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Numerical solutions to singular reaction–diffusion equation over elliptical domains

Matthew A. Beauregard

Department of Mathematics and Statistics, Stephen F. Austin State University, Nacogdoches, TX 75962, USA

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ABSTRACT

Solid fuel ignition models, for which the dynamics of the temperature is independent of the single-species mass fraction, attempt to follow the dynamics of an explosive event. Such models may take the form of singular, degenerate, reaction–diffusion equations of the quenching type, that is, the temporal derivative blows up in finite time while the solution remains bounded. Theoretical and numerical investigations have proved difficult for even the simplest of geometries and mathematical degeneracies. Quenching domains are known to exist for piecewise smooth boundaries, but often lack theoretical estimates. Rectangular geometries have been primarily studied. Here, this acquired knowledge is utilized to determine new theoretical estimates to quenching domains for arbitrary piecewise, smooth, connected geometries. Elliptical domains are of primary interest and a Peaceman–Rachford splitting algorithm is then developed that employs temporal adaptation and nonuniform grids. Rigorous numerical analysis ensures numerical solution monotonicity, positivity, and linear stability of the proposed algorithm. Simulation experiments are provided to illustrate the accomplishments.

1. Introduction

Nonlinear evolution equations that form a singularity in finite time are ubiquitous in nature. Applications are broad appearing in models from chemistry, physics, biology, rocket, and combustion engineering. Solid fuel ignition models attempt to approximate an explosive event, identified as the rate of change of the temperature increasing without bound and forming a singularity in finite time. The formation of the singularity equates to ignition in the combustor. Moreover, the finite time ignition is triggered if the temperature reaches a critical threshold. The sophistication of combustion models can be reduced considerably if one examines asymptotically close to the ignition time. In such cases, the equation for the temperature decouples from the chemistry and mass-species fraction [5,19]. The final result is a highly nonlinear differential equation, in particular,

$$s(x,y)u_t = \Delta u + f(u), \quad t > 0, \ (x,y,t) \in \Omega \times (0,T), \tag{1}$$
$$u(x,y,0) = u_0(x,y), \quad (x,y) \in \Omega, \tag{2}$$

where $\Omega \in \mathbb{R}^2$, Dirichlet boundary conditions specified on the boundary $\partial\Omega$, and $0 \leqslant u_0(x,y) < 1$ for $(x,y) \in \Omega$. The source term, $f(u)$, is a highly nonlinear function. It is positive and strictly increasing for $0 \leqslant u < 1$. Most importantly, it tends to infinity when $u \to 1^-$. The degeneracy function $s(x,y) \geqslant 0$ and models particular heat transportation characteristics within

E-mail address: beauregama@sfasu.edu

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the domain. While it remains positive within the domain it may vanish or become singular on a countable subset of points on the boundary. If the degeneracy function vanishes this is seen as a defect in the transportation of heat, while if it becomes singular it is a defect in the diffusion of heat. In either case, the degeneracy indicates a defect at a particular location of the combustor or, common to combustion engine designs, a special material concentration point [2,14,19].

A sufficient condition for the singularity to form in the temporal derivative is that $u \to 1^-$ as $t \to T^- < \infty$ in $\tilde{\Omega} \subseteq \Omega$ [24]. In such cases, the solution u is said to quench at the *quenching time* T over the domain Ω. The set $\tilde{\Omega}$ is called the *quenching location set,* and in this study involves a single point in the domain. On one hand, given an initial condition and domain shape there is no guarantee that the solution will quench. One the other hand, it is known that for a piecewise smooth and connected domain there does exists a critical size for which the solution will always quench for all sizes larger [10]. This was originally observed and proven in the one-dimensional case by Kawarada [13] for a particular $f(u)$, and then was extended to general source terms by Levine and Montgomery [15]. In higher dimensions, the results are not nearly as precise and finding estimates to the critical size that quenching persists for a particular shape is problematic. Fortunately, there are known theoretical estimates for rectangular domains [9]. Numerical approximations have been employed to extend and resolve these estimates further [2,17]. In this paper, stemming from the creation of lower and upper bound solutions to the singular problem, theoretical estimates of the critical quenching domain are established in Section 2 for arbitrary domains. This provides an avenue of creating novel estimates for arbitrary domains, in particular when the domain shape is convex and will be used to provide additional verification of the numerical algorithm in the experiments of Section 6.

This paper is also interested in the development and analysis of an adaptive splitting algorithm that can accurately be used to explore the singular problem posed over an elliptical domain. To date, numerical explorations have primarily focused on rectangular domains while circular and elliptical geometries may be more applicable to realistic applications. In addition, the analysis of Section 2 provides valuable estimates to the critical quenching domains and are used to further validate the numerical scheme in the experiments of Section 6. Moreover, the intricate numerical methodologies, such as splitting, adaptation, and nonuniform grids requires extensions to such geometric considerations. Indeed, after careful design, the numerical analysis shows that the numerical scheme is indeed reliable, accurate, monotonically increases toward a steady state or quenching, and is weakly stable.

The paper is organized as follows. In the following section theoretical estimates for quenching domains for piecewise smooth, connected domains are given. It is evident that these results can be extended to blow-up problems. In addition, as a corollary to the theorems, quenching time estimates can be established for arbitrary domain shapes and sizes. In Section 3 the study begins its focus on elliptical domains. The equations are then written in elliptical coordinates. Hence, the computation is designed over the rectangular grid generated by the coordinate transformation. Appropriate boundary conditions are then established. In Section 4 the adaptive, second order, splitting algorithm is given. The numerical analysis of the algorithm is in Section 5. In Section 6 numerous numerical experiments are offered, namely a statistical analysis of introduced errors, critical quenching domain calculations for elliptical domains of certain ratios of minor to major axes, and experimentally studying the effect of the mathematical degeneracy on the solution's fundamental characteristics. The paper is then concluded in Section 7.

2. Theoretical estimates of quenching domains

For singular, reaction–diffusion equations of the quenching type one of most interesting features is the existence of a critical quenching domain size for a particular domain shape. As one might expect, showing that this is indeed the case for arbitrary domains is a difficult task, especially in higher dimensions. Recently, in [10], it has been shown that for connected piecewise smooth domains there exists a critical quenching domain size. In realistic domain shapes, this novel result indicates this phenomena will persist, however, theoretical estimates of the critical size are lacking. Even so, reliable theoretical estimates have been established for rectangular domains. These estimates have been verified numerically in a number of resources [2,11,17].

The use of upper and lower solutions to differential equations has a long history in analysis of blow-up problems [1]. The fundamental idea can be traced back to [22]. Consider the solution $u(x,y,t)$ of (1) and (2).

Let $w(x,y,t)$ be a time-dependent lower bound of $u(x,y,t)$. Then if $w(x,y,t) \to 1$ in finite time T then the quenching singularity forms in $u(x,y,t)$ at a quenching time of $T^* \leqslant T$. Therefore, if one can establish a time-dependent lower bound of u that approaches a value of one in finite time then u will quench. Similarly, let $v(x,y,t)$ be a time-dependent upper bound of $u(x,y,t)$. Then if $v(x,y,t) < 1$ for all time then clearly $u(x,y,t)$ will not quench.

Definition 1. A lower solution of (1) and (2) is a function $v(x,y,t)$ that satisfies

$$\begin{aligned} &v_t \leqslant \Delta v + f(v), \quad (x,y) \in \Omega, t > 0, \\ &v \leqslant 0, \quad (x,y) \in \partial\Omega, \ t > 0, \\ &v \leqslant 0, \quad (x,y) \in \bar{\Omega}, \ t = 0. \end{aligned}$$