nu} \theta + \sigma(\theta - \theta_w) &= 0 & \text{on } \partial\Omega \times (0, T); \\ \theta(x, 0) &= \theta_0 & \text{in } \partial\Omega \end{cases}$$

and

$$(5.8) \quad \begin{cases} P_t &= \gamma(1 - P) \int_0^t \alpha(\theta)(t - \tau)^2 d\tau & \text{in } \Omega \times (0, T); \\ P(0) &= 0 & \text{in } \Omega \end{cases}$$

where the symbols take the values of  $\Omega = (-1, 1)$ ,  $L = 151.099$ ,  $\kappa = 0.125$ ,  $\sigma = 1$ ,  $\theta_w = 20$ ,  $\theta_0 = 800$  and  $\gamma = 4\pi$ . Our choice of these data reflects the cooling of a eutectoid carbon steel, which is known to exhibit one diffusive phase transition below the temperature  $\theta_0$ , see, e.g., [11]. Moreover, we assume a uniform growth rate  $\rho = 1$ . To realize the forward problem we let the nucleation rate, also the control,  $\alpha(\theta) = 6 \exp(-0.02(\theta - 650)^2)$  and discretize the coupled system with the finite element method by the Matlab pde toolbox. In order to save the computational time we adjust the cost functional with a weighted constant  $W = 10^3$  such that

$$(5.9) \quad J(\theta(\alpha)) = \frac{W}{2} \int_0^T \int_{\omega} (\theta - \theta_m)^2 dx dt$$

where the adjoint system is adjusted accordingly in the numerical realization. The measurement domain  $\omega$  is a circle centered at  $(0, 0.6)$  with a radius of 0.2. In Figures 1 and 2, we collect the complete domain, the measurement  $\theta_m$  at  $T = 3$  and the temperature distribution  $\theta(x, t)$ , phase volume fraction  $P(x, t)$  at  $x = (0, 0.6)$ . As one

can observe in the left penal of Figure 2 the cooling process is disturbed by the latent heat induced by the phase volume fraction  $P$  especially at  $t \in (0.5, 1.5)$ .

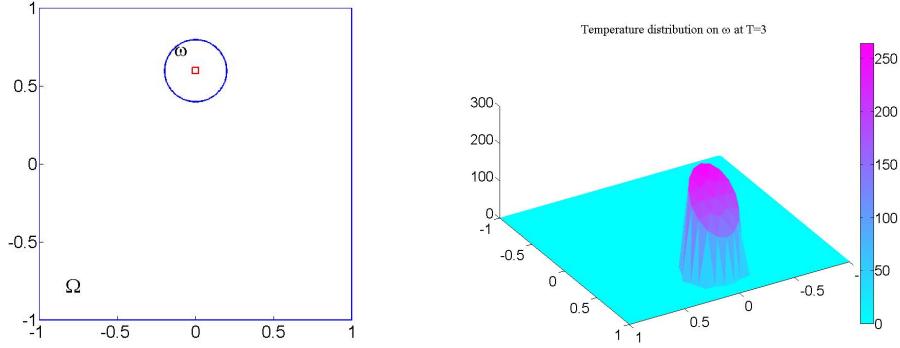


FIGURE 1. Left: the whole domain  $\Omega$  and the observation domain  $\omega$ . Temperature distribution and phase volume fraction at  $\square$  ( $x = (0, 0.6)$ ) is presented in Figure 2. Right: Measurement  $\theta_m(x, T)$  for  $x \in \omega$  and  $T = 3$ .

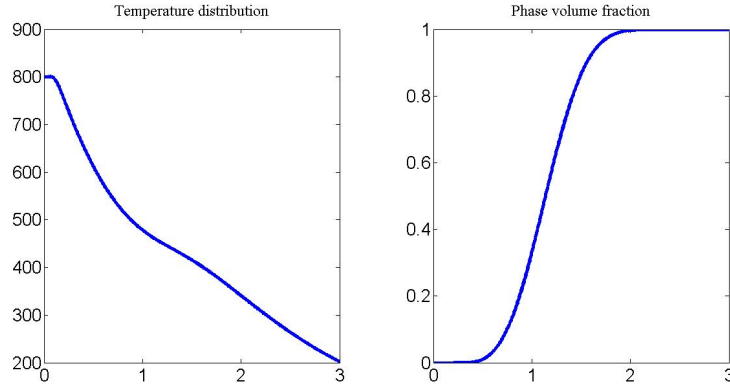


FIGURE 2. Left: Temperature distribution  $\theta(x, t)$ . Right: Phase volume fraction  $P(x, t)$  for  $x = (0, 0.6)$  and  $t \in [0, 3]$ .

In order to identify the nucleation rate  $\alpha(\theta)$  with respect to the measured temperature distribution on  $\omega$  we define the support of the control  $\text{supp}(\alpha) = [\theta_-, \theta_+]$  with  $\theta_- = 650$  and  $\theta_+ = 750$ . We then discretize the domain  $[\theta_-, \theta_+]$  with equal-distance distributed points  $\theta_- := \tau_0 \leq \tau_1 < \dots < \tau_N := \theta_+$  and approximate  $\alpha$  with cubic B-splines of basis functions  $\varphi_i(\tau)$  such that

$$\alpha^N(\tau) = \sum_{i=1}^N \alpha_i \varphi_i(\tau), \quad \tau \in [\theta_-, \theta_+]$$

with  $N = 9$ .

We thus define a finite-dimensional set of admissible controls

$$\alpha_{ad}^N = \{\alpha^N = (\alpha_1, \dots, \alpha_N)^T \in \mathbb{R}^N : 0 \leq \alpha_i \leq M \text{ for } i = 1, \dots, N\}$$

with the upper and lower constraints  $M$  and  $m$ . The original (infinite-dimensional) optimal control problem (4.1) is reduced into a finite form such that  $J_{dis}(\alpha^N) = J(\theta(\alpha^N), \alpha^N)$  and define  $\bar{\alpha}^N$  to be the optimal control. By choosing  $\alpha^N$  satisfying  $\alpha_j = \bar{\alpha}_j$  for  $j \neq l$ , the first order necessary optimality condition in Theorem 4.4 yields

$$(\alpha_l - \bar{\alpha}_l) \int_0^T \int_{\Omega} \varphi_l(\bar{\theta}) \zeta dx dt \geq 0.$$

The feasible gradient for  $J_{dis}(\alpha^N)$  thus can be defined by

$$(5.10) \quad \frac{\partial J_{dis}}{\partial \alpha_l} = \int_0^T \int_{\Omega} \varphi_l(\bar{\theta}) \zeta dx dt, \quad 1 \leq l \leq N,$$

which allows us to solve the optimal control problem with a quasi-Newton method routinely by calling Matlab command *fmincon*. In Figure 3, we displayed four snapshots of the approximated solution towards the exact measured data. Quantitative information of the iteration is collected in Table 1 with objective function value as well as the gradient value.

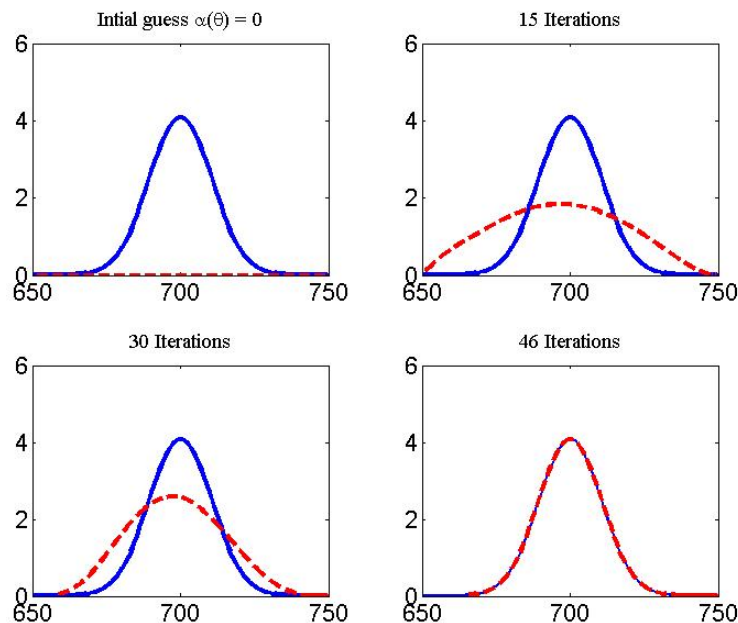


FIGURE 3. 4 snapshots of the approximated solution towards the exact measured data. The solid line is the exact solution, the dashed line is the approximated one.

Finally to investigate the robustness of our proposed method we tested our algorithm with noisy perturbed data. The noisy data is generated by adding the exact measurements with uniformly distributed noise whose absolute noise levels are 0.1 and 0.4 respectively. In Figure 4 we collected the the optimization results for perturbed data where the stable performance can be observed.

TABLE 1. Quantitative information of the objective functional  $J_i$  and error in the gradient  $e_i = \|\bar{G}(\theta) - G_i(\theta)\|$ 

Iteration $i$	$J_i$	$e_i$
1	2608.62	650
15	0.0393	0.0070
30	0.0068	0.0003
46	$3.2 \times 10^{-10}$	$3.15 \times 10^{-6}$

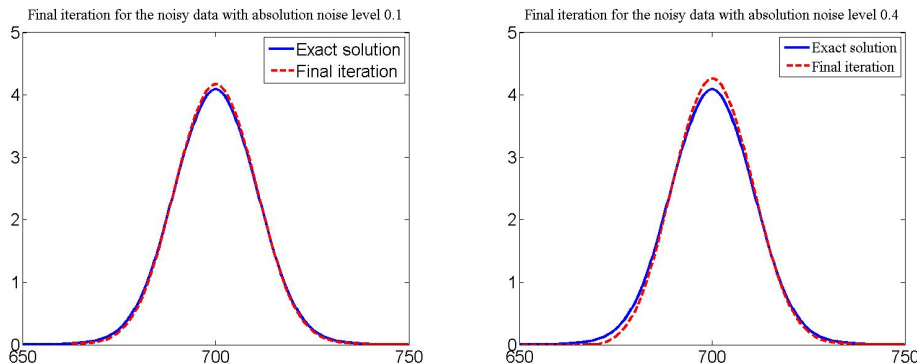


FIGURE 4. Final iteration of the optimization problem for noisy data. Left: absolute noise level 0.1; Right: absolute noise level 0.4.

## 6. CONCLUSIONS

In the present paper we have investigated the identification of the temperature dependent nucleation rate for the generalised Avrami model. We have shown its unique identifiability and derived an optimal control based approximation scheme. Numerical results with model data prove the feasibility of this approach.

The next step will be the utilisation of experimental data which have been derived from dilatometer experiments as in [11]. From modelling point of view an interesting task is the generalisation of the present model to multiphase nucleation and growth models. This would allow to describe the phase evolution in modern multi-phase steels. Finally, the ultimate goal is to study the optimal control problem for the production of multi-phase steels. In other words one would like to compute optimal cooling conditions to produce a steel with desired micro structural composition.

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## APPENDIX A. PROOF OF LEMMA 3.5

First we show a Carleman estimate. Let  $d \in C^2(\bar{\Omega})$  such that  $|\nabla d| \neq 0$  on  $\bar{\Omega}$ . We set

$$\begin{aligned} \psi(x, t) &= d(x) - \beta t^2, \quad \varphi(x, t) = e^{\lambda \psi(x, t)}, \\ D &= \{(x, t) : x \in \bar{\Omega}, t > 0, \psi(x, t) > \varepsilon\} \end{aligned}$$

with some  $\beta > 0$  and  $\varepsilon > 0$ . We fix sufficiently large  $\lambda > 0$ . We assume that  $\overline{D} \subset \overline{\Omega} \times [0, T]$ . We set  $Lu = \partial_t u - \kappa \Delta u$ . Then, there holds

**Lemma A.1.** *There exists a constant  $s_0 > 0$  such that there exists a constant  $C = C(s_0) > 0$  such that*

$$\begin{aligned} & \int_D (s|\nabla u|^2 + s^3|u|^2)e^{2s\varphi} dxdt \\ \leq & C \int_D |Lu|^2 e^{2s\varphi} dxdt + Ce^{Cs} \int_{\partial D} (|\nabla_{x,t} u|^2 + |u|^2) dSdt \end{aligned}$$

for all  $s > s_0$  and  $u \in H^{2,1}(D)$ .

The proof is found e.g., as Theorem 3.2 in Yamamoto [25].

Let  $\Omega_0$  be an arbitrary bounded domain such that  $\partial\Omega_0$  is smooth and

$$(1) \quad \Gamma := \partial\Omega_0 \cap \omega \supset \partial\Omega_0 \cap \{x \in \mathbb{R}^3 : |x - x_0| < \varepsilon_0\}$$

with some  $x_0 \in \mathbb{R}^3$  and  $\varepsilon_0 > 0$ . By  $z = 0$  in  $\omega \times (0, T)$ , we have

$$(2) \quad z = |\nabla_{x,t} z| = 0 \quad \text{on } \Gamma \times (0, T).$$

It suffices to prove that

$$(3) \quad z = 0 \quad \text{in } \Omega_0 \times (0, T).$$

In fact, since  $\Omega$  is covered by a family of  $\Omega_0$  satisfying (1), the conclusion (3) implies that  $z = 0$  in  $\Omega \times (0, T)$ .

Let  $\Omega_1$  be a bounded domain with smooth boundary such that

$$\overline{\Omega_1} \subset \Omega_0 \cup \Gamma,$$

$\partial\Omega_1 \cap \partial\Omega_0 \neq \emptyset$  is an open subset of  $\partial\Omega_0$ , and is a proper subset of  $\Gamma$ .

For proving (3), we have only to prove

$$(4) \quad z = 0 \quad \text{in } \Omega_1 \times (0, T).$$

Because we can choose  $\Omega_1$  arbitrarily close to  $\Omega_0$ .

Let  $\Omega_2$  be a union of  $\Omega_0$  and a bounded domain  $\widehat{\Omega} \subset \overline{\mathbb{R}^3} \setminus \overline{\Omega_0}$  such that  $\partial\widehat{\Omega} \cap \overline{\Omega_0} = \Gamma$  and  $\widehat{\Omega}$  contains some non-empty open set. Then

$$(5) \quad \overline{\Omega_0} \subset \Omega_2, \quad \overline{\Gamma} = \overline{\partial\Omega_0} \cap \overline{\Omega_2}, \quad \partial\Omega_0 \setminus \Gamma \subset \partial\Omega_2.$$

Choose  $\omega_0$  satisfying  $\overline{\omega_0} \subset \Omega_2 \setminus \overline{\Omega_0}$ . Then there exists  $d \in C^2(\overline{\Omega_2})$  satisfying

$$d(x) > 0, \quad x \in \Omega_2, \quad d(x) = 0, \quad x \in \partial\Omega_2,$$

$$(6) \quad |d(x)| > 0, \quad x \in \overline{\Omega_2} \cap \overline{\Omega_0}.$$

The existence of such  $d$  is proved e.g., in Imanuvilov [12].

Then, since  $\overline{\Omega_1} \subset \Omega_2$  and  $d|_{\partial\Omega_2} = 0$ , we can choose a sufficiently large  $N > 1$  such that

$$(7) \quad \{x \in \Omega_2 : d(x) > \frac{4}{N} \|d\|_{C^1(\overline{\Omega_2})}\} \cap \overline{\Omega_0} \supset \Omega_1.$$

We choose  $\beta > 0$  and  $\varepsilon > 0$  such that

$$(8) \quad \beta > \frac{\|d\|_{C(\overline{\Omega_2})}}{T^2}, \quad 0 < \varepsilon < \sqrt{\frac{3\|d\|_{C(\overline{\Omega_2})}}{N\beta}}.$$

We set  $\mu_k = \frac{k}{N} \|d\|_{C(\overline{\Omega_2})}$ ,  $k = 1, 2, 3, 4$  and

$$(9) \quad D = \{(x, t) : x \in \overline{\Omega_0}, t > 0, \psi(x, t) > \mu_1\}.$$

Then we can prove

$$(10) \quad \Omega_1 \times (0, \varepsilon) \subset D \subset \overline{\Omega_0} \times (0, T).$$

**Proof of (10).** Let  $(x, t) \in \Omega_1 \times (0, \varepsilon)$ . Then, by (7), we see that  $x \in \overline{\Omega_0}$  and

$$d(x) \geq \frac{4}{N} \|d\|_{C(\overline{\Omega_2})}.$$

Hence

$$\begin{aligned} \psi(x, t) &= d(x) - \beta t^2 > \frac{4}{N} \|d\|_{C(\overline{\Omega_2})} - \beta \varepsilon^2 \\ &> \frac{1}{N} \|d\|_{C(\overline{\Omega_2})} + \left( \frac{3}{N} \|d\|_{C(\overline{\Omega_2})} - \beta \varepsilon^2 \right) > \frac{1}{N} \|d\|_{C(\overline{\Omega_2})} = \mu_1 \end{aligned}$$

by (8). Therefore  $(x, t) \in D$ . Next let  $(x, t) \in D$ . Then by the definition of  $D$ , we have  $x \in \overline{\Omega_0}$  and  $d(x) - \beta t^2 > \mu_1$ . Hence  $\|d\|_{C(\overline{\Omega_2})} - \beta t^2 > \mu_1 = \frac{1}{N} \|d\|_{C(\overline{\Omega_2})}$ , and so

$$\|d\|_{C(\overline{\Omega_2})} > \frac{N-1}{N} \|d\|_{C(\overline{\Omega_2})} > \beta t^2,$$

that is,

$$0 < t < \sqrt{\frac{\|d\|_{C(\overline{\Omega_2})}}{\beta}}.$$

The first condition in (8) yields  $0 < t < T$ . Therefore (10) is verified.

Next we have

$$(11) \quad \partial D \subset \Sigma_1 \cup \Sigma_2 \cup \Sigma_3,$$

where

$$\Sigma_1 \subset \Gamma \times (0, T), \quad \Sigma_2 = \{(x, t) : x \in \overline{\Omega_0}, t \geq 0, \psi(x, t) = \mu_1\}$$

and

$$\Sigma_3 \subset \Omega_0 \times \{0\}.$$

In fact, it is sufficient to prove that  $\partial D \cup \{t > 0\} \subset \Sigma_1 \cup \Sigma_2$ . In fact, let  $(x, t) \in \partial D \cap \{t > 0\}$ . Then  $x \in \overline{\Omega_0}$ ,  $t > 0$  and  $\psi(x, t) \geq \mu_1$ . We separately consider the cases  $x \in \Omega_0$  and  $x \in \partial\Omega_0$ . First let  $x \in \Omega_0$ . If  $\psi(x, t) > \mu_1$ , then  $(x, t)$  is an interior point of  $D$ . Therefore if  $x \in \Omega_0$ , then  $\psi(x, t) = \mu_1$ . Next let  $x \in \partial\Omega_0$ . Let  $x \in \partial\Omega_0 \setminus \Gamma$ . Then  $x \in \partial\Omega_2$  by the third condition in (5), and  $d(x) = 0$  by the second condition in (6). On the other hand,  $\psi(x, t) \geq \mu_1$  yields that

$$d(x) - \beta t^2 = -\beta t^2 \geq \frac{1}{N} \|d\|_{C(\overline{\Omega_2})}.$$

By  $t > 0$ , this is impossible. Therefore we must have  $x \in \Gamma$ . In terms of (10), we have  $t \in (0, T)$ . Thus the verification of (11) is completed.

We apply Lemma A.1 in  $D$ . Henceforth  $C > 0$  denotes generic constants, which are independent of  $s$  and choices of  $g, p, \kappa$ . For it, we need a cut-off function because we

have no data on  $\partial D \setminus (\Gamma \times (0, T))$ . Let  $\chi_0 \in C^\infty(\mathbb{R})$  be monotone increasing,  $0 \leq \chi_0 \leq 1$ , and satisfy

$$\chi_0(\eta) = \begin{cases} 1, & \eta > \mu_3, \\ 0, & \eta < \mu_2. \end{cases}$$

Then setting  $\chi(x, t) = \chi_0(\psi(x, t))$ , we see that  $\chi \in C^\infty(\mathbb{R}^{n+1})$ ,  $0 \leq \chi \leq 1$  and

$$(12) \quad \chi(x, t) = \begin{cases} 1, & \psi(x, t) > \mu_3, \\ 0, & \psi(x, t) < \mu_2. \end{cases}$$

Since  $\psi(x, \tau) \geq \psi(x, t)$  for  $0 \leq \tau \leq t$  and  $x \in \overline{\Omega}_1$  and  $\chi_0$  is monotone increasing, we have

$$(13) \quad \chi(x, \tau) \geq \chi(x, t), \quad 0 \leq \tau \leq t, x \in \overline{\Omega}_1.$$

We set  $v = \chi z$ , and have

$$(14) \quad \begin{aligned} & \partial_t v - \kappa \Delta v \\ &= (\partial_t \chi)z - 2\kappa \nabla \chi \cdot \nabla z - \kappa z \Delta \chi \\ &+ \int_0^t A(x, t, \tau) z(x, \tau) d\tau \quad \text{in } D. \end{aligned}$$

Since  $z(x, 0) = 0$ ,  $x \in \Omega$ , we have  $z(x, 0) = \partial_t z(x, 0) = 0$ ,  $x \in \Omega$  by substituting  $t = 0$  in  $\partial_t z - \kappa \Delta z = \int_0^t A(x, t, \tau) z(x, \tau) d\tau$ . Consequently by (3) and (11), we have  $z = |\nabla z| = \partial_t z = 0$  on  $\partial D$ . Hence applying Lemma 1 in (14), we obtain

$$\begin{aligned} & \int_D s^3 |v|^2 e^{2s\varphi} dx dt \\ & \leq C \int_D |(\partial_t \chi)z - 2\kappa \nabla \chi \cdot \nabla z - \kappa z \Delta \chi|^2 e^{2s\varphi} dx dt \\ & + C \int_D \left| \chi(x, t) \int_0^t A(x, t, \tau) z(x, \tau) d\tau \right|^2 e^{2s\varphi} dx dt \end{aligned}$$

for all large  $s > 0$ . By (12), the first terms on the right-hand side includes the derivatives of  $\chi$  as factors and so does not vanish only if  $\mu_2 < \psi(x, t) < \mu_3$ . Hence

$$\int_D |(\partial_t \chi)z - 2\kappa \nabla \chi \cdot \nabla z - \kappa z \Delta \chi|^2 e^{2s\varphi} dx dt \leq C M e^{2s\theta_3},$$

where we set

$$\theta_k = e^{\lambda \mu_k}, \quad k = 1, 2, 3, 4$$

and

$$M = \|z\|_{L^2(0, T; H^1(\Omega))}^2.$$

Therefore

$$(15) \quad \begin{aligned} & \int_D s^3 |v|^2 e^{2s\varphi} dx dt \\ & \leq C M e^{2s\theta_3} + C \int_D \left| \chi(x, t) \int_0^t A(x, t, \tau) z(x, \tau) d\tau \right|^2 e^{2s\varphi} dx dt \end{aligned}$$

for all large  $s > 0$ . We estimate the second term on the right-hand side. First by (9) we note that  $(x, t) \in D$  if and only if

$$0 < t < g(x) := \sqrt{\frac{d(x) - \mu_1}{\beta}}, \quad x \in \overline{\Omega}_0.$$

Therefore by (13) and  $v(x, \tau) = \chi(x, \tau)z(x, \tau)$ , we obtain

$$\begin{aligned}
J &:= \int_D \left| \chi(x, t) \int_0^t A(x, t, \tau) z(x, \tau) d\tau \right|^2 e^{2s\varphi} dx dt \\
&\leq \int_D \left( |\chi(x, t)| \int_0^t |A(x, t, \tau) z(x, \tau)| d\tau \right)^2 e^{2s\varphi} dx dt \\
&\leq \int_D \left( \int_0^t |\chi(x, \tau)| |A(x, t, \tau) z(x, \tau)| d\tau \right)^2 e^{2s\varphi} dx dt = \int_D \left( \int_0^t |A(x, t, \tau) v(x, \tau)| d\tau \right)^2 e^{2s\varphi} dx dt \\
&\leq \int_D \left( \int_0^t |v(x, \tau)| d\tau \right)^2 e^{2s\varphi(x, t)} dx dt.
\end{aligned}$$

At the last inequality, we used  $A \in L^\infty(\Omega \times (0, T)^2)$  and the Cauchy-Schwarz inequality. Hence, since  $\varphi(x, t) \leq \varphi(x, \tau)$  for  $0 \leq \tau \leq t$ , we have

$$\begin{aligned}
J &\leq C \int_{\Omega_0} \left( \int_0^{g(x)} \left( \int_0^t |v(x, \tau)|^2 d\tau \right) e^{2s\varphi(x, t)} dt \right) dx \\
&\leq C \int_{\Omega_0} \int_0^{g(x)} \left( \int_0^t e^{2s\varphi(x, \tau)} |v(x, \tau)|^2 d\tau \right) dt dx \leq C \int_{\Omega_0} \int_0^{g(x)} \left( \int_0^{g(x)} e^{2s\varphi(x, \tau)} |v(x, \tau)|^2 d\tau \right) dt dx \\
&\leq C \max_{x \in \Omega_0} g(x) \int_{\Omega_0} \int_0^{g(x)} e^{2s\varphi(x, \tau)} |v(x, \tau)|^2 d\tau dx \leq C_1 \int_D |v|^2 e^{2s\varphi} dx dt.
\end{aligned}$$

Consequently by (15), we have

$$(16) \quad s^3 \int_D |v|^2 e^{2s\varphi} dx dt \leq CM e^{2s\theta_3} + C_1 \int_D |v|^2 e^{2s\varphi} dx dt$$

for all large  $s > 0$ . Choosing  $s > 0$  large, we can absorb the second term on the right-hand side into the left-hand side, and we have

$$s^3 \int_D |v|^2 e^{2s\varphi} dx dt \leq C_2 M e^{2s\theta_3}.$$

Since  $D(\mu_4) := \{(x, t) \in D : \psi(x, t) > \mu_4\} \subset D$ , we obtain

$$s^3 e^{2s\theta_4} \int_{D(\mu_4)} |v|^2 dx dt \leq C_2 M e^{2s\theta_3},$$

that is,

$$\int_{D(\mu_4)} |v|^2 dx dt \leq \frac{C_2 M}{s^3} e^{-2s(\theta_4 - \theta_3)}$$

for all large  $s > 0$ . Letting  $s \rightarrow \infty$ , noting that  $\chi = 1$  in  $D(\mu_4)$  by (12), we have  $v = 0$  in  $D(\mu_4)$ , that is,  $z = 0$  in  $D(\mu_4)$ . We can choose  $N > 0$  arbitrarily and so  $\mu_4 > 0$  is arbitrary. Therefore we have  $z = 0$  in  $D = D(\mu_1)$ . Hence  $z = 0$  in  $\Omega_1 \times (0, \varepsilon)$  by (10). Therefore  $z$  satisfies

$$\partial_t z - \kappa \Delta z = \int_\varepsilon^t A(x, t, \tau) z(x, \tau) d\tau, \quad x \in \Omega_1, \varepsilon < t < T,$$

and

$$z(x, \varepsilon) = 0, \quad x \in \Omega_1.$$

After fixing  $N > 0$  sufficiently large, we choose  $\varepsilon > 0$  by (8) and we repeat the previous argument to have  $z = 0$  in  $\Omega_1 \times (\varepsilon, 2\varepsilon)$ . Continuing this argument until  $m\varepsilon \geq T$  with some  $m \in \mathbb{N}$ , we obtain (4). Thus the proof of Lemma 3.5 is completed.

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