

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

DMITRY GLOTOV, WILLIS E. HAMES, A. J. MEIR, AND SEDAR NGOMA

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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:

$$\begin{aligned} (1) \quad & u_t - c(t)\Delta u = s(t), \quad (x, t) \in \Omega_T, \\ (2) \quad & u = 0, \quad (x, t) \in \Gamma_T, \\ (3) \quad & u(x, 0) = u_0(x), \quad x \in \Omega. \end{aligned}$$

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

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

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

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 ($f_{\text{Ar}} \approx 10.9\%$). 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

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

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 $s(t) = \lambda_K f_{\text{Ar}} e^{-\lambda_K t}$, 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