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An integral constrained parabolic problem with applications in thermochronology

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We dedicate this paper to Max Gunzburger, the third author's thesis advisor, on the occasion of his 70th birthday. A teacher, colleague, and friend, who so kindly shared his wisdom

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ABSTRACT

We investigate an inverse source problem with an integral constraint for a parabolic equation. The constraint is motivated by an application in thermochronology, a branch of geology. The existence and uniqueness of weak solutions are established by means of the Rothe method and an energy method, respectively. The elliptic problem resulting from the time discretization is solved by homogenizing the integral constraint. The implicit scheme used in the proof of existence lends itself readily for numerical studies and we present the results of numerical experiments. We also report on the errors and convergence rates.

1. Introduction

Let Ω be a domain in $\mathbb{R}^d$ with a C^2 boundary $\partial\Omega$. We consider an inverse source problem corresponding to the equation:

$$\partial_t u - \Delta u = F(x,t) + f(t), \quad x \in \Omega,\ t > 0 \tag{1}$$

$$u(x,t) = g(x,t), \quad x \in \partial\Omega,\ t > 0 \tag{2}$$

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

$$\int_\Omega u(x,t)\,dx = \mu(t), \quad t > 0. \tag{4}$$

The problem is as follows: given the known component $F(x,t)$ of the source, the Dirichlet boundary conditions $g(x,t)$, the initial condition $u_0(x)$, and a scalar function $\mu(t)$, find the pair $(u(x,t), f(t))$ that satisfies (1)–(4). In this paper, our focus is on the numerical scheme for solving this system. This scheme also allows us to prove existence via Rothe's method.

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The problem of finding the solution of (1)–(4) with a non-linear source term and a constant in time integral constraint was considered by Švadlenka and Omata in [1]. These authors addressed existence, regularity, and presented results of numerical studies. The case of a non-constant integral constraint was developed by Ginder in [2] who proved existence and regularity under the assumption that $\mu(t) \in C^1[0,T]$. In both [1,2], the method of discrete Morse flow, which we refer to as Rothe's method, was applied. Numerical results using finite difference schemes in two dimensions are presented in [3] and an application of the boundary element method in one dimension is treated in [4]. An inverse parabolic source problem in which the source depends on both time and space with a final overdetermination is treated by Cao, Gunzburger, and Turner [5]. The authors used optimal control theory to prove exact controllability. Inverse problems of determining the time-dependent conductivity coefficient in one dimension with integral overdetermination are discussed in [6,7]. A related inverse source problem involving data in the form of an internal measurement is dealt with, for example, in [8,9]. The case of a source that depends only on the space variable or only on the time variable for both elliptic and parabolic equations is considered in [10]. An elliptic problem with an integral constraint is solved in [11].

This paper is organized as follows. In Section 2, we establish a link between the inverse source problem (1)–(4) and a problem arising in geology. The reader interested only in the mathematical part of this paper may safely skip to Section 3, where we solve a related elliptic problem with an integral constraint. In Section 4, we homogenize the initial and boundary conditions in the parabolic problem, prove the uniqueness of weak solutions, and introduce a semi-discretization in time based on the solution of the elliptic problem. In Section 5, we use the time discretization to obtain a bound on the unknown source via eigenfunction expansions, which, in turn, allows us to prove existence using Rothe's method. Finally, in Section 6, we present the results of numerical studies and comment on the rate of convergence of the scheme.

2. Motivation

The problem originated in thermochronology, a branch of geology wherein the thermal history of minerals is evaluated on the basis of the concentration of daughter isotopes that are susceptible to loss via diffusion at elevated temperature. The thermal history is of considerable interest to studies of the crustal history due to the proxy relationship between temperature and depth beneath Earth's surface (ca. 30 °C/km in stable, continental regions). By constraining the temperature of geologic samples as a function of time, we are able to reconstruct the various processes they have been subject to and to better understand Earth history.

The K–Ar dating method is based on the decay of radiogenic ^{40}K with half-life 1.25 Ga to stable ^{40}Ar, and is among the most widely used as potassium is abundant within rocks and minerals from a variety of crustal settings. As ^{40}Ar is chemically inert, it tends to be excluded from many minerals at the time of crystallization, and then to accumulate as a radiogenic product that is unaffected by chemical processes but can migrate within crystals by thermally activated lattice diffusion. The ^{40}Ar/^{39}Ar dating method is a variation of traditional K–Ar dating, in which samples are irradiated with fast neutrons in the core of a nuclear reactor to produce ^{39}Ar from ^{39}K, the stable and most abundant potassium isotope, to serve as a proxy for ^{40}K [12]. The ^{40}Ar/^{39}Ar dating method is extremely useful as it permits measurement of the parent–daughter ratio on single, small quantities of samples; current laser sampling methods permit measurement of ^{40}Ar/^{39}Ar age at scales of tens of microns within single crystals. The spatial distribution of ^{40}Ar within crystals, and its concentration relative to the parent, presents a record of the sample's thermal history. The complete distribution of ^{40}Ar/^{39}Ar within crystals corresponds to the problem of final overdetermination considered in [5,8,10].

To set up a model of argon diffusion, we think of a mica crystal as occupying a domain $\Omega \subset \mathbb{R}^d$, where $d = 2$ or 3. The concentration of argon $u(x,t)$ satisfies the following partial differential equation

$$\partial_t u - c(t)\,\Delta u = s(t), \quad x \in \Omega,\ t > 0 \tag{5}$$

$$u(x,0) = u_0(x), \quad x \in \Omega \tag{6}$$

$$u(x,t) = 0, \quad x \in \partial\Omega. \tag{7}$$

Here, the coefficient $c(t)$ is a composition of a function $D(\cdot)$ with temperature T, which itself is a function of time, i.e., $c(t) = D(T(t))$; the dependence of D on T is given by the Arrhenius law

$$D(T) = D_0\, e^{-E/RT}, \tag{8}$$

where the activation energy E, the gas constant R, and the frequency factor D_0 are parameters; the source term has the form

$$s(t) = \lambda_K f_{\mathrm{Ar}}\, e^{-\lambda_K t}, \tag{9}$$

where λ_K is the rate of radiogenic decay of ^{40}K and f_{Ar} is the fraction of the parent isotope ^{40}K decays that yield ^{40}Ar. Without loss of generality, the initial concentration of the parent isotope is scaled to one.

We perform a change of variables that transforms Eq. (5) with an unknown *coefficient* $c(t)$ into Eq. (1) with unknown *source* $f(t)$. For a given function $c(\cdot)$, let y be the solution of the ordinary differential equation

$$c(y)\dot{y} = 1, \qquad y(0) = 0, \tag{10}$$

and define $v(x,t) = u(x,y(t))$ so that u is a solution of (5) if and only if v is a solution of

$$\partial_t v - \Delta v = f(t), \quad x \in \Omega,\ t > 0, \tag{11}$$