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AN INVERSE DIFFUSION COEFFICIENT PROBLEM FOR A PARABOLIC EQUATION WITH INTEGRAL CONSTRAINT

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We dedicate this paper to Bill Layton on the occasion of his 60th birthday and take the opportunity to thank him for generously sharing his expertise and advice.

Abstract. We consider a problem of recovering the time-dependent diffusion coefficient in a parabolic system. To ensure uniqueness the system is constrained by the integral of the solution at all times. This problem has applications in geology where the parabolic equation models the accumulation and diffusion of argon in micas. Argon is generated by the decay of potassium and the diffusion is thermally activated. We introduce a time discretization, on which we base an application of Rothe's method to prove existence of solutions. The numerical scheme corresponding to the semi-discretization exhibits convergence that is consistent with that in Euler's method.

Key words. Inverse problems, integral constraint, parabolic equation, Rothe's method, geochronology.

1. Introduction

Suppose Ω is a bounded domain in $\mathbb{R}^d$ with a smooth boundary. While in general we consider $d \geq 1$, the cases $d = 2$ and $d = 3$ are the most relevant for applications in geology. Let $T > 0$ and denote $\Omega_T = \Omega \times (0, T]$ and $\Gamma_T = \partial\Omega \times (0, T]$. We consider an inverse problem for the following system:

$$u_t - c(t)\Delta u = s(t), \qquad (x,t) \in \Omega_T, \tag{1}$$

$$u = 0, \qquad (x,t) \in \Gamma_T, \tag{2}$$

$$u(x,0) = u_0(x), \quad x \in \Omega. \tag{3}$$

The problem is as follows: given the source $s(t)$ and the initial condition $u_0(x)$, we seek the coefficient $c(t)$. As stated, the problem admits multiple solutions. To ensure unique solvability we impose an additional constraint for the integral of the solution with respect to the space variable, namely

$$\int_\Omega u(x,t)\, dx = \mu(t), \quad t \in (0, T], \tag{4}$$

where the function $\mu(t)$ is also given.

The equations in system (1)-(3) arise as a model for the diffusion of ^{40}Ar produced by radioactive decay of ^{40}K. This isotope is found in mica that is a silicate mineral with nearly perfect basal cleavage. This property renders micas highly amenable to *in situ* analyses in a geology laboratory setting, in which the concentrations for both ^{40}Ar and ^{39}Ar, a proxy for ^{40}K, can be measured. We summarize the description of the model as found in [8]. In this model, the function $u(x,t)$ corresponds to the concentration of argon, which diffuses in the crystalline lattice

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with a thermally activated rate, and satisfies equation (1). The specific dependence of the diffusion coefficient $c(t)$ on temperature $T(t)$ is given by

$$c(t) = D_0 e^{-E/RT(t)}.$$

Here D_0, E, and R are parameters with experimentally determined or empirically postulated values. We are interested in recovering $c(t)$ since this function gives us the thermal history that the sample underwent. The thermal history in turn provides the exhumation history, i.e., the distance to surface as a function of time, due to the proxy relationship between the depth and the temperature: the sample can be assumed to cool as it rises to the surface with an almost linear rate of 30°C per km for a certain range of depths.

When a crystal is formed, it is natural to assume that the initial concentration of potassium is constant in space. Following crystallization, potassium decays with the exponential rate λ_K to either ^{40}Ar or ^{40}Ca. We denote by f_{Ar} the fraction of decays that yield ^{40}Ar ($f_{\mathrm{Ar}} \approx 10.9\%$). We note that, in the model with no diffusion, i.e., in the case of the ordinary differential equation, the age of a sample is determined using the formula

$$A(u, v) = \frac{1}{\lambda_K} \ln \left(1 + \frac{1}{f_{\mathrm{Ar}}} \frac{u}{v} \right),$$

where u and v are the concentrations of the daughter and parent isotopes, respectively. Consequently, only the ratio u/v is relevant and, without loss of generality, we can take the initial concentration of ^{40}K to be unity. Since potassium is weakly chemically bonded in the lattice, its concentration remains constant in space. As a product of ^{40}K decay, argon is generated at the rate $s(t) = \lambda_K f_{\mathrm{Ar}} e^{-\lambda_K t}$, which appears as the source term in equation (1). In a slight generalization of this model, which does not affect our analysis, we can consider a source term that depends both on the space variable x and on time t. This generalization is justified, for example, when potassium has a known non-constant initial concentration $g(x)$. In this case, the source term has the product representation $s(t)g(x)$. Argon, being chemically inert, tends to have negligible concentration at the time of crystallization, which results in the initial condition $u_0 = 0$ in (3).

Next, we provide a motivation for the integral constraint (4). In addition to the aforementioned *in situ* analyses, which are essentially spot measurements of the concentration, *bulk* age measurement is another popular method of estimating the age of a sample. This method involves crushing it to obtain a single measurement of the age. The *bulk* age corresponds to the integral $\mu(t)$ of the solution in (4). Eusden and Lux reported in [2] the bulk age data they obtained for samples collected on the slopes of Mount Washington, New Hampshire. These geologists observed that the mica ages increase progressively from the bottom to the top of the mountain and used them to estimate the exhumation rate. These data afford an interpretation of the geological history for these samples that possibly included upward movement with similar temperature regimes in the relevant temperature range that was followed by erosion or another event that exposed the samples along the slope with similar histories but with different starting times of their development.

We illustrate this scenario in Figure 1 and note that the problem we are considering presently involves three assumptions, namely, we suppose that (1) the samples followed the same temperature history but with different starting points in time; (2) there are samples available with any starting point between now and the age of the oldest sample; and (3) the exact ages of the samples, e.g., the times of crystallization, are known. The first of these assumptions is not unrealistic. The second assumption, if satisfied, would imply that the erosion event, which exposed the samples, spanned the depth of about 15 km, which is not feasible. This assumption can be relaxed in practice to requiring that the event that resulted in rapid cooling in samples and halted diffusion in them affected the samples in the temperature range from the onset of retention to closure. In this case, we can hope to recover the temperature history only for that interval. In order to supply the sample ages, as required in the third assumption, some additional data may need to be interpreted. For example, the elevations at which the samples were collected may provide a basis for estimating their relative ages.

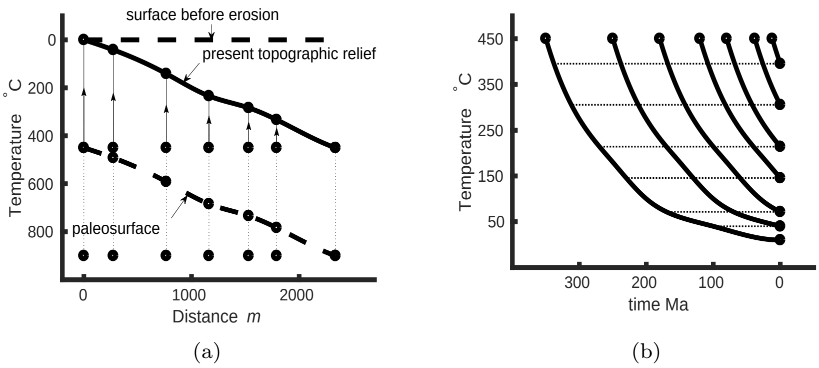

Figure 1. (a) Stages of development of a paleosurface containing the future samples collected on the present topographic surface; (b) Terminal points of the temperature histories for the younger samples correspond to the intermediate points on the temperature history of the oldest sample.

Ivanchov [5] treated the problem of recovering the unknown diffusion coefficient in the one-dimensional case for non-local boundary conditions and proved existence using Schauder fixed point theory. Kanca and Ismailov [6] also proved well-posedness in 1d using the separation of variables method. Cannon and Rundell [1] considered this problem in the case of arbitrary dimension. They imposed the assumption of additional data in the form of the heat flux at a single point on the boundary. Their method is based on the Banach fixed point theorem and existence and uniqueness are proved for the choices of boundary values that effectively amount to pumping energy into the system. This technical condition allows the application of a monotonicity argument. Their initial conditions must satisfy rather restrictive assumptions: in particular, the case of a constant initial condition is not covered. The authors state that their method also works for the integral constraint under consideration in this paper. We considered in [4] the problem of recovering an unknown source in the parabolic system. The inverse source problem with an integral constraint is also addressed in [3, 9].

Our main result is an iterative scheme that both gives rise to the existence of solutions and allows us to compute approximate solutions. The assumptions that we impose on the data are fairly intuitive and they allow examples not covered elsewhere in the literature. The rest of the paper is organized as follows. In Section 2, we develop an iterative scheme, whose convergence depends on the estimates developed in Section 3. We prove existence of solutions by applying Rothe's method in Section 4. Section 5 contains the results of numerical experiments motivated by the scheme.

2. Semi-discretization in time

We will establish well-posedness for the problem using Rothe's method, which requires semi-discretization in time. This section contains an outline of a procedure for discretizing this system. In the first step, we let

$$0 = t^0 < t^1 < t^2 < \cdots < t^{N-1} < T \le t^N$$

be the times to be determined later and let $\tau^k = t^k - t^{k-1}$, $k = 1, \ldots, N$ be the discretization time steps. Due to the variable time step, we assume that the source $s(t)$ and the data $\mu(t)$ are defined on an interval slightly larger than $(0, T]$. We approximate $u(t^k)$ by u^k, $c(t^k)$ by c^k, and $\int_{t_{k-1}}^{t^k} s(t)\,dt$ by S^k. The backward Euler scheme for equation (1) takes the form:

$$u^k - \tau^k c^k \Delta u^k = u^{k-1} + S^k. \tag{5}$$

This equation as well as all elliptic equations appearing below are understood to be taken with the zero Dirichlet boundary condition. We cannot solve this elliptic equation as stated since the coefficient c^k is unknown. To solve the equation we transfer the uncertainty from the coefficient in front of the Laplacian to the *variable* time step. Specifically, we fix a discretization parameter $\alpha = \tau^k c^k$ and rewrite the last equation as

$$u^k - \alpha \Delta u^k = u^{k-1} + S^k. \tag{6}$$

Next, we separate the contributions of the two terms in the right-hand side by considering two equations:

$$\hat{u}^k - \alpha \Delta \hat{u}^k = u^{k-1}, \tag{7}$$

$$\tilde{u} - \alpha \Delta \tilde{u} = 1, \tag{8}$$

which depend only on the parameter α, and look for the solution of (6) in the form

$$u^k = \hat{u}^k + S^k \tilde{u}. \tag{9}$$

In order to satisfy the integral constraint (4) we approximate $\frac{1}{\tau^k}\int_{t^{k-1}}^{t^k} \mu(t)\,dt$ by μ^k, denote

$$\hat{\mu}^k = \int_\Omega \hat{u}^k\,dx, \quad \tilde{\mu} = \int_\Omega \tilde{u}\,dx,$$

and integrate (9) over Ω to get

$$\mu^k = \hat{\mu}^k + S^k \tilde{\mu}. \tag{10}$$

This equation is satisfied when t^k is the root of the function of a single variable

$$G^k(t) = \mu(t) - \hat{\mu}^k - \tilde{\mu} \int_{t^{k-1}}^{t} s(\tau)\,d\tau. \tag{11}$$

Adopting the notation $u^0 = u_0$, we assemble the solution process in the following three steps on each time iteration $k = 1, 2, \ldots, N$:

Step 1. Solve $\hat{u}^k - \alpha \Delta \hat{u}^k = u^{k-1}$, $x \in \Omega$.
Step 2. Find the smallest $t^k > 0$ such that $G^k(t^k) = 0$, for $G^k(t)$ given by (11).
Step 3. Let $u^k = \hat{u}^k + S^k \tilde{u}$.

It is easy to verify that u^k obtained in Step 3 is the solution of equation (6) and it satisfies the integral constraint, i.e., $\int_\Omega u^k\,dx = \mu(t^k)$.

3. Preliminary estimates

The convergence of this iteration procedure hinges on the solution of the nonlinear equation in Step 2 having the property that, as the discretization parameter α goes to zero, $\tau^k = t^k - t^{k-1}$ also goes to zero but not too fast. We address this property in Lemmas 2 and 3 below by considering eigenfunction expansions using the following notation.

Let ψ_j and λ_j be the eigenfunctions and eigenvalues of the Laplace operator acting on $H_0^1(\Omega)$, that is,

$$-\Delta\psi_j = \lambda_j\psi_j \quad \text{for } j = 1, 2, \dots .$$

With appropriate scaling, the functions ψ_j form an orthonormal basis in $L^2(\Omega)$. We expand the solutions of equations (6), (7), and (8) as the series

$$u^k = \sum_{j\geq 1} U_j^k \psi_j, \quad \hat{u}^k = \sum_{j\geq 1} \hat{U}_j^k \psi_j, \quad \tilde{u} = \sum_{j\geq 1} \tilde{U}_j \psi_j.$$

Using the corresponding equations, we can solve for the coefficients in these expansions:

$$U_j^k = \frac{U_j^{k-1} + S^k\omega_j}{1+\alpha\lambda_j}, \quad \hat{U}_j^k = \frac{U_j^{k-1}}{1+\alpha\lambda_j}, \quad \tilde{U}_j = \frac{\omega_j}{1+\alpha\lambda_j},$$

where $\omega_j = (1, \psi_j)$ and (u, v) denotes the scalar product in $L^2(\Omega)$. Without loss of generality, assume $\omega_j > 0$. Iterating on the recursive relationship for U_j^k, we get

$$U_j^k = \frac{S^k\omega_j}{1+\alpha\lambda_j} + \frac{S^{k-1}\omega_j}{(1+\alpha\lambda_j)^2} + \dots + \frac{S^1\omega_j}{(1+\alpha\lambda_j)^k} + \frac{U_j^0}{(1+\alpha\lambda_j)^k}. \tag{12}$$

We note that the integrals of u^k, $\hat{u}^k$, and $\tilde{u}$ have representations

$$\mu^k = \sum_{j\geq 1} U_j^k\omega_j, \quad \hat{\mu}^k = \sum_{j\geq 1} \frac{U_j^{k-1}\omega_j}{1+\alpha\lambda_j}, \quad \tilde{\mu} = \sum_{j\geq 1} \frac{\omega_j^2}{1+\alpha\lambda_j}. \tag{13}$$

In the following lemma, we establish a bound for $\tilde{\mu}$ that is independent of $\alpha > 0$.

Lemma 1. *The solution $\tilde{u}$ of (8) has the property $\tilde{u} \leq 1$ in Ω. In particular, the integral $\tilde{\mu}$ of $\tilde{u}$ satisfies $\tilde{\mu} < |\Omega|$.*

Proof. Suppose $\tilde{u}$ attains its maximum at $x_0 \in \Omega$. Considering the equation at this point

$$\tilde{u}(x_0) - \alpha\Delta\tilde{u}(x_0) = 1,$$

we note that $\tilde{u} > 0$ in Ω by the maximum principle and $\Delta\tilde{u}(x_0) \leq 0$ from calculus considerations. Therefore $\tilde{u}(x_0) \leq 1$ and the conclusion follows.

Alternatively, just for the second part of this lemma, we integrate equation (8) and apply the divergence theorem in the second term to get

$$\tilde{\mu} - \alpha\int_{\partial\Omega} \frac{\partial\tilde{u}}{\partial\nu}\, ds = |\Omega|.$$

Since $\tilde{u} > 0$ in Ω, we have $\displaystyle\int_{\partial\Omega} \frac{\partial\tilde{u}}{\partial\nu}\, ds < 0$ and thus obtain the desired estimate. □

We need the following assumptions.

Assumption 1. *Assume $s \in L^\infty(0, T)$ and $\mu \in C^1[0, T]$ have the properties:*

(1A) $s(t) \geq 0$ for all $t \in (0, T)$;

(1B) there exists a constants $m > 0$, such that $m < \mu(t)$ for all $t \in [0, T]$;

(1C) there exist two constants $|\Omega|\|s\|_\infty < \gamma_1 < \gamma_2$ *such that*

$$\mu'(t) + \gamma_1 \le \tilde{\mu}s(t) < \mu'(t) + \gamma_2 \quad \text{for all } t \in [0, T].$$

Assumption 2. *Assume* $u_0(x)$ *has the eigenfunction expansion* $u_0 = \sum_{j\ge1} U_j^0 \psi_j$ *with coefficients that satisfy* $\delta := \sum_{j\ge1} \lambda_j \omega_j |U_j^0| < \infty$.

Remark 1. *The condition (1A) is consistent with the assumption that argon is* generated *as a product of decay of potassium and the rate of production is positive. Assumption (1B) that* μ *is bounded away from zero is essential in ensuring that the function* $G^k(t)$ *in* (11) *has a root and that the time step is not too small. Assumption (1C) can be interpreted as follows: the scaled rate of production of argon* $s(t)$ *is within a constant of the rate at which the diffusant escapes the sample through the boundary. This condition is crucial for controlling the size of the time step.*

In the next lemma, we show that τ^k converges to zero as α goes to zero.

Lemma 2. *Suppose* μ *and* s *satisfy Assumption 1 and* u_0 *satisfies Assumption 2. Then* $\tau^k < C_1\alpha$ *and* $S^k < C_2\alpha$ *for* $k = 1, \dots, N$*, where* $C_1 = \dfrac{\delta}{\gamma_1 - |\Omega|\|s\|_\infty}$ *and* $C_2 = C_1\|s\|_\infty$.

Proof. Recall that $\tau^k = t^k - t^{k-1}$ and t^k is the root of the function $G^k(t)$ defined by (11). Rewrite $G^k(t)$ as

$$G^k(t) = \mu^{k-1} - \hat{\mu}^k + \int_{t^{k-1}}^{t} (\mu'(\tau) - \tilde{\mu}s(\tau))\, d\tau. \tag{14}$$

The idea is to majorize $G^k(t)$ by a linear function. In particular, the integral in the right-hand side is estimated using Assumption (1C), namely,

$$\int_{t^{k-1}}^{t} (\mu'(\tau) - \tilde{\mu}s(\tau))\, d\tau \le -\gamma_1(t - t^{k-1}). \tag{15}$$

We note that the intercept $\mu^{k-1} - \hat{\mu}^k$ is positive. Indeed, using induction and Assumption (1A) we get that the right-hand side of (6) is positive and the maximum principle gives us that $u^k > 0$ in Ω. Therefore, the solution $\hat{u}^k$ of (7) is also positive again by the maximum principle. Integrating (7) over Ω, we get

$$\mu^{k-1} - \hat{\mu}^k = -\alpha \int_\Omega \Delta \hat{u}^k\, dx = -\alpha \int_{\partial\Omega} \frac{\partial \hat{u}^k}{\partial \nu}\, ds > 0,$$

where the last inequality follows since $\hat{u}^k > 0$ in Ω and $\hat{u}^k = 0$ on $\partial\Omega$ as in Lemma 1. Thus the smallest positive root of $G^k(t)$ is smaller than the horizontal intercept of the decreasing linear function, which can be determined explicitly.

Hence we need only to find a uniform bound for the difference $\mu^{k-1} - \hat{\mu}^k$ from above. To that end, we argue by induction and assume $S^n \le C_2\alpha$ for $n = 1, \dots, k-1$, where C_2 is to be specified later. Then expanding $\mu^{k-1} - \hat{\mu}^k$ as in (13), we have

$$\begin{aligned}\mu^{k-1} - \hat{\mu}^k &= \sum_{j\ge1} \frac{\alpha\lambda_j\omega_j}{1+\alpha\lambda_j} U_j^{k-1} \\ &= \alpha \sum_{j\ge1} \frac{\lambda_j\omega_j^2 S^{k-1}}{(1+\alpha\lambda_j)^2} + \cdots + \frac{\lambda_j\omega_j^2 S^2}{(1+\alpha\lambda_j)^{k-1}} + \frac{\lambda_j\omega_j^2 S^1}{(1+\alpha\lambda_j)^k} + \frac{\lambda_j\omega_j U_j^0}{(1+\alpha\lambda_j)^k},\end{aligned}$$

where we used the representation (12) for U_j^k. Next, we apply the induction hypothesis and collect the resulting geometric series to get

$$\mu^{k-1} - \hat{\mu}^k \le C_2\alpha \sum_{j\ge 1} \frac{\omega_j^2}{1+\alpha\lambda_j} - \sum_{j\ge 1} \frac{C_2\alpha\omega_j^2}{(1+\alpha\lambda_j)^k} + \alpha \sum_{j\ge 1} \frac{\lambda_j\omega_j U_j^0}{(1+\alpha\lambda_j)^k}. \tag{16}$$

Recalling that $\omega_j > 0$, we estimate $\dfrac{\lambda_j\omega_j U_j^0}{(1+\alpha\lambda_j)^k} \le \lambda_j\omega_j|U_j^0|$. Recognizing $\tilde{\mu}$ in the first sum in (16), dropping the second sum, and using Assumption 2 for the last term, we get

$$\mu^{k-1} - \hat{\mu}^k \le C_2\alpha\tilde{\mu} + \alpha\delta \le \alpha(C_2|\Omega| + \delta), \tag{17}$$

where we have also used Lemma 1 in the last inequality. Combining the estimates (15) and (17), we get

$$G^k(t) \le \alpha(C_2|\Omega| + \delta) - \gamma_1(t - t^{k-1}).$$

Therefore, the root of $G^k(t)$ must be less than the root of the linear function on the right, i.e.,

$$\tau^k \le \frac{C_2|\Omega| + \delta}{\gamma_1}\,\alpha. \tag{18}$$

We have obtained one estimate for the conclusion of this lemma. In order to complete the induction step we estimate

$$S^k = \int_{t^{k-1}}^{t^k} s(\tau)\,d\tau \le \|s\|_\infty \frac{C_2|\Omega| + \delta}{\gamma_1}\,\alpha.$$

Thus the induction step $S^k \le C_2\alpha$ is verified if we take

$$C_2 = \frac{\delta\|s\|_\infty}{\gamma_1 - |\Omega|\|s\|_\infty}.$$

The denominator of this expression is positive by Assumption (1C). We substitute the value of C_2 in (18) to calculate the constant C_1. □

Remark 2. *Assumption 2 may be replaced, for example, with the requirement that $u_0 \in C^2(\Omega)$ with $\Delta u_0 \in L^2(\Omega)$. In this case, a uniform bound for the last term in* (16) *may be obtained by the Cauchy-Schwarz inequality as follows:*

$$\left(\sum_{j\ge 1} \frac{\lambda_j\omega_j U_j^0}{(1+\alpha\lambda_j)^k}\right)^2 \le \sum_{j\ge 1} \frac{\omega_j^2}{(1+\alpha\lambda_j)^2} \cdot \sum_{j\ge 1} \frac{\lambda_j^2 (U_j^0)^2}{(1+\alpha\lambda_j)^{2(k-1)}}. \tag{19}$$

We recognize the first sum on the right as the integral $\int_\Omega \tilde{u}^2\,dx$, where $\tilde{u}$ is the solution of equation (8)*. By Lemma 1, this integral is bounded by $|\Omega|$. For the second sum, we consider the sequence of equations*

$$v^k - \alpha\Delta v^k = v^{k-1}, \quad k = 1, 2, \ldots,$$

where $v^0 = \Delta u_0$. Multiplying this equation by v^k, integrating over Ω, and applying the Cauchy-Schwarz inequality, we get $\|v^k\| \le \|v^{k-1}\|$, where $\|\cdot\|$ denotes the norm in $L^2(\Omega)$. Applying this inequality recursively, we obtain $\|v^k\| \le \|\Delta u_0\|$. The second sum in (19) *corresponds to the integral $\int_\Omega (v^{k-1})^2\,dx$. Combining the two estimates, we have*

$$\sum_{j\ge 1} \frac{\lambda_j\omega_j U_j^0}{(1+\alpha\lambda_j)^k} \le |\Omega|^{1/2}\|\Delta u_0\|.$$

This modification covers the important example of the constant initial condition.

In the lemma below, we prove that for any value of the discretization parameter $\alpha > 0$, the iteration has finitely many time steps on the interval $(0, T]$.

Lemma 3. *Let μ, s, and u_0 be as in Lemma 2. Then for any $\alpha > 0$, we have $\tau^k > C_3$ for $k = 1, \ldots, N$, for some positive constant C_3 that depends on α.*

Proof. The idea is similar to that in Lemma 2. Using Assumption (1C), we estimate $G^k(t)$ in (14) from below as follows:

$$G^k(t) \geq \mu^{k-1} - \hat{\mu}^k - \gamma_2(t - t^{k-1}). \tag{20}$$

Thus the lower bound for τ^k is derived from the lower bound on $\mu^{k-1} - \hat{\mu}^k$. We obtain the absolute minimum of this difference through the following construction.

Let $\mathcal{P} = \{u \in L^2(\Omega) : \; u > 0 \text{ and } \|u\| = 1\}$. Here and throughout, we adopt the convention that $\|\cdot\|$ denotes the norm in $L^2(\Omega)$. Let

$$l_\alpha = \inf_{u \in \mathcal{P}} \left\{ \int_\Omega (u - \hat{u})\, dx : \; \hat{u} - \alpha\Delta\hat{u} = u \right\}.$$

We claim that $l_\alpha > 0$. Indeed, suppose $u \in \mathcal{P}$ and $\hat{u}$ is the solution of $\hat{u} - \alpha\Delta\hat{u} = u$. Multiplying this equation by $\hat{u}$, integrating over Ω, and using Young's inequality with ε, we have

$$\|\hat{u}\|^2 + \alpha\|\nabla\hat{u}\|^2 = \int_\Omega u\hat{u}\, dx \leq \varepsilon\|\hat{u}\|^2 + \frac{1}{4\varepsilon}\|u\|^2.$$

Choosing $\varepsilon < 1$ so that $\alpha < 1 - \varepsilon$, we have $\|\hat{u}\|^2_{H^1(\Omega)} < 1/4\alpha\varepsilon$. Let $\{u_j, \hat{u}_j\}$ be a minimizing sequence for l_α, that is, $u_j \in \mathcal{P}$, $\hat{u}_j - \alpha\Delta\hat{u}_j = u_j$ and $\int_\Omega (u_j - \hat{u}_j)\, dx \to l_\alpha$. By weak compactness, there exist subsequences, without loss of generality also denoted by $\{u_j, \hat{u}_j\}$, such that $u_j \rightharpoonup u$ weakly in $L^2(\Omega)$ and $\hat{u}_j \rightharpoonup \hat{u}$ weakly in $H^1(\Omega)$. Taking the limit in the weak equation

$$(\hat{u}_j, v) + \alpha(\nabla\hat{u}_j, \nabla v) = (u_j, v), \quad \text{for all } v \in H^1_0(\Omega),$$

we have

$$(\hat{u}, v) + \alpha(\nabla\hat{u}, \nabla v) = (u, v), \quad \text{for all } v \in H^1_0(\Omega),$$

i.e., $\hat{u} - \alpha\Delta\hat{u} = u$ and the infimum l_α is attained by the weak limit $\{u, \hat{u}\}$. Integrating the equation, we get

$$l_\alpha = -\alpha \int_{\partial\Omega} \frac{\partial\hat{u}}{\partial\nu}\, ds,$$

where the right-hand side is strictly positive since $\hat{u} > 0$ in Ω.

Returning to the equation $\hat{u}^k - \alpha\Delta\hat{u}^k = u^{k-1}$ in Step 2 of the iterative procedure, we first note that, due to Assumption (1B), we have

$$m \leq \int_\Omega u^k\, dx \leq |\Omega|^{1/2}\|u^k\|.$$

The conclusion in the previous paragraph yields the estimate

$$\mu^{k-1} - \hat{\mu}^k \geq \frac{m l_\alpha}{|\Omega|^{1/2}}.$$

The final step is the same as in the proof of the previous lemma: we conclude from the estimate (20) that

$$\tau^k \geq \frac{m l_\alpha}{\gamma_2|\Omega|^{1/2}}.$$

In closing we point out that, although this construction produces a positive lower bound for τ^k that is not explicit in α, the fact that it depends only on α, the lower bound m for μ, and the domain Ω is sufficient for our purposes. ∎

4. Existence of solutions

The application of Rothe's method presented here is based on [7, p.287] and it is a simplified version of the arguments found in [4]. We state the main result in the following theorem and outline the essential points of the proof for the sake of completeness.

Theorem 1. *Suppose μ, s, and u_0 satisfy Assumptions 1 and 2. There exists a weak solution (u, c) of equations (1)-(4) in the sense that $u \in L^2(0,T;H_0^1(\Omega))$ with $u_t \in L^2(0,T;H^{-1}(\Omega))$ and $c \in L^\infty(0,T)$ satisfy*

$$\int_0^T \langle u_t, \phi\rangle + c(t)(\nabla u, \nabla\phi)\,dt = \int_0^T (s,\phi)\,dt, \quad \textit{for all } \phi \in L^2(0,T;H_0^1(\Omega)),$$

$$\int_\Omega u(x,t)\,dx = \mu(t), \quad \textit{for a.e. } t \in (0,T].$$

Proof. We first establish the existence of solutions for the equation with a scaled time variable. Replace u^k by v^k in (6) and rewrite it in the form

$$v_{\bar{t}}^k - \Delta v^k = f^k, \quad k = 1,\dots,N, \tag{21}$$

where $v_{\bar{t}}^k = (v^k - v^{k-1})/\alpha$ and $f^k = S^k/\alpha$. The idea is to establish uniform in α energy estimates for the solutions of elliptic equations (21), then extract weakly convergent subsequences for $\alpha \to 0$, and finally show that the limit satisfies the parabolic equation. To obtain the estimates, as in [4], we multiply (21) by v^k and integrate over Ω. The summation of resulting identities in the range $k = 1,\dots,n$, for some $n \le N$, yields

$$\sum_{k=1}^n \int_\Omega v_{\bar{t}}^k v^k\,dx + \sum_{k=1}^n \int_\Omega |\nabla v^k|^2\,dx = \sum_{k=1}^n f^k \mu^k. \tag{22}$$

Applying the identity $2\alpha \sum_{k=1}^n v_{\bar{t}}^k v^k = (v^n)^2 - (v^0)^2 + \alpha^2 \sum_{k=1}^n (v_{\bar{t}}^k)^2$ to the first term and rearranging, we get

$$\begin{aligned} I_\alpha^n &:= \int_\Omega (v^n)^2\,dx + 2\alpha \sum_{k=1}^n \int_\Omega |\nabla v^k|^2\,dx + \alpha^2 \sum_{k=1}^n \int_\Omega (v_{\bar{t}}^k)^2\,dx \\ &= \int_\Omega (v_0)^2\,dx + 2\sum_{k=1}^n S^k \mu^k. \end{aligned}$$

Thus we have the estimate

$$I_\alpha^n \le \|v_0\|_{L^2(\Omega)}^2 + 2T \cdot \sup s \cdot \sup \mu, \quad n = 1,\dots,N.$$

The rest of the proof for establishing existence of weak solutions follows the arguments in [4] and we refer to the proof of Theorem 1 in that paper for details. As a result of passing to the limit as $\alpha \to 0$, we extract for sequences of piece-wise constant functions with values $\{v^k, f^k\}_{k=1}^N$ the limit functions $\{v(x,t), f(t)\}$ that satisfy the following equation together with the initial and boundary conditions:

$$v_t - \Delta v = f(t), \quad (x,t) \in \Omega_{\tilde{T}}, \tag{23}$$

$$v = 0, \quad (x,t) \in \Gamma_{\tilde{T}} \tag{24}$$

$$v(x,0) = u_0(x), \quad x \in \Omega, \tag{25}$$

where $\tilde{T} = \alpha N$. We note that these equations arise from a change of the time variable in the original system (1)-(3). Indeed, given $c(t)$ let $y(t)$ be the solution of

$c(y)\dot{y} = 1$, $y(0) = 0$ and define $v(x,t) = u(x, y(t))$. Then u is a solution of (1)-(3) if and only if v is a solution of (23)-(25) with

$$f(t) = \frac{s(y(t))}{c(y(t))}. \tag{26}$$

To recover $y(t)$ from $f(t)$ we use the definition of y and rearrange the terms in (26) as follows:

$$s(y)\dot{y} = f(t), \quad y(0) = 0.$$

This equation has a solution y implicitly defined as a function of t in terms of $f(t)$ in the relation

$$S(y(t)) = \int_0^t f(\tau)\, d\tau,$$

where $S(\cdot)$ is the integral of $s(\cdot)$ with $S(0) = 0$. Finally, we solve for $c(\cdot)$ using the relation (26). □

Remark 3. *For the specific choice of* $s(t) = \lambda_K f_{Ar} e^{-\lambda_K t}$, *we can solve for* $y(t)$ *explicitly*

$$y(t) = -\frac{1}{\lambda_K} \ln\left(1 - \frac{1}{f_{Ar}} \int_0^t f(\tau)\, d\tau\right) \quad \textit{and} \quad c(y(t)) = \frac{\lambda_K}{f(t)}\left(f_{Ar} - \int_0^t f(\tau)\, d\tau\right).$$

5. Numerical studies

In this section, we present the results of some numerical experiments. We recall the computational algorithm as derived and described in Section 2. We choose $0 < \alpha < 1$ and solve the following elliptic equation

$$\tilde{u} - \alpha\Delta\tilde{u} = 1,\ x \in \Omega, \quad \tilde{u} = 0,\ x \in \partial\Omega \quad \text{and compute} \quad \tilde{\mu} = \int_\Omega \tilde{u}\, dx.$$

Next, we set $t^0 = 0$, $u^0 = u_0$ and follow the steps below for $k \geq 1$.

Step 1. Solve $\hat{u}^k - \alpha\Delta\hat{u}^k = u^{k-1},\ x \in \Omega,\ \hat{u}^k = 0,\ x \in \partial\Omega$ and compute $\hat{\mu}^k$.

Step 2. Solve the nonlinear equation $\mu(t^k) = \hat{\mu}^k + \tilde{\mu} \int_{t^{k-1}}^{t^k} f(t)\, dt$ for t^k.

Step 3. Compute the approximate solution $u^k = \hat{u}^k + \tilde{u} \int_{t^{k-1}}^{t^k} f(t)\, dt$.

Step 4. Find the time step $\tau^k = t^k - t^{k-1}$ and the approximate diffusion coefficient $c^k = \alpha/\tau^k$.

The Steps 1-4 are repeated as long as t^k satisfies $t^k \leq T$.

We consider several examples to illustrate the accuracy of our scheme. For the domain Ω we consider the square $[-1,1] \times [-1,1]$ in $\mathbb{R}^2$. The final time is taken to be $T = 1$, and the source function is $f(t) = e^{-t}$. The assumption that μ is uniformly bounded away from zero was essential for proving convergence and it is also important in the numerical experiments. When this condition is violated, the numerical procedure breaks down in Step 2. In our experiments, we choose the initial data $u_0(x,y) = \cos\frac{\pi}{2}x \cos\frac{\pi}{2}y$. The examples of the coefficient functions we use in our experiments are given in Table 1 and they are chosen so that they all have the same maximum value of 3 on the temporal interval $[0,T]$. The algorithm employs a finite element discretization in space as implemented in the PDE toolbox in Matlab and the time discretization corresponds to the implicit Euler method with variable time step. The triangular mesh on the spatial domain Ω has maximum mesh size of 0.4 resulting in 82 elements and 52 unknowns. To generate the data for each diffusion coefficient in Table 1, we run the forward model to obtain a numerical approximation of the direct problem, which we treat as the exact solution. We then compute the numerical integral of the solution which is used as the data for

TABLE 1. Rates of convergence estimated using linear regression.

c	$2t+1$	$\frac{9}{4}t^2+\frac{3}{4}$	$2\sin\left(\frac{\pi}{2}t\right)+1$	e^t+3-e
s_u	0.8837	0.9608	0.8547	0.9783
s_c	1.0088	1.0130	1.0090	1.0031

our scheme. In our computational algorithm, we use the built-in Matlab functions *parabolic*, *assempde*, and *fzero* to solve the parabolic equation, the elliptic equations, and to find roots of the nonlinear equation, respectively.

We note that the discretization parameter α can be taken as the time step. Error estimates for the standard implicit scheme suggest that

$$\left(\int_0^T \|u(\cdot,t)-u^\alpha(\cdot,t)\|^2_{L^2(\Omega)}\,dt\right)^{1/2} = \mathcal{O}(\alpha^{s_u}), \quad \max_{0\le t\le T}|c(t)-c^\alpha(t)| = \mathcal{O}(\alpha^{s_c})$$

for some $s_u, s_c > 0$, where u and c denote the exact solution and the exact diffusion coefficient, respectively, and u^α is the approximate solution obtained in Step 3 and c^α is the approximate diffusion coefficient given in Step 4 of this section. The log-log plots of these errors versus the discretization parameter α are depicted in Figure 2. We also report the slopes s_u and s_c which correspond to the rates of convergence that we estimate using linear regression and summarize in Table 1. Both s_u and s_c are close to one which is consistent with the rate of convergence in the Euler scheme.

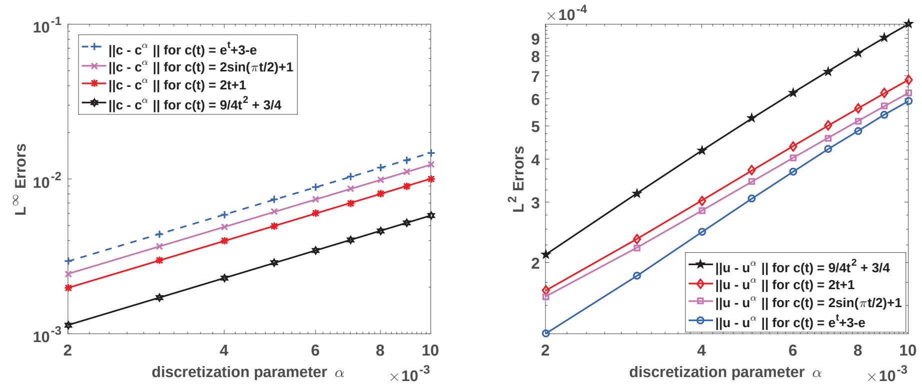

FIGURE 2. Log-log error plots for the diffusion coefficient c (left); log-log error plots for the solution u (right).

6. Conclusions and future work

We investigated the problem of recovering the time-dependent diffusion coefficient in a parabolic equation subject to an integral constraint. This problem has applications in geochronology, an area of geology, which specializes in determining the age of rocks. We introduced a time discretization using the implicit Euler scheme with a variable time step. This discretization essentially transfers the uncertainty from the unknown coefficient to the time step. With an application of the

Rothe method, we proved existence of weak solutions. Using the scheme together with a finite element discretization in the space variable, we computed numerical approximations of the solutions and estimated the rates of convergence for several examples. Having computed the errors and observing the nearly linear convergence, our next step in this project is to perform the error analysis and compare the theoretical rates with the observations. Another interesting direction for future work is a modification of the scheme that removes the restriction that the integral of the solution $\mu(t)$ is bounded away from zero uniformly in t. In particular, this would allow for a geologically relevant zero initial condition.

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