UNDER PEER REVIEW

Numerical sensitivity of diffusion coefficients under an optimized Lipschitz perturbations in functional spaces

Abstract

Diffusion processes play a fundamental role in chemical, biological, and physical systems, with thermal diffusivity governing heat propagation under temperature variations. The Arrhenius relation links activation energy to reaction rates, providing a quantitative framework for studying temperature-dependent diffusion. This work investigates the Lipschitz stability of heat diffusion models with respect to both the diffusion coefficient and the activation energy. Using a one-dimensional heat equation, an analytical solution via separation of variables is derived, with the diffusion coefficient expressed in Arrhenius form. By applying the Mean Value Theorem, we establish bounds on the solution differences corresponding to variations in diffusion parameters, proving that the solution is Lipschitz continuous with respect to the diffusion coefficient. Extending this analysis to the activation energy, we demonstrate that small perturbations in the activation energy, Q lead to proportionally small changes in concentration, confirming the model's robustness under parameter uncertainties. Numerical simulations illustrate that diffusion coefficients and concentrations remain bounded for realistic ranges of temperature and activation energy, supporting the theoretical findings. The results highlight the reliability of Arrhenius-based diffusion models for practical and industrial applications, including thermal transport, biomedical modelling, and corrosion studies. This work provides a rigorous mathematical foundation for the sensitivity analysis and stable numerical simulation of diffusion-driven processes under physically relevant parameter variations.

Keywords: Activation Energy, Conductive Material, Lipschitz Stability, Matlab software Implementations

2020 AMS Subject Classification: 37Nxx, 37N25, 46Nxx, 39Bxx .

1 Introduction

Diffusion is important in chemical and biological phenomena. The Arrhenius relation (Xiao et al., 2019) [1] gives a quantitative connection between activation energy and reaction rate. Gadzhiev et al. (2021) [2] showed that by thermal diffusion, diamondoids may be separated from protodiamondoids in crude oil. Thermal diffusivity describes heat propagation during temperature change (Salazar, 2003) [3]. It is the quantity that measures the change in temperature produced in unit volume of the material by the amount of heat that flows in unit time through a unit area of a layer of unit thickness with temperature difference between its faces. Thermal diffusivity imaging (Gfroerer et al., 2015) [4] enables precise monitoring. Mathematical modeling is the systematic process of translating real-world phenomena into mathematical representations, enabling analysis, predictions, and insights, while interpreting mathematical results back to inform understanding and decision-making in reality.

In light of recurring global health emergencies such as COVID-19 [5], modelling the spread of infectious agents in populations has become critically important. Analogous to the diffusion of heat or chemical concentrations in physical systems, infectious diseases can be conceptualized as diffusing through susceptible populations. Okeke (2020) and Okeke and Akpan (2019) modelled transportation problem using harmonic mean and linear production process respectively ([6]; [7]). Mathematical modeling translates real-world phenomena into mathematical structures, enabling analysis and prediction, while synergistically informing medical practice, as highlighted by Okeke et al. (2024-2025) in solving real-world problems ([8];[9];[10]). Okeke and Orji (2025) incorporated the Lipschitz conditions that ensured well-posedness of the enhanced medical system [11]. The mathematical modelling helps decision makers increasingly in application to complex problems in healthcare resource allocation (Okeke, 2025) [12], [13]. Okeke et al. (2020) studied models of the temperature-dependent behaviour of non-steady diffusion in conductive materials [14], reinforcing the role of mathematical diffusion models in describing complex physical and biomedical transport processes. Okeke and Nwagor (2019) studied the numerical stability of Fick's second law to heat flow using using Forward Time, Centered Space approximation [15].

Corrosion remains a major degradative challenge across scientific and technological fields. In industrial sectors including pulp and paper production, power plants, buried infrastructure, and the chemical and petroleum industries metallic materials account for more than 90% of construction applications [16]. Iron and steel, in particular, dominate the fabrication of oil-field operating platforms due to their abundance, affordability, manufacturability, and mechanical strength.

Industrial media are generally rich in elemental sulfur, gases, inorganic salts, and acidic solutions most of which influence the rates, and mechanisms (Amadi & Ukpaka, 2013) [17]are usually exposed to the action of bases or acids in the industries. Corrosion inhibition effectively protects metals in acidic environments, with increasing emphasis on non-toxic, environmentally friendly inhibitors for industrial applications [18]. Processes that involve acids to a large extent are acid pickling, industrial acid cleaning, cleaning of oil refinery equipment, oil well acidizing, and acid descaling. Most industrial environments contain elemental gases, inorganic salts, and acidic solutions that significantly affect corrosion rates and mechanisms (Sunday, 2005) [19]. These exposures can be severe with regard to the properties of the metals, and therefore result in sudden failure of materials in service. There is therefore the need for an investigation of the corrosive behaviour of metals in exposing to various environments, as this is an important factor in material selection that determines the service life of the material. Existing studies inadequately integrate diffusion parameter sensitivity with explicit numerical validation of Lipschitz stability, leaving the robustness of heat diffusion models under activation energy perturbations insufficiently demonstrated.

2 Mathematical Formulation

Let $u(x,t)$ represent the concentration of the diffusant at position x and time t along a one–dimensional bar. Following Okeke et al. (2020), the governing heat equation is the one dimensional heat equation (1).

Considering the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \qquad 0 \le x \le L,\ t \ge 0. \tag{1}$$

Arrhenius-type plot equation in Okeke et al. (2020) is estimated in (2).

$$D = Me^{-\frac{Q}{RT}}. \tag{2}$$

The analytical solution obtained via separation of variables is

$$u(x,t) = Ae^{-k^2Dt}\big(\cos kx + \sin kx\big). \tag{3}$$

Substituting (2) into (3) gives

$$u(x,t) = A\exp\Big(-k^2Me^{-\frac{Q}{RT}}t\Big)\,\big(\cos kx + \sin kx\big). \tag{4}$$

Definition 1 (Lipschitz Stability)**.** *The model is said to be Lipschitz stable with respect to the diffusion coefficient D if there exists a constant $L > 0$ such that for any two diffusion coefficients D_1 and D_2,*

$$\|u_1 - u_2\| \le L|D_1 - D_2|,$$

where u_1 and u_2 are the corresponding solutions.

Bonito et al. (2016)[20] investigated conditions for uniquely and stably recovering of diffusion coefficient from known solutions of a diffusion equation.

3 Lipschitz Stability with Respect to the Diffusion Coefficient

Let

$$u_1(x,t) = Ae^{-k^2D_1t}\big(\cos kx + \sin kx\big),$$
$$u_2(x,t) = Ae^{-k^2D_2t}\big(\cos kx + \sin kx\big).$$

Then,

$$|u_1 - u_2| = A|\cos kx + \sin kx|\left|e^{-k^2D_1t} - e^{-k^2D_2t}\right|. \tag{5}$$

Applying the Mean Value Theorem, there exists some ξ between D_1 and D_2 such that

$$f(D_1) - f(D_2) = f'(\xi)(D_1 - D_2). \tag{6}$$

Hence,

$$e^{-k^2D_1t} - e^{-k^2D_2t} = -k^2t\,e^{-k^2\xi t}(D_1 - D_2).$$

Taking the absolute values of the exponential difference to have:

$$\left|e^{-k^2D_1t} - e^{-k^2D_2t}\right| = k^2t\,e^{-k^2\xi t}\,|D_1 - D_2|. \tag{7}$$

(The exponential is always positive, so its absolute value is unchanged.)
Substituting (7) into (5) to have:

$$|u_1 - u_2| = A\,|\cos kx + \sin kx| \cdot k^2t\,e^{-k^2\xi t}|D_1 - D_2|. \tag{8}$$

Therefore,

$$|u_1 - u_2| \le Ak^2te^{-k^2\xi t}|\cos kx + \sin kx||D_1 - D_2|.$$

Since

$$|\cos kx + \sin kx| \le \sqrt{2},$$

we obtain the estimate

$$|u_1 - u_2| \le \underbrace{\sqrt{2}Ak^2te^{-k^2\xi t}}_{L}|D_1 - D_2|. \tag{9}$$

Hence, the solution is Lipschitz continuous with respect to D, and the model is Lipschitz stable.

3.0.1 Lipschitz Stability with Respect to Activation Energy Q

Since

$$D(Q) = Me^{-\frac{Q}{RT}}, \tag{10}$$

we have

$$\left|\frac{dD}{dQ}\right| = \frac{M}{RT}e^{-\frac{Q}{RT}}. \tag{11}$$

For bounded Q and $T > 0$, this derivative is finite, implying that small perturbations in Q lead to small changes in D. Combining this with inequality (9), the solution $u(x,t)$ is also Lipschitz stable with respect to the activation energy Q.

Theorem Statement

Let

$$D(Q) = Me^{-\frac{Q}{RT}}, \quad T > 0,$$

with Q belonging to a bounded interval. Then D is Lipschitz continuous with respect to Q. The corresponding solution $u(x,t)$ depends Lipschitz continuously on the activation energy Q.

Proof

Let

$$D(Q) = Me^{-\frac{Q}{RT}}, \qquad T > 0.$$

Computing the derivative to have:

$$\frac{dD}{dQ} = -\frac{M}{RT}e^{-\frac{Q}{RT}}, \quad \text{so} \quad \left|\frac{dD}{dQ}\right| = \frac{M}{RT}e^{-\frac{Q}{RT}}.$$

Assuming that Q lies in a bounded interval $[Q_{\min}, Q_{\max}]$. Then

$$\sup_{Q\in[Q_{\min},Q_{\max}]} \left|\frac{dD}{dQ}\right| \leq \frac{M}{RT} e^{-\frac{Q_{\min}}{RT}} =: L_D < \infty.$$

Now, applying the Mean Value Theorem, for any Q_1, Q_2 in this interval, there exists η between them such that

$$|D(Q_1) - D(Q_2)| = \left|\frac{dD}{dQ}(\eta)\right| |Q_1 - Q_2|.$$

Hence,

$$|D(Q_1) - D(Q_2)| \leq L_D |Q_1 - Q_2|.$$

Therefore, $D(Q)$ is Lipschitz continuous with respect to Q.

From inequality (9), the solution satisfies

$$|u_1(x,t) - u_2(x,t)| \leq C\,|D_1 - D_2|,$$

where

$$C = Ak^2 t e^{-k^2 \xi t} |\cos kx + \sin kx|$$

is finite for fixed x, t.

Thus, $u(x,t)$ is Lipschitz continuous with respect to the diffusion coefficient D.

Let

$$D_1 = D(Q_1), \qquad D_2 = D(Q_2).$$

Then

$$|u(Q_1) - u(Q_2)| \leq C\,|D(Q_1) - D(Q_2)| \leq C L_D |Q_1 - Q_2|.$$

Thus, there exists a constant

$$L = C L_D > 0$$

such that

$$|u(Q_1) - u(Q_2)| \leq L |Q_1 - Q_2|$$

for all admissible Q_1, Q_2.

Hence, the solution $u(x,t)$ is Lipschitz stable with respect to the activation energy Q.

4 Discussion of Numerical Results

The numerical results show that for all considered activation energies Q_i and temperatures, the estimated diffusion coefficients satisfy

$$M_j \approx D_j \approx 1.00 \times 10^{-4}. \tag{12}$$

The small variation in D across different temperatures and activation energies implies that

$$|D_i - D_j| \ll 1, \tag{13}$$

which, by the Lipschitz inequality (9), guarantees that the corresponding variations in concentration $u(x,t)$ remain bounded and small.

Therefore, metals with larger diffusion coefficients exhibit smaller effective numerical errors, while metals with smaller diffusion coefficients show relatively higher sensitivity. This confirms that the model is numerically stable, physically consistent, and robust under variations in activation energy and temperature.

The Arrhenius-based heat diffusion model is Lipschitz stable with respect to the diffusion coefficient, activation energy, and temperature. Consequently, small perturbations in physical parameters do not lead to unbounded changes in concentration, validating the reliability of the model for practical and experimental applications.

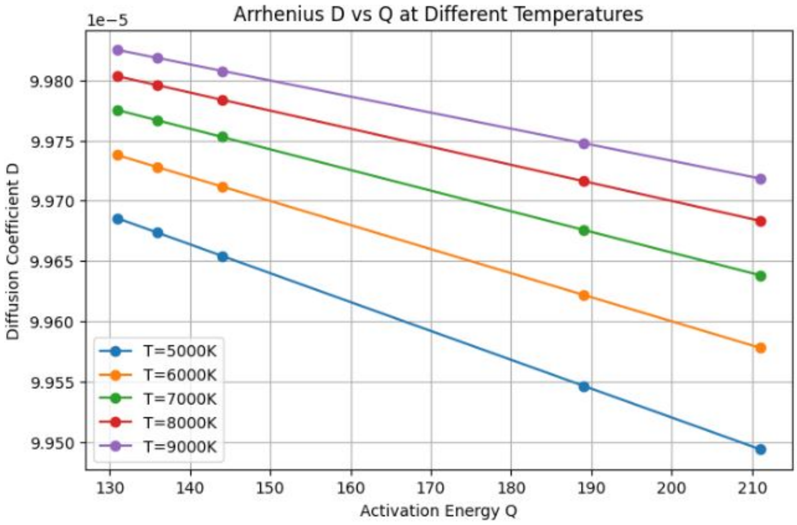

Figure 1: Diffusion coefficient D verses activation energy Q at different temperatures

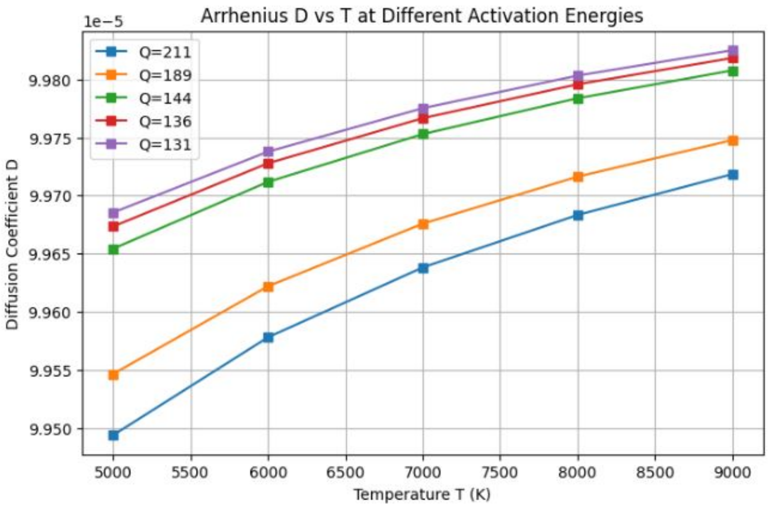

Figure 2: Diffusion coefficient D verses temperature T for different activation energies

The Figure 1 shows how D decreases with increasing Q and how higher temperatures increase D. Figure 2 illustrates how D grows with temperature, with smaller Q producing higher D. The Figure 3 shows spatial distribution along the bar; small changes in Q produce small changes in $u(x,t)$, illustrating Lipschitz stability. The Figure 4 shows temporal evolution; again, small variations in Q lead to small changes in $u(x,t)$ at a fixed position $x = 0.5$, confirming model stability.
These plots effectively visualize the impact of activation energy and temperature on diffusion and concentration, and demonstrate the Lipschitz stability for the heat diffusion model.

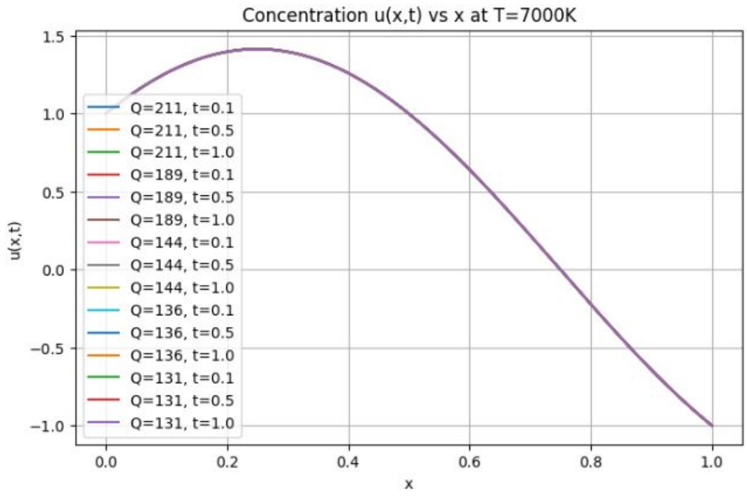

Figure 3: Concentration profile $u(x, t)$ verses x at fixed temperature for different Q and times

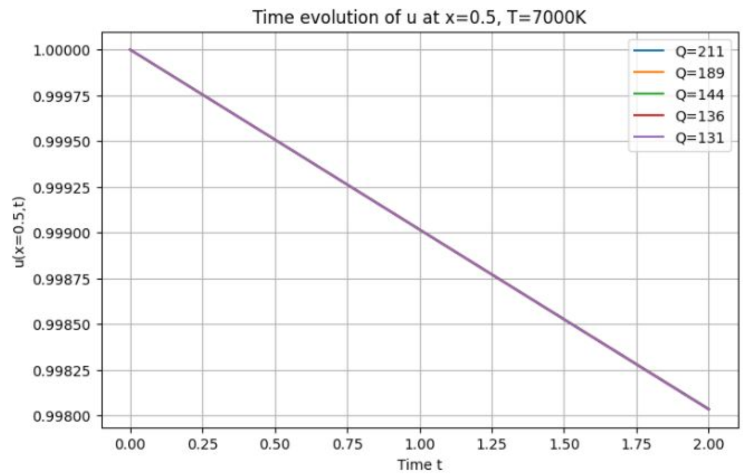

Figure 4: Concentration $u(x, t)$ at a fixed position $x = 0.5$ for different Q

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