APPLICATION OF BOUNDARY VALUE PROBLEM IN THERMODYNAMICS & KINETICS

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Abstract

Boundary value problems (BVP) are a robust mathematical framework that describes and solves challenging physical phenomena in various scientific areas. BVPs are critical in understanding and modeling a wide range of phenomena in thermodynamics and kinetics, from heat transfer and phase transitions to chemical reactions and reaction rates. In the context of BVP in thermodynamics and kinetics, we introduce a mathematical framework to describe thermodynamic processes occurring in deformable systems. This framework includes the influence of dissipative effects on the development of near-surface phenomena. Expressions describing the local state (LS) and the description of dissipative processes (DP) can be derived by integrating kinetic energy and applying thermodynamic principles. Furthermore, utilizing the variational approach, we can builds a function, when minimized, that provides those connections relating to the LS, the description and the application of natural boundary conditions. We explain the requisite conditions for the convexity of this function.

Keywords: ***Thermodynamics, Kinetics, Boundary value problem (BVP), Local and Variational Formulation***

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1. Introduction

The BVP demonstrates the enormous potential of mathematics in explaining complex physical phenomena and improves our understanding of scientific concepts. These mathematical problems have evolved into indispensable tools, equipping scientists and engineers to address many problems associated with energy transfer, phase transitions, chemical reactions and the evolution of systems with time [1]. These mathematical problems were initially presented as problems in the field of mathematics. Our understanding of the physical universe is supported by the investigation of thermodynamics, a critical component of physics and engineering [2]. The scientific analysis of thermodynamics aims to understand the complex movement of energy and the behavior of matter. The mathematical theory of thermodynamics is an encompassing field of research that goes into the fundamental complexities of heat, temperature and the spatial distribution of thermal energy in various materials and systems. The concepts of heat conduction are essential to the investigation of thermodynamics. This concept is crucial to an extensive range of natural processes, which play a central role in thermodynamics [3].

Heat conduction involves the movement of thermal energy through matter, which is an essential part of thermodynamic studies. The ability to describe and anticipate the direction of thermal energy is the most significant importance since it serves as the basis for much work done in the scientific and technological fields [4]. BVP In thermodynamics, issues are potent tools that help researchers and engineers understand and discover solutions to complex heat conduction challenges. These types of problems involve the use of materials that possess a variety of different properties as well as complex geometries, making it necessary to employ a robust mathematical framework that can adjust these complexities [5].

By defining exact boundary conditions at interfaces and the materials themselves, BVPs make it possible to create mathematical models that can simulate and forecast temperature distributions and heat transport mechanisms. This capacity is essential in a variety of engineering disciplines, including the design of efficient thermal management systems, the optimization of the performance of electronic equipment and the development of the efficiency of energy generation and storage [6].The investigation of the velocity at which chemical reactions occur and the mechanisms that are responsible for their regulation comes under the scope of chemical kinetics, a field of thermodynamics. It provides fundamental insights into how reactants transform into products and whether the precise conditions of a reaction influence the general course of a chemical process. Chemical reactions within the area of kinetics prove to be subtle and multifaceted, demanding the involvement of BVPs to navigate these difficulties [7].

BVP is an effective tool for illustrating complicated reaction kinetics within the context of chemical kinetics, where it is considered as a subfield. An infinite number of rate-determining steps, intermediate products and branching paths might be found in chemical reactions ranging from the most fundamental to the most complicated and multi-step processes. These complexities challenge chemists and engineers as they work toward their objective of understanding and controlling reactions for various applications, such as the synthesis of novel chemicals, the creation of pharmaceuticals and the cleanup of polluted environments [8].The significance of BVP in resolving complex thermodynamic and kinetic challenges becomes transparent as technology develops and research in these fields advances.

This paper organizes our discussion into the following sections: Section 2 presents an overview of related works. Section 3 delves into the application of BVP. Section 4 is dedicated to conclusions, summarizing the key insights derived from our study.

2. Related works

The mathematical investigations of the study [9] were related to linear issues of equilibrium dynamics and vibrations of elastic bodies subjected to surface stresses. They extended their previous research on BVP using the Gurtin-Murdoch model.The paper [10] focused on analyzing a mixed initial boundary problem in the context of dipolar thermo-elasticity. The fundamental equations and limitations of the issue were established and the particularity of the results was demonstrated. Those results were achieved without placing any requirements on the elastic coefficients regarding definiteness and without requiring the heat conductivity tensor to be positive, as usually happened.Research [11] investigated local and non-local BVP related to hyperbolic equations of a general form characterized by changing coefficients and featuring a "Caputo fractional derivative."

Article [12] focused on developing global solutions without a vacuum that exhibited significant amplitude for the initial boundary value issues associated with the “one-dimensional compressible Navier-Stokes” equations. Those equations involved degenerate transport coefficients.A study [13] demonstrated that the equations of motion, boundary conditions and constitutive equations defining the behavior of polarized time-dependent thermo-elastic materials were obtained from two fundamental laws of thermodynamics.The equilibrium equation and the associated natural boundary conditions were obtained again via the "Lagrange variational" principle, which had been revised to include the coupled linear strain gradient continua [14].

Research [15] proposed two techniques, the "Embedded Perturbed Chebyshev Integral Collocation Method and the Embedded Perturbed Bernstein Integral Collocation Method," as practical computational approaches to solve nonlinear BVP of high order.The paper [16] focused on the computerized calculation of a high-temperature plasma's thermodynamic properties with a density similar to a solid object. The Thomas-Fermi model served as the foundation for the analysis, the framework contained quantum exchange corrections while considering the impact of an external magnetic field. They developed a numerical solution that was both straightforward and efficient for solving the given BVP.The study [17] analyzed the time differential three-phase-lag thermal transfer model, identifying the constraints necessary for its thermodynamic consistency. They demonstrated the continuous dependence of the solutions on the initial data and the supply term for the BVP that corresponded to the initial data.

Paper [18] presented a mathematical simulation of a reduced internal combustion engine. Superficial relationships were derived for confined motions that contributed to understandthe engine kinematics and its geometry. The equation governing the action of the piston could be characterized as a singular BVP. They simulated an engine working while subjected to constant torque and poly-tropic expansions, which revealed high-frequency piston vibration when certain circumstances were met.Research [19] provided a mathematical model incorporating fractional differential equations to describe the dynamics of domain structure in ferroelectric materials. The mathematical model, derived from the "Landau-Ginzburg-Devonshire-Khalatnikov approach," was formulated as an initial BVP for "a semi-linear time-fractional differential equation." The study [20] examined a BVP for a continuous equation that served as a representation of grain boundary motion. Theirequation included the "microscopic mechanisms of line defects" and considered the influence of several thermodynamic driving forces.

3. Application of BVP

Across the range of engineering specialties, BVP is popular. BVPs provide unparalleled analysis across disciplines, from electronics and control engineering to kinetics as well as thermodynamics. Their wide range of uses stems from their remarkable precision in simulating various physical events and engineering concepts. BVP can be addressed in two typical ways: the local formulation and the variational formulation.

3.1 Local Formulation

Consider the interaction between a thermo-elastic body $\ell_*$and its surrounding atmosphereℓ_*^+. The reference thermodynamic state of the body, denoted as (s), is defined as its natural homogeneous condition. This stage is characterized by various properties presented in Table 1.

Table 1: Properties and its variables

Property	Absolute Temperature	Entropy Density	Chemical Potential	Mass Density	Pressure	Specific Volume
Variables	$S_{(0)}$	$T_{(0)}$	$\mu_{(0)}$	$\rho_{(0)}$	$O_{(0)}$	$U_{(0)} = \rho_{(0)}^{-1}$

The occurrence of "near-surface phenomena" within the $\ell_* \cup \ell_*^+$ system in time $s_1 < s \leq s_2 (s_1 > s_2)$ is a result of the interaction with the thermoelastic body ℓ_* and its surrounding atmosphere ℓ_*^+as the body ℓ_* transitions from its original natural (homogeneous) state to a "gradient-type stationary state".

3.1.1 Kinetic Energy Balance

The energy of the body ℓ_* is considered a fundamental indicator of its thermostressed conditionfor $s > s_0$.

$\varepsilon(\ell_*.s) = \varepsilon[W_*(s) \cup \partial W_*(s)],$ (1)

The space region covered by the "thermo-elastic body"ℓ_* is denoted as $W_*(s) \cup \partial W_*(s)$ at the specific time $s \in (s_1, s_2)$. The energy of system $\varepsilon(\ell_*, s)$ can be described as a "positive-definite cumulative measure" of its state. The description of the term variable is displayed in Table 2.

$c\varepsilon(\ell_* \;\; , s) = \delta R_*{}^{(+)} + \delta B_*^{(+)}$ (2)

Table 2: Description

Term	Description
$\varepsilon(\ell_*, s)$	Energy linear part
$\delta R_*^{(+)}$	Thermal interaction between thermo-elastic body $\ell_*$and its environment
$\delta B_*^{(+)}$	Mechanical interaction between bodyℓ_* and its environment ℓ_*^+

$c\varepsilon(\ell\,, s) = \delta R_*{}^{(+)} + \delta B_*^{(+)}$ (3)

Linear components $\delta R^{(+)}$ and $\delta B^{(+)}$ represent the energy gain of the system ℓ due to interactions with the environment$\ell^+ = \ell_*^+ \cup \ell_* \backslash \ell$. Component $\delta R^{(+)}$ describes heat. On the other hand, component $\delta B^{(+)}$illustrates the increase in kinetic energy resulting from mass transfer.

$c\varepsilon(\delta\ell, s) = c[F(q, s)\delta U]$ (4)

Consider q represents the radius vector of a specific location occupied by an arbitrary material point, denoted as $l \in \ell_*$, at a given moment, referred to as s. let$F(q, s)$represent the energy associated with a physically tiny subsystem, denoted as $\delta\ell$, divided by the volume of this subsystem, referred to as $\delta U(q, s)$, at a particular moment in time, represented as$s$.

$c\varepsilon(\delta\ell, s) = cF_0 \delta U_0$ (5)

$cF_0 = D_U dS + D_U^* d\mu + \hat{\sigma} \ldots . c(\nabla_0 \otimes q)^{\intercal} + (\nabla_0 . \hat{\sigma} + e^+). dv$ (6)

The variables and their corresponding descriptions are presented in Table 3. The scalar is indicated by a "dot between numbers, the tensor (dyadic) product" is designated in$\otimes$ and the tensor operation $\nabla_0 \otimes q$"transposition" is expressed in $\intercal$.

Table 3: Description of variables

Variables	Description
$F_0 = F_0(q_0, s)$	The density subsystem is at a small physical size.
$D_U = D_U(q_0, s)$	Specific heat density
$D_U^* = D_U^*(q_0, s)$	Density of mass kinetic energy subsystem content
$S = S(q_0, s)$	Absolute temperature
$\mu = \mu(q_0, s)$	Chemical potential
$\hat{\sigma} = \hat{\sigma}(q_0, s)$	Tensor of the stress of the Piola-Kirchhoff type

$e^+ = e^+(q_0, s)$	Bulk-force density Vector
$\nabla_0 \otimes q$	Site gradient Tensor
$v = q - q_0$	Displacement vector

3.1.2 Thermodynamic State Equations

$\rho = \rho_{(0)}(1-f),\ o = o\left(\frac{1}{\rho_0(1-f)}\right),\ \sigma = 3Lf,$ (7)

Where L represents the dilatation modulus,

The differential representing the kinetic energy in the "linear approximation"can exhibit the following equation,

$dE = \frac{1}{3}\sigma^* df \ + \ \hat{\sigma}_0^c \,..\, d\hat{f}^c + \left(\mu - \mu_{(0)}\right)d(-\nabla_0 \,.\, \Pi_M),$ (8)

Where,

$\frac{1}{3}\sigma^* = \ -\frac{o_{(0)}}{\rho_{(0)}} + L_* f,\ L_* = L - \frac{2o_{(0)}}{\rho_{(0)}} - \frac{1}{\rho_{(0)}^2}\frac{\partial o}{\partial(1\rho)}\Big|_{\left(\frac{1}{\rho_{(0)}}\right)}$ (9)

If the function of state $E = E\left(f, \hat{f}^c, -\nabla_0 . \Pi_N\right)$ is provided, we can express the following system of determining connections based on the differential (12).

$\sigma^* 3\frac{\partial E}{\partial f} = \sigma^*(A),\ \hat{\sigma}_0^c = \frac{\partial E}{\partial \hat{f}^c} = \hat{\sigma}_0^c(A),\ \mu - \mu_{(0)} = \frac{\partial E}{\partial(-\nabla_0 . \Pi_N)} = \left(\mu - \mu_{(0)}\right)(A)$ (10)

To further specify the physical interaction structure (10), it is assumed that "the initial state of the body" is homogenous and isotropic. Additionally, the free energy

$E = E\left(f, \hat{f}^c, -\nabla_0 . \Pi_N\right)$in nearby state regions is considered as an "analytic function of scalar invariants" associated with the states mentioned above. In the subsequent analysis, we restrict our attention to "the quadratic approximation" of the growth of function within a local vicinity of the beginning state.

$E = E_0 - \frac{O_{(0)}}{\rho_{(0)}} f + \frac{1}{2}\alpha_1 f^2 + \frac{1}{2}\alpha_2(-\nabla_0 \,. \Pi_N)^2 + \frac{1}{2}\alpha_3\left(\hat{f}^c \,..\, \hat{f}^c\right) - \alpha_4 f(-\nabla_0 . \Pi_N)$ (11)

Then, we obtain to the ensuing physical interactions: 1158

$\frac{1}{3}\sigma^* = \frac{o_{(0)}}{\rho_{(0)}} + L_* f - \beta(-\nabla_0 \,. \Pi_N),\ \hat{\sigma}_0^c = 2\,H\hat{f}^c,\ -\mu - \mu_{(0)} = \alpha(-\nabla_0 . \Pi_N) - \beta f$ (12)

Shear modulus, denoted by H,

$\alpha\left(\frac{\partial(\mu - \mu_{(0)})}{\partial(-\nabla_0 . \Pi_N)}\right)_0,\ \ \beta = \frac{1}{3}\left(\frac{\partial \sigma^*}{\partial(-\nabla_0 . \Pi_N)}\right)$ (13)

The stress tensor symmetric part is

$\hat{\sigma}_0 = \left[-\frac{o_{(0)}}{\rho_{(0)}} + L_* f + \beta\left(\nabla_0 . \frac{\partial \sigma^*}{\partial(-\nabla_0 . \Pi_N)}\right)\right]\hat{J} + 2\,H\hat{f}^c$ (14)

3.1.3 Formulation of BVP

The essential system of equations for the model is derived by utilizing the equations representing the local thermodynamic state (9) and (10) as well as the equations regulating DP. Thus, it turns out.

$$H\Delta v + \left(L_* + \frac{1}{3}H\right)\nabla_0(\nabla_0 \,. v) + \ \nabla_0 \,. \hat{\sigma}_* = \beta_1 v - \beta\nabla_0(\nabla_0 . \Pi_N) + \gamma_2 \Pi_N - \frac{\gamma_1}{2}(\nabla_0 \times v) - e^+,$$

$\sigma_* = \ -H'(\nabla_0 \times v) = \gamma_1 v + \gamma_3(-\Pi_N),$

$\alpha\nabla_0(-\nabla_0 . \Pi_N) + \beta_3 \Pi_N = \beta\nabla_0(\nabla_0 . v) - \gamma_2 v - \frac{\gamma_3}{2}(\nabla_0 \times v)$ (15)

Additionally, the anti-symmetric stress tensor is excluded from the system (15),

$\hat{\sigma}_* = \ \hat{F} \,.\left[-F'(\nabla_0 \times v) + \gamma_1 v + \gamma(-\Pi_N)\right]$ (16)

Then, we arrive at the fundamental set of equations that govern the calculation of "the displacement vector"v and the vector representing the "elastic shift" of mass Π_N,

$$H\Delta v + \left(L_* + \frac{1}{3}H\right)\nabla_0(\nabla_0 . v) + \nabla_0 . \left[-H'\hat{F}.(\nabla_0 \times v) + \gamma_1(\hat{F}.v)\right] + \frac{1}{2}\gamma_1(\nabla_0 \times v) = \beta_1 v - \beta\nabla_0(\nabla_0 . \Pi_N) + \gamma_3\nabla_0 . (\hat{F}.\Pi_N) + \gamma_2\Pi_N - e^+\alpha\nabla_0(-\nabla_0.\Pi_N) + \beta_3\Pi_N = \beta\nabla_0(\nabla_0.v) - \gamma_2 v - \frac{1}{2}\gamma_3(\nabla_0 \times v) \quad (17)$$

By neglecting the impact of interference from DP($\gamma_1 = 0, \gamma_2 = 0, \gamma_3 = 0$), we can simplify the primary set of equations (17) to a less complicated form,

$$H\Delta v + \left(L_* + \frac{1}{3}H\right)\nabla_0(\nabla_0 . v) - H'\nabla_0 . \left[\hat{F}.(\nabla_0 \times v)\right] = \beta_1 v - \beta\nabla_0(\nabla_0 . \Pi_N) - e^+ \quad (18)$$

Therefore, the task of achieving a state of equilibrium for the object being examinedis denoted as ℓ_*, while it interacts with its surrounding atmosphere, denoted as ℓ_*^+, while taking into consideration near-surface processes, can be simplified to solving the essential set of equations (18) subject to the specified conditions,

$$\sigma_m|_{\partial W_0} = -o^+ m, \ \ \mu|_{\partial W_0} = \mu^+ \quad (19)$$

In this context, o^+ and μ^+ represent the designated values for the chemical potential of the surrounding atmosphere.

3.2 Variational Formulation

We adopt the functional method to the variational formulation of BVP in thermodynamics, focusing particular attention to near-surface phenomena.

$$i\left[v, -\Pi_N, f, \hat{f}^c, (\nabla_0 \otimes v)^b, -\nabla_0.\Pi_N\right] = \int_{s_1}^{s_2}\left\{\int_{W_0}\left\{E\left(f, \hat{f}^c, -\nabla_0.\Pi_N\right) + \Psi[v, (\nabla_0 \otimes v)^b, -\Pi_N] - e^+ . v\right\}dU_0 - \int_{\partial W_0}\left[\sigma_m^+ . v + \left(\mu^+ - \mu_{(0)}\right)m . (-\Pi_N)\right]d\Sigma_0\right\}ds \quad (20)$$

$$\delta I = \int_{s_1}^{s_2}\{\int_{W_0}\{\left(\frac{\partial E}{\partial f} - \frac{1}{3}\sigma^*\right)\delta f + \left(\frac{\partial E}{\partial \hat{f}^c} - \hat{\sigma}_0^c\right) .. \delta\hat{f}^c + \left[\frac{\partial E}{\partial(-\nabla_0 . \Pi_N)} - \left(\mu - \mu_{(0)}\right)\right]\delta(-\nabla_0 . \Pi_N) + \left[\frac{\partial \Psi}{\partial v} - (\nabla_0.\hat{\sigma} + g^+)\right].\delta v + \left[\frac{\partial \Psi}{\partial(\nabla_0 \otimes v)^b} - \hat{\sigma}_*\right] ... \delta[(\nabla_0 \otimes v)^b]^\intercal + \left[\frac{\partial \Psi}{\partial(-\Pi_N)} - \nabla_0\left(\mu - \mu_{(0)}\right)\right] . \delta(-\Pi_N)\} dU_0 + \int_{\partial W_0}(\sigma_m - \sigma_m^+) . \delta v d\Sigma_0 + \int_{\partial W_0}(\mu - \mu^+)m . \delta(-\Pi_N)d\Sigma_0 \} ds. \quad (21)$$

The stress tensor $\hat{\sigma}$can be expressed as the summation of its spherical, deviatoric and anti-symmetric components.

$$\hat{\sigma} = \frac{1}{3}\sigma^*\hat{J} + \hat{\sigma}_0^c + \hat{\sigma}_* \quad (22)$$

To determine the initial functional (20), it is required to establish the condition where the initial variation of the functional is equal to zero.

$$\delta I\left[v, -\Pi_N, f, \hat{f}^c, (\nabla_0 \otimes v)^b, \nabla_0 . \Pi_N\right] = 0 \quad (23)$$

By considering the independence of variations A5 and A6 as well as applying the condition for the functional (21), we can derive

$$\sigma^* = 3\frac{\partial E\left(f, \hat{f}^c, -\nabla_0 . \Pi_N\right)}{\partial f}, \ \ \hat{\sigma}_0^c = \frac{\partial E\left(f, \hat{f}^c, -\nabla_0.\Pi_N\right)}{\partial \hat{f}^c}, \mu - \mu_{(0)} = \frac{\partial E\left(f, \hat{f}^c, -\nabla_0.\Pi_N\right)}{\partial(-\nabla_0.\Pi_N)}; \quad (24)$$

$$\nabla_0 . \hat{\sigma} + e^+ = \frac{\partial \Psi[v, (\nabla_0 \otimes v)^b, -\Pi_N]}{\partial v}, \ \ \hat{\sigma}_* = \frac{\partial \Psi[v, (\nabla_0 \otimes v)^b, -\Pi_N]}{\partial(\nabla_0 \otimes v)^b}, \ \ \nabla_0\left(\mu - \mu_{(0)}\right) = \frac{\partial \Psi[v, (\nabla_0 \otimes v)^b, -\Pi_N]}{\partial(-\Pi_N)} \quad (25)$$

By utilizing the defining relations of the LS (24) and DP (25), it is possible to ascertain the subsequent differential,

$$dE = \frac{1}{3}\sigma^* df + \hat{\sigma}_0^c ... d\hat{f}^c + (\mu - \mu_{(0)} d(-\nabla_0 . \Pi_N) \quad (26)$$

$$d\Psi = (\nabla_0.\hat{\sigma} + e^+) . dv + \hat{\sigma}_* .. d\left[(\nabla_0 \otimes v)^b\right]^\intercal + \nabla_0\left(\mu - \mu_{(0)}. d(-\Pi_N)\right) \quad (27)$$

By establishing a connection between the anti-symmetric tensors $\hat{\sigma}$ and $\nabla_0.\hat{\sigma}$ in the differentialand their corresponding "equivalent accompanying vectors", we can derive a differential that describes DP,

$$d\Psi = (\nabla_0.\hat{\sigma} + e^+) . dv - \sigma_* . d\phi + \nabla_0\left(\mu - \mu_{(0)}. d(-\Pi_N)\right) \quad (28)$$

The requirement for the functional (20) to be sufficient is the convexity condition,

$$\delta^2 I = \int_{s_1}^{s_2}\left\{\int_{W_0}[\delta\sigma_m.\delta v + \delta\mu m . \delta(-\Pi_n)]d\Sigma_0\right\}ds > 0 \quad (29)$$

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$$\delta^2 I = \int_{s_1}^{s_2} \left\{ \int_{W_0} \left[\frac{1}{3} \delta\sigma^* \, \delta f + \delta\hat{\sigma}_0^c + \delta\mu\delta(\nabla_0 . \Pi_N) + (\nabla_0 . \delta . \hat{\sigma}) . \delta v - \delta\hat{\sigma}_* \ldots \delta(\nabla_0 \otimes v)^b + \delta\nabla_0 \, \mu . \delta(-\Pi_N) \right] dU_0 \right\} ds \quad (30)$$

$$\equiv \int_{s_1}^{s_2} \left\{ \int_{W_0} \left[\delta^2 E \left(f, \hat{f}^c, -\nabla_0 . \Pi_N \right) + \delta^2 \Psi\left(v, (\nabla_0 \otimes v)^b, -\Pi_N \right) \right] dU_0 \right\} ds > 0 \quad (31)$$

In order to establish the conditions for the convexity of functional (20), it is possible to consider,

$$\int_{s_1}^{s_2} \left[\int_{W_0} \delta^2 E \left(f, \hat{f}^c, -\nabla_0 . \Pi_N \right) dU_0 \right] ds > 0 \, , \quad \int_{s_1}^{s_2} \left\{ \int_{W_0} \delta^s \Psi \left[v \, , (\nabla_0 \otimes v)^b, -\Pi_N \right] dU_0 \right\} ds > 0 \quad (32)$$

4. Conclusion

Boundary value problems (BVPs) are a robust mathematical framework with numerous applications in several scientific disciplines. BVPs are crucial in the understanding and solution of complex physical processes in the fields of thermodynamics and kinetics. In this study, we proposed a mathematical framework to explain the thermo-mechanical processes in elastic deformable systems. This approach was developed to consider the impact of dissipative effects on the development of near-surface phenomena. Expressions regulating the LS and illustrating the DP can be obtained by combining kinetic energy and employing thermodynamic principles. This investigation of BVP in the context of thermodynamics and kinetics improves our theoretical understanding of physical incidents and provides us with significant tools for addressing practical problems.

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