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Quenching Reaction-Diffusion Systems in Bioengineering and Life Sciences

Samiha Djemai[1], Salim Mesbahi[2*], Khaoula Imane Saffidine[3]
[1,2]Ferhat Abbas University, Faculty of Sciences, Department of Mathematics, LMFN Laboratory, Setif, Algeria
[3]Abdelhamid Mehri University, Faculty of New Information and Communication Technologies,Constantine, Algeria

ABSTRACT: This research paper revolves around investigating the phenomenon of quenching in reaction-diffusion systems and highlighting its significance. The primary focus is on analyzing a specific type of parabolic singular reaction-diffusion model that incorporates positive Dirichlet boundary conditions. The objective is to establish the sufficiency of certain conditions for quenching to occur within a finite time frame and to demonstrate the global existence of solutions. The novelty of this paper lies in the simplicity of the conditions imposed on the nonlinearity. This simplicity allows us to choose it from a wide range of possibilities, thus facilitating the application of the model to numerous singular reaction-diffusion phenomena. To bolster our findings, we will present various real-world applications in the fields of bioengineering and life sciences, showcasing the practical relevance of quenching phenomena. Finally, the paper ends with a conclusion and some potential future perspectives for further research in this area.

KEYWORDS: singular reaction-diffusion equation, quenching phenomenon, global existence, parabolic problem

I. INTRODUCTION

Quenching is a rapid cooling process that alters specific properties of materials by manipulating the cooling rate. The material is heated above the recrystallization temperature but below the melting point to allow grain restructuring, followed by controlled cooling to a predetermined temperature. The exploration of this significant phenomenon commenced in 1975 when Kawarada [12] published a paper that focused on a one-dimensional model. This publication served as an initial stepping stone for extensive investigations into the quenching problem conducted by numerous researchers across various scientific disciplines. The phenomenon of quenching is observed in many fields, such as metallurgy, biology, medicine, ecology, bioengineering, the manufacture of medical devices, instruments, and contact lenses, particularly in the context of polymerization processes. In this context, quenching refers to the rapid cooling or solidification of a material, typically a polymer, to halt or control a chemical reaction. We find sufficient information about this in Liščić et *al*. [14], Banasiak and Mokhtar-Kharroubi [1]. In the production of contact lenses, polymerization is a key step in forming the lens material. The polymerization reaction involves the conversion of monomers, small molecules with reactive groups, into a polymer network. This reaction is often initiated by heat or light, and it proceeds through a process known as reaction-diffusion. The monomers are dispersed in a liquid solution, and the polymerization reaction occurs as the monomers diffuse and react with each other. During the polymerization process, it is crucial to control the reaction to achieve the desired properties of the contact lens material, such as their mechanical strength, transparency, and water content. Quenching is employed as a means to stop the polymerization reaction at a specific stage. By rapidly cooling or solidifying the material, the diffusion of monomers and reaction products is effectively halted, preventing further polymerization. Quenching can be accomplished through various methods, such as immersion in a cooling bath or exposure to cold air or liquid nitrogen. The specific quenching technique used depends on the manufacturing process and the desired properties of the contact lenses. For some examples and additional details, see Barka et *al*. [2], Rouabah et *al*. [21].

Quenching in reaction-diffusion systems can manifest in different ways, depending on the specific characteristics of the system. In simultaneous quenching, the quenching of different components can occur simultaneously, meaning that the concentrations of all the substances involved in the reaction become zero at the same time. This type of quenching is often studied to understand the overall behavior of the system and the underlying mechanisms. Non-simultaneous quenching occurs when the concentrations of different substances in the system become zero at different times. This type of quenching can lead to more complex dynamics and is also the subject of research in reaction-diffusion systems. Different types of quenching rates can lead to different behaviors and can be studied to understand the system's dynamics. In many cases, the solution of a reaction-diffusion system quenches in finite time, meaning that the concentration of one or more substances becomes zero after a certain amount of time has passed. This type of quenching is often of interest in practical applications, as it can lead to the system reaching a steady state more quickly. Understanding these and other quenching species in reaction-diffusion systems is essential for studying their behavior and can have implications for various fields, such as engineering, chemistry, biology, ecology, and medicine. See Chan [4], Liščić et *al*. [14],

The spatial distribution of quenching, which refers to the location and extent of the regions where the concentration of one or more substances in a reaction-diffusion system becomes zero, can have various effects on the behavior of these systems. In some cases, it can lead to the formation of complex patterns, such as spots, stripes, or spirals. This is due to the interaction between the quenching regions and the diffusion of the substances involved in the reaction. The spatial distribution of quenching can also affect the stability of the system, as it can lead to the formation of unstable regions where the concentration of one or more substances becomes zero. Understanding the effect of quenching on stability is important for predicting the behavior of the system and for designing control strategies. See Cross and Greenside [6].

The phenomenon of quenching in bioengineering is the application of heat treatment quenching to biological or biomimetic materials. For example, quenching can be used to create bioactive glasses, which are materials capable of chemically bonding with living tissues. Bioactive glasses are obtained by melting a mixture of silicon, calcium, sodium, and phosphorus salts, and then rapidly cooling to prevent crystallization. Bioactive glasses can be used as implants, drug delivery agents, or tissue regeneration scaffolds. See Jones [11], Hench and Jones [8] and the references mentioned therein. Another example of quenching in bioengineering is the production of silk nanofibers. Silk is a natural protein produced by certain insects and spiders, which possesses exceptional mechanical properties. Silk can be dissolved in an aqueous solution, then stretched and rapidly cooled to form nanofibers. Silk nanofibers can be used as reinforcement materials, sensors, filters, or matrices for cell culture.

Therefore, quenching in bioengineering is a process that allows for the creation of innovative and high-performance materials, drawing inspiration from the principles of metallurgy. Quenching can modify the structure and properties of materials at the nanoscale or micrometer scale, depending on the temperature, cooling rate, and chemical composition parameters. In Kundu [13], we find a lot about this content.

Here are some phenomena that can be modeled using reaction-diffusion equations:

(i) Protein Folding and Unfolding: Quenching can refer to the rapid cooling or sudden change in environmental conditions that leads to the folding or unfolding of proteins. The process of protein folding involves the formation of a three-dimensional structure, while unfolding refers to the disruption of the native protein structure. Reaction-diffusion equations can be used to model the conformational changes and kinetics of protein folding and unfolding.

(ii) Cell Signaling and Receptor-Ligand Binding: Quenching can also describe the attenuation or termination of cell signaling pathways or the binding of ligands to receptors. In these cases, reaction-diffusion equations can be used to model the diffusion of signaling molecules or ligands, as well as their binding kinetics with receptors. The equations can capture the spatial and temporal dynamics of the signaling or binding process and provide insights into the quenching mechanisms.

(iii) Fluorescence Quenching in Biosensors: Quenching can occur in biosensors that rely on fluorescence-based detection. When a fluorescent molecule or fluorophore is in close proximity to a quencher molecule, the fluorescence emission can be attenuated. Reaction-diffusion equations can be employed to model the diffusion of the fluorescent and quencher molecules, as well as the quenching kinetics. This allows for the optimization of biosensor designs and the prediction of fluorescence quenching patterns.

It's important to note that these examples are just a few instances where reaction-diffusion equations can be applied to model quenching phenomena in bioengineering. The specific equations and parameters would depend on the particular system and the underlying mechanisms involved. We find many details, real models, and techniques used to study such problems in Barka et *al*. [2], Berestycki et *al*. [3], de Bonis [7], Ji et *al*. [10], Kawarada [12], Mesbahi [15,16], Murray [17,18], Pei and Li [19], Salin [22], Wang [24], Zhou et *al*. [26], Zhu et *al*. [27], as well as in the sources mentioned there.

In this paper, we will mathematically investigate a problem that aligns with the previously discussed concept of quenching. Our focus lies on examining a reaction-diffusion model that incorporates singular nonlinearity and positive Dirichlet boundary conditions:

$$\begin{cases} u_t - \Delta u = -f(x) & in\ (0,T)\times\Omega \\ u = 1 & on\ (0,T)\times\partial\Omega \\ u(0,x) = u_0(x) & in\ \Omega \end{cases} \quad (1)$$

with

$$\begin{cases} u_0 \in C^2(\Omega)\cap C^1(\overline{\Omega}) & \\ u_0 = 1 & on\ (0,T)\times\partial\Omega \\ 0 < u_0 \leq 1 & in\ \overline{\Omega} \\ \Delta u_0 - f(u_0) < 0 & in\ \Omega \end{cases} \quad (2)$$

where Ω is a smooth and bounded domain in $\mathbb{R}^N$ $(N \geq 2)$, and f is a positive function on $(0,1]$.

The remaining sections of this paper are structured as follows. In the subsequent section, we will showcase real-life applications of the investigated model in the fields of bioengineering and biology. Following that, in the third section, we will present our main result and demonstrate them in detail. The fourth section focuses on the numerical study conducted. Finally, the paper concludes with concluding remarks and perspectives.

II. REAL-LIFE APPLICATIONS

We can explore several examples of quenching phenomena that can be effectively modeled using reaction-diffusion equations. For more in-depth information and comprehensive details about these examples, we can refer to the works of Chenna et *al*. [5], Hussain et *al*. [9], Purich [20], Suckart et *al*. [23], Williams [25], Zhou et *al*. [26], and in the sources mentioned there.

(i) The extinguishing of a chemical flame: When a flame is quenched, it undergoes a rapid transition from a state of combustion to an extinguished state due to the removal of one or more essential components for sustaining the flame, such as fuel or oxygen. This quenching process can be described by a singular reaction-diffusion equation that models the chemical reactions and diffusion of species involved in the combustion process. The equation used to model flame quenching depends on the specific combustion chemistry and the reaction mechanism of the fuel being burned. However, a simplified example can be represented by the reaction-diffusion equation (1) with a single species, such as the fuel concentration (denoted as u), and a reaction term that accounts for the combustion reaction. In this case, $-f(u)$ is the reaction term that describes the combustion reaction. The specific form of $f(u)$ depends on the combustion chemistry and can involve nonlinear terms to capture the reaction kinetics. Modeling flame quenching using reaction-diffusion equations aids in understanding the dynamics of combustion processes, optimizing fire safety measures, and designing efficient fire suppression systems.

(ii) The diffusion-limited quenching of reactive oxygen species (ROS) by antioxidants: Reactive oxygen species, such as hydrogen peroxide H_2O_2 and superoxide radicals $O_2^{\bullet-}$, are highly reactive molecules that can cause oxidative damage to cells and tissues. Antioxidants are substances that can neutralize or scavenge these ROS, protecting cells from oxidative stress. The reaction-diffusion equation (1) can describe the diffusion of ROS and antioxidants and the quenching process. The quenching effect is modeled by a reaction term that becomes singular when the concentration of ROS is high and the concentration of antioxidants is low. In this case, $-f(u)$ dominates and leads to a decrease in the ROS concentration. This behavior represents the quenching of ROS by antioxidants, where the antioxidants act as scavengers to neutralize the reactive species.

(iii) The enzyme inhibition: Enzymes play a crucial role in biological processes by catalyzing chemical reactions. However, enzymes can be inhibited by various factors, such as inhibitors or regulatory molecules, leading to a decrease in their activity. The reaction-diffusion equation (1) can be used to model the spatial distribution of the enzyme concentration and the inhibitor concentration, as well as the quenching effect due to enzyme inhibition. The quenching effect is modeled by a reaction term that becomes singular when the concentration of the inhibitor is high. In this case, the reaction term $-f(u)$ dominates and leads to a decrease in the enzyme activity. This behavior represents the quenching of enzyme activity due to inhibition.

(iv) The quenching in fluorescence resonance energy transfer (FRET) assays: FRET is a widely used technique to study molecular interactions and proximity in biological systems. It relies on the transfer of energy between a donor fluorophore and an acceptor fluorophore, which are typically attached to biomolecules of interest. However, the fluorescence signal can be quenched when the donor and acceptor fluorophores come into close proximity or interact with each other. The reaction-diffusion equation (1) can describe the diffusion of the donor and acceptor fluorophores and the quenching process in FRET assays. The quenching effect is modeled by a reaction term that becomes singular when the concentration of the acceptor fluorophore is high. In this case, term $-f(u)$ dominates and leads to a decrease in the fluorescence signal of the donor fluorophore. This behavior represents the quenching of fluorescence in FRET assays, where the proximity or interaction between the donor and acceptor fluorophores results in energy transfer and a reduction in the donor fluorescence intensity.

(v) The diffusion-limited quenching of free radicals by antioxidants: Free radicals, such as reactive oxygen species (ROS), are highly reactive molecules that can cause damage to cellular components and contribute to various diseases. Antioxidants are molecules that can neutralize free radicals by donating an electron, thereby reducing their reactivity and preventing cellular damage. The reaction-diffusion equation (1) can describe the diffusion of free radicals and antioxidants and the quenching process. When the concentration of free radicals is sufficiently high and the concentration of antioxidants is low, the reaction term $-f(u)$ dominates and leads to a decrease in the concentration of free radicals. This behavior represents the quenching of free radicals by antioxidants, where the antioxidants act as scavengers to neutralize the reactive species and reduce their harmful effects.

III. STATEMENT OF MAIN RESULTS

The finite-time quenching phenomenon is caused by singular nonlinearity in the absorption term of (1). Therefore, we present the concept of a quenched solution to our problem.

A. Assumptions

Definition: A solution u of problem $(1)-(2)$ is said to be quenche if u exists in the classical sense and is positive on $[0,T)$, and also satisfies $\inf_{t\to T} \min_{x\in[0,1]} u(t,x) = 0$. In this case, T is called quenching time.

To study problem $(1)-(2)$, we also assume that the positive function $f:(0,1] \to (0,+\infty)$ satisfies the following two hypotheses (H_1) and (H_2):

(H_1) f is a strictly decreasing and locally Lipschitzian function on $(0,1]$.
(H_2) $\lim_{s\to 0^+} f(s) = +\infty$.

To make our findings more easily understandable, we denote by ϕ the first eigenfunction associated with the first eigenvalue λ_1 of the problem:

$$\begin{cases} \Delta\phi + \lambda\phi = 0 & in\ \Omega \\ \phi = 0 & on\ \partial\Omega \end{cases}$$

normalized by $\int_\Omega \phi(x)dx = 1$, with $\phi(x) > 0\ in\ \Omega$.

B. The main results

An adequate condition for finite-time quenching is provided by the following theorem.

Theorem 1: Under hypotheses $(H_1)-(H_2)$, the solution of problem $(1)-(2)$ quenches in finite time for any initial data provided that λ_1 is small enough.

Proof. Let u be the solution of problem $(1)-(2)$ with the maximal existence time T. By the maximum principle, we have $0 \le u \le 1$ in $(0,T)\times\Omega$. Let

$$\xi(t) = \int_\Omega (1-u)\phi(x)dx\ , t \in [0,T) \qquad (3)$$

By Assumptions $(H_1)-(H_2)$ and the corresponding Taylor expansions, we get easily

$$f(u) \ge \delta(1-u) + \beta \qquad (4)$$

where δ and β are positive constants. By a straight-forward computation and (4), we obtain

$$\begin{aligned} \frac{d\xi}{dt} &= -\int_\Omega u_t.\phi(x)dx \\ &= -\int_\Omega \Delta u.\phi(x)dx + \int_\Omega f(u)\phi(x)dx \\ &= \int_\Omega \Delta(1-u).\phi(x)dx + \int_\Omega f(u)\phi(x)dx \\ &\ge -\lambda_1\int_\Omega (1-u)\phi(x)dx + \delta\int_\Omega (1-u)\phi(x)dx \\ &\quad + \beta\int_\Omega \phi(x)dx \\ &= (\delta-\lambda_1)\xi(t) + \beta \end{aligned}$$

Since $0 \le u \le 1$ then $0 \le 1-u \le 1\ in\ (0,T)\times\Omega$. This is confirmed by (3) that $0 \le \xi(t) \le 1$. Since λ_1 is small enough, it is obvious that $(\delta-\lambda_1)\xi(t)+\beta > 0$. This gives us

$$\frac{d\xi}{(\delta-\lambda_1)\xi(t)+\beta} \ge dt\ , t \in [0,T)$$

which gives, by integration from 0 to T,

$$T \le \begin{cases} \frac{1}{\delta-\lambda_1} log\left(\frac{(\delta-\lambda_1)\xi(T)+\beta}{(\delta-\lambda_1)\xi(0)+\beta}\right) & if\ \delta \ne \lambda_1 \\ \frac{1}{\beta}(\xi(t)-\xi(0)) & if\ \delta = \lambda_1 \end{cases} \qquad (5)$$

Now, letting $t \to T^-$ in (5) and combining $\lim_{t\to T^-} \xi(t) \le 1$, we obtain

$$T \le \begin{cases} \frac{1}{\delta-\lambda_1} log\left(\frac{\delta-\lambda_1)+\beta}{(\delta-\lambda_1)\xi(0)+\beta}\right) & if\ \delta \ne \lambda_1 \\ \frac{1}{\beta}(1-\xi(0)) & if\ \delta = \lambda_1 \end{cases} \qquad (6)$$

The positivity of the right-hand side of (6), which illustrates the finite time quenching of the solutions of problem $(1)-(2)$ can be readily reached since $1 \le \xi(t) \le 1$. This is what is required.

Remark: Many quenching studies confirm that time-derivatives blow-up while the solution itself remains bounded. We refer, for example, to Chan [4] and Kawarada [12].

The global existence of solutions can be described by the following theorem.

Theorem 2: If the diameter of Ω is small enough and the initial data satisfies $0 < \varepsilon \le u_0 \le 1\ in\ \Omega$, then under hypotheses $(H_1)-(H_2)$, the solution of problem $(1)-(2)$ does not quench in finite time. In this case, we say that the solution u exists globally.

Proof. Consider the auxiliary problem:

$$\begin{cases} \bar{u}_t = \Delta\bar{u} - f(\bar{u}) & in\ (0,T)\times\Omega \\ \bar{u} = 1 & on\ (0,T)\times\partial\Omega \\ \bar{u}(0,x) = 1 & in\ \bar{\Omega} \end{cases}$$

According to the comparison principle, we have $u \le \bar{u}$.
Now, we consider the following problem:

$$\begin{cases} \Delta\bar{u}^* = f(1) & in\ B_\rho \\ \bar{u}^* = 1 & on\ \partial B_\rho \end{cases}$$

with

$$B_\rho = \{x \in \mathbb{R}^N : |x| < \rho\}\ and\ \rho \ge \left(\frac{2N}{f(1)}\right)^{\frac{1}{2}}$$

By Green's function, the solution is $\bar{u}^*$ denoted as follows:

$$\bar{u}^* = \frac{f(1)(|x|^2-\rho^2)}{2N} + 1$$

and

$$\min \bar{u}^* = \frac{-f(1)\rho^2}{2N} + 1$$

Clearly, $\bar{u}^*$ is a super solution of $(1)-(2)$. The solution u of $(1)-(2)$ is global only if $\bar{u}^* > 0$.

IV. CONCLUSION AND PERSPECTIVES

(i) This research work focuses on understanding and studying quenching phenomena, which involve rapid changes in temperature or physical conditions and can lead to complex phenomena in different systems. The study contributes to a deeper understanding of the mathematical principles underlying quenching processes, advancing research in this area.

(ii) The results obtained in this study have wider implications beyond quenching phenomena alone. They can be applied to the study of other singular reaction-diffusion phenomena. This opens up new avenues for investigating and understanding various physical and chemical processes where similar mathematical principles may be at play.

(iii) The study's findings and insights provide a foundation for further theoretical and numerical investigations under different conditions. This deeper dive into the problem aims to achieve additional progress in the field and expand our knowledge. This deeper dive into the problem aims to push the boundaries of current understanding and potentially uncover new phenomena or mechanisms.

(iv) The primary goal of the research is to contribute to the advancement of quenching technology and modeling in diverse scientific disciplines. Quenching phenomena have practical implications in fields such as bioengineering, biology, and many others. By deepening the understanding of quenching through mathematical research, the study can potentially lead to improved techniques, methodologies, and models that benefit these scientific fields. The advancements may enable better control and optimization of quenching processes, which can have practical applications in various industries.

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