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Mathematical Modeling of High-Energy Shaker Mill Process with Lumped Parameter Approach for One-Dimensional Oscillatory Ball Motion with Collisional Heat Generation

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Abstract: This study presents an advanced mathematical model for the high-energy shaker mill process, incorporating thermal interactions among the milling ball, shaker mill vial, and the air contained within. Unlike previous models focusing solely on the ball's temperature, this research emphasizes the heat produced by impacts and the thermal exchange among all three components. Incorporating these thermal interactions allows the model to provide a more comprehensive depiction of the energy dynamics within the system, leading to more precise predictions of temperature changes. Utilizing a lumped parameter method, the study simplifies complex airflow dynamics and non-uniform temperature distributions in the milling system, enabling efficient numerical analysis. Hamilton's equations are extended to include supplementary state variables that account for the internal energies of both the vial and the air, in addition to the thermomechanical state variables of the ball. High-energy milling techniques are essential in mechanochemical synthesis and various industrial applications, where the optimization of heat transfer and energy efficiency is crucial. Numerical simulations computed using the Bogacki–Shampine integration algorithm significantly align with experimental data, confirming the model's accuracy. This comprehensive framework enhances understanding of heat transfer in one-dimensional ball motion, optimizing milling parameters for better performance. The mathematical model facilitates the computation of heat production due to collisions, based on operational parameters like shaking frequency and amplitude, thereby allowing for the anticipation of chemical reaction activation potential in mechanochemistry.

Keywords: mathematical modeling; high-energy mill; collisional heating; lumped-parameter modeling; Hamiltonian mechanics; thermomechanical coupling

MSC: 37M05



Academic Editor: Irina G. Nizovtseva

Received: 28 December 2024

Revised: 23 January 2025

Accepted: 28 January 2025

Published: 28 January 2025

Citation: Son, K.L. Mathematical Modeling of High-Energy Shaker Mill Process with Lumped Parameter Approach for One-Dimensional Oscillatory Ball Motion with Collisional Heat Generation.

Mathematics **2025**, *13*, 446. <https://doi.org/10.3390/math13030446>

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1. Introduction

High-energy ball milling has increasingly been acknowledged as a versatile method in mechanochemical applications, particularly in the alloying of metal components [1–5]. In addition, extensive studies have examined such an energetic milling process, particularly to synthesize ammonia through nitrogen fixation and subsequent hydrogenation [6–8]. This technique exploits the substantial impact energies generated during milling not only to pulverize materials [9–12], but also to produce thermal activation energy, thus promoting chemical reactions [13,14]. Consequently, high-impact milling has increasingly been recognized as a more sustainable method for synthesizing ammonia compared to the

conventional Haber–Bosch process, offering enhanced efficiency at relatively moderate temperatures and pressures [15].

Analyzing the mechanics and thermodynamics associated with milling balls is essential to optimize milling processes. However, experimental obstacles, including the challenge of real-time monitoring of the position, velocity, and temperature of the grinding ball, complicate detailed evaluations of their thermomechanical conditions [16]. Although quasireal-time experiments have succeeded in obtaining periodic temperature data by occasionally stopping the milling process [17,18], computational simulations have become essential to investigate complex particle interactions that occur during milling [19–22]. The discrete element method (DEM) is a well-established computational approach commonly utilized to simulate contact forces, collisions, and the behavior of particulate materials. Recent progress in the field of DEM encompasses investigations into interparticle conductive heat transfer [23–25] as well as fluid–structure interactions (FSI) [26–29]. Only a few models have been developed to examine the interplay between the heat generated by collisions and convective heat transfer [30–32]. For example, the previous research of the author formulated a mathematical model to simulate heat production during collisions of an individual spherical milling ball within an oscillating vial [33]. However, that mathematical model mainly focused on the milling ball itself, neglecting the thermal interactions with both the vial and the surrounding air. To overcome these limitations, this study expands upon previous research by applying a lumped parameter methodology to capture heat transfer among the ball, vial, and surrounding air. This extensive framework integrates extra state variables for both vial and air temperatures, as well as the ball’s thermomechanical state variables, allowing for a more detailed assessment of thermal behavior in the high-energy shaker mill process.

The introduced model simplifies the dynamics occurring in the shaker milling process by expressing them as a series of first-order non-linear differential equations. The generation of collisional heat is associated with the energy dissipation mechanisms present in a non-linear viscoelastic contact model. In addition, a heat convection model is integrated into the energy balance equations, relying on the translational velocity of the milling ball. The vial and the air are considered uniform-state thermal reservoirs that absorb heat through convection. This study deviates from conventional Newtonian mechanics by employing a Hamiltonian mechanics approach that focuses on energy to formulate the governing equations, which are subsequently integrated numerically. The validation of numerical results is achieved through experimental data, which confirm the precision of the model and help identify potential limitations.

The organization of this paper is outlined as follows. The problem of high-speed collisions with a single degree of freedom is initially defined in Section 2. In Section 3, mathematical models based on Hamiltonian mechanics are formulated, incorporating elements such as viscoelastic contact, collision-induced heat generation, and convective heat transfer. Subsequently, Section 4 offers a comprehensive presentation and analysis of the numerical results and their significance. Finally, Section 5 provides the concluding remarks and suggests potential directions for future investigation.

2. Problem Description

The aim of this study is to construct a mathematical framework to examine the multi-physics of a shaker mill, consisting of a cylindrical vial, enclosed air, and a spherical milling ball. This analysis focuses on the 8000 M Mixer/Mill, produced by Spex CertiPrep located in Metuchen, NJ, USA, which is frequently employed in research involving high-energy milling [17,34,35]. Table 1 provides a comprehensive overview of the main specifications of the milling system. The mill functions through a kinematic system where the vial follows a

curved trajectory and engages in oscillatory yawing, resulting in an intricate and coordinated three-dimensional roto-translational movement [34,35]. To simplify the modeling process, this study considers the motion to be one-dimensional, assuming that the vial undergoes sinusoidal oscillations along its longitudinal axis, while the milling ball follows the same path. The employment of a one-dimensional translational motion model is a strategic simplification intended to improve mathematical clarity and interpretability. Although the real three-dimensional roto-translational motion occurring in a shaker mill involves intricate dynamics, reducing it to a one-dimensional model enables a focus on primary heat-generating mechanisms. In particular, collisions at the end of the vial play a significant role in affecting the milling ball's momentum change and the resulting heat generation. Meanwhile, collisions with sidewalls and friction-induced heat have a comparatively lesser effect. This modeling strategy mirrors simplifications found in physics, such as representing sphere collisions by the coefficient of restitution, while disregarding local deformations, wave propagation, and other factors. Despite these constraints, one-dimensional analysis offers valuable insights into the primary dynamics of the system with a satisfactory degree of approximation. Within this simplified framework, the milling ball's dynamics are predominantly dictated by its interaction with the vial, neglecting gravitational influences. The milling ball exclusively interacts with the cylindrical vial on its circular end faces with a diameter of 19 mm. Moreover, it is assumed that the convective heat transfer surface areas on both the inner and outer sides are approximately the same.

Table 1. Specifications of Spex 8000M Mixer/Mill system.

Specification	Symbol	Value	Unit
Milling ball radius	R	6.35	mm
Cylindrical vial length	l_v	58	mm
Vial inner contact area	A_i	567.06	mm ²
Vial outer surface area	A_o	567.06	mm ²
Vial oscillation amplitude	X_v	25	mm
Vial oscillation frequency range	ω	90–130	rad/s

Figure 1 illustrates a fundamental schematic that depicts a milling ball located within a vial exhibiting sinusoidal motion. When the milling ball impacts either the left or right edge of the vial, an overlap occurs at the contact point, and the contact force is determined using a contact force model. These impacts produce heat at the contact point, which is then split; some heat is transferred to the milling ball, while the remainder is absorbed by the vial, causing their temperatures to rise. Beyond interactions with the vial boundaries, the milling ball also engages in convective heat exchange with the air within the vial. The vial, in turn, has thermal interactions with the internal air and engages in convective heat transfer with the outside air. In the context of employing the lumped parameter modeling technique, the thermal reservoirs within the system are divided into three components: the milling ball, the vial, and the internal air. The heat formed at the contact points is transferred to both the ball and the vial, while convective heat exchange happens between these three thermal reservoirs. This modeling technique simplifies the complex dynamics of heat transfer and mechanical interactions into an analytically tractable system. The coordinates and momentum of the milling ball, denoted by x and p , are determined by the application of Hamiltonian mechanics. The internal energy, U_b , incorporates the effects of heating due to collisions and loss of convective heat. Unlike the earlier model by the author [33], this research integrates the thermal properties of the vial and the internal air. These components are treated as uniform thermal entities, defined by lumped internal energy parameters U_v and U_a for the vial and the internal air, respectively.

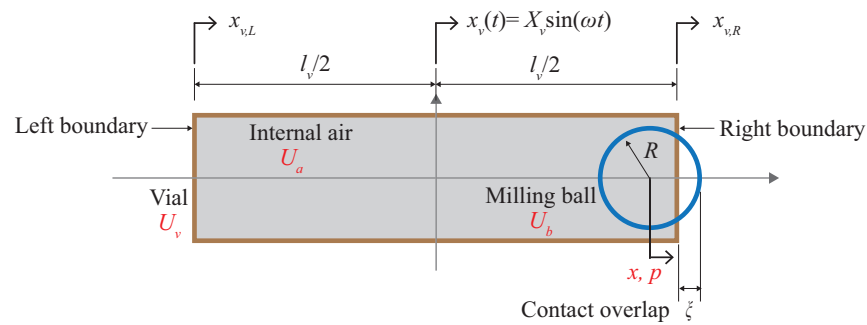


Figure 1. Diagram of simplified one-dimensional collisional heating problem involving milling ball in shaker mill.

The system is solely driven by the movement at the boundaries of the vial, symbolized as $x_{v,L}$ and $x_{v,R}$, and described by a sinusoidal function:

$$x_v(t) = x_{v,L} = x_{v,R} = X_v \sin \omega t, \quad (1)$$

where X_v indicates the oscillation amplitude, ω is the angular frequency, and t denotes time. Equation (1) describes a holonomic constraint that varies with time, thus qualifying as a rheonomic constraint, indicating that the force related to this constraint does non-zero work. However, since this constraint force is operative only during impacts, it qualifies as an inequality constraint.

Figure 2 illustrates the equivalent circuit model of the system shown in Figure 1, which is commonly used in lumped-parameter analysis in mechatronics and control engineering. This model effectively represents heat dissipation and storage between the three media: the milling ball, the vial, and the internal air. Specifically, while the resistive and capacitive elements of this circuit behave linearly, the resistance between the milling ball and the internal air is an exception, as it exemplifies the complex mechanisms of non-linear velocity-dependent heat transfer.

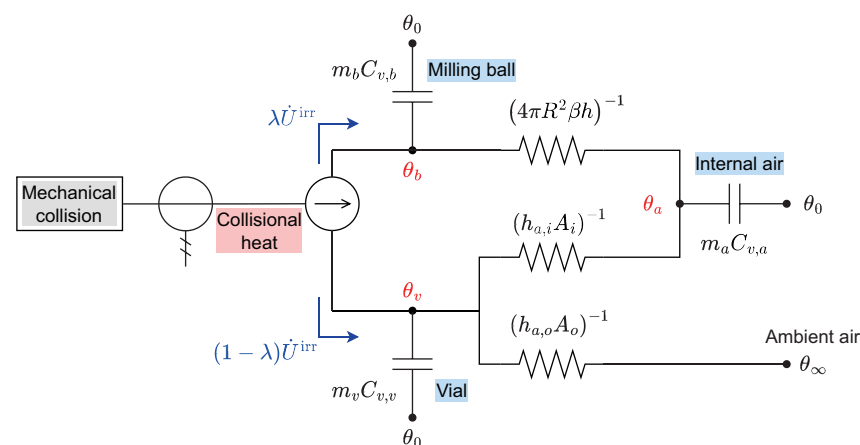


Figure 2. Lumped-parameter model equivalent circuit for 1D shaker mill system.

This research utilizes the notion of contact overlap, commonly known as penetration depth, a metric widely employed in contact computations in DEM and the finite element method (FEM). It is instrumental in assessing the impact and repulsive forces between the milling ball and the vial. During penetration, a viscoelastic contact force is activated to oppose and reduce further overlap. The force is determined by both the overlap distance and its velocity.

3. Mathematical Modeling

The mathematical model examined in this study closely corresponds to the methodologies outlined in the earlier research by the author [33]. However, to improve clarity and understanding, the modeling framework has been fully presented. Significantly, this study broadens the thermodynamic modeling perspective by not only focusing on the milling ball, but also integrating the thermodynamic states of the vial and surrounding air. This broadened approach increases the number of thermal reservoirs considered in the model from one to three, thereby enabling a more comprehensive portrayal of the system's thermal response. Furthermore, significant improvements have been made to the conduction and convection heat transfer models to accurately characterize the heat exchange between these three entities. These improvements lead to a notably enhanced model, providing deeper insight into the thermodynamic interactions among the components within the shaker mill system.

3.1. Particle Contact Model

The interaction between the milling ball and the vial walls is characterized by Boolean operators, which define contact conditions. The mathematical representation of these operators is given by:

$$\alpha_L = \langle R - (x - x_{v,L}) \rangle^0, \quad (2)$$

$$\alpha_R = \langle R - (x_{v,R} - x) \rangle^0, \quad (3)$$

where $\langle \rangle^0$ signifies a zeroth-order singular bracket function, analogous to the Heaviside step function, and the variables $x_{v,L}$ and $x_{v,R}$ represent the coordinates of the left and right boundaries of the vial, respectively. Contact with the left wall occurs when $\alpha_L = 1$, whereas $\alpha_R = 1$ indicates contact with the right wall. It is physically impossible for the milling ball to touch both walls simultaneously, as shown in Figure 1, which means α_L and α_R cannot be equal to each other at the same time.

The variable ζ denotes the penetration depth during the interaction between the sphere and the wall. It is defined mathematically as follows:

$$\zeta = \zeta_L + \zeta_R = \langle R - (x - x_{v,L}) \rangle^1 + \langle R - (x_{v,R} - x) \rangle^1, \quad (4)$$

where the operator $\langle \rangle^1$ acts as a first-order singular bracket, maintaining the value of the expression when positive and assigning zero when it is not. The parameters ζ_L and ζ_R denote the respective extents of overlap in the left and right contact regions, and they are constrained by mutual exclusivity principles akin to the restrictions imposed on α_L and α_R .

The rate of change of contact overlap, represented as $\dot{\zeta}$, is obtained by performing a time differentiation of Equation (4), resulting in:

$$\dot{\zeta} = \alpha_L(\dot{x}_v - \dot{x}) + \alpha_R(\dot{x} - \dot{x}_v), \quad (5)$$

where $\dot{x}$ represents the velocity of the milling ball, and $\dot{x}_v$ denotes the vial's translational velocity. This velocity, $\dot{x}_v$, is derived from the sinusoidal motion expressed in Equation (1), leading to:

$$\dot{x}_v = \omega X_v \cos \omega t. \quad (6)$$

The study employs a non-linear viscoelastic force model with two terms, known as the Hertz–Mindlin model, to characterize the interactions between particles and surfaces [36–39]. The contact force acting in the normal direction, denoted as F_c , can be separated into a

conservative elastic component, F_e , and a non-conservative damping component, F_d , and is represented by:

$$F_c = F_e + F_d = \frac{4}{3} \sqrt{R E_{\text{eff}}^2 \xi^{\frac{3}{2}}} n_w - \sqrt{\frac{20}{3}} \left(\frac{\ln e}{\ln^2 e + \pi^2} \right) \left(m_b^2 R E_{\text{eff}}^2 \xi \right)^{\frac{1}{4}} \dot{\xi} n_w, \quad (7)$$

where n_w pertains to the outward normal at the contact location, R stands for the ball's radius, e indicates the restitution coefficient, and m signifies the mass of the milling ball. The effective elastic modulus, denoted as E_{eff} , is expressed by the equation:

$$\frac{1}{E_{\text{eff}}} = \frac{1 - \nu_b^2}{E_b} + \frac{1 - \nu_v^2}{E_v}, \quad (8)$$

where E_b and E_v represent the elastic moduli of the ball and the vial, respectively, while ν_b and ν_v are their respective Poisson's ratios.

The direction of the contact force, represented by n_w , is established via a mathematical examination that includes the Boolean operations α_L and α_R :

$$n_w = \alpha_L - \alpha_R, \quad (9)$$

which confirms that the directional components of the force vectors on the left and right sides are in opposition.

The component of the elastic force F_e aligns with the classical Hertzian contact force [40], which explains the interaction between a sphere and a flat plane. The damping component F_d represents the energy loss due to material deformation, governed by the restitution coefficient e [36]. This comprehensive model successfully integrates the conservative and dissipative components of particle–wall interactions, providing a robust foundation for the simulation of milling dynamics.

3.2. Collision-Induced Heating Model

An inelastic collision is characterized by a coefficient of restitution that is less than unity, resulting in the dissipation of some of the initial kinetic energy. The energy dissipation results from a variety of mechanisms, such as the plastic deformation of materials, frictional forces at the surfaces of contact, and the inherent damping characteristics of the materials used. This study suggests that material damping serves as the fundamental process for energy dissipation during collisions. The damping-related non-conservative force, represented as F_d , is detailed in Equation (7). This force is utilized to define the power loss associated with damping as follows:

$$\dot{U}^{F_d} = F_d v, \quad (10)$$

where $v = \dot{x}$ denotes the milling ball velocity.

The parameter η represents the portion of power loss transformed into irreversible thermal energy during collisions, thus serving as a measure of the efficiency of internal heat generation. With this parameter, the rate of irreversible heat production, symbolized as $\dot{U}^{\text{irr}}$, can be described by the subsequent equation:

$$\dot{U}^{\text{irr}} = \eta \dot{U}^{F_d} = -\eta \sqrt{\frac{20}{3}} \left(\frac{\ln e}{\ln^2 e + \pi^2} \right) \left(m_b^2 R E_{\text{eff}}^2 \xi \right)^{\frac{1}{4}} \dot{\xi} n_w v. \quad (11)$$

The previous study on mathematical modeling [33] considered the parameter η as an adaptable numerical variable to align with experimental results. In contrast, the current study uses heat transfer coefficients as adjustable parameters, allowing η to remain a

constant value. In particular, η is set to 0.9, aligning with the commonly accepted estimate that approximately 90% of energy is transformed into heat due to inelastic deformation in collisions [41,42].

3.3. Heat Transfer Model

The transfer of heat due to convection from a sphere moving within a fluid can be characterized by the convection heat transfer coefficient, which measures the rate at which thermal energy is dispersed to the surrounding medium. The dimensionless Nusselt number (Nu) frequently represents this coefficient and is influenced by both the Reynolds number (Re) and the Prandtl number (Pr), as outlined in [43,44]. For a spherical body, these dimensionless quantities can be defined by the following equations:

$$Nu = \frac{2Rh}{k}, \quad Re = \frac{2R\rho v}{\mu}, \quad Pr = \frac{C_p\mu}{k}, \quad (12)$$

where h signifies the convective heat transfer coefficient, k is the thermal conductivity, μ is the dynamic viscosity, and C_p denotes the specific heat at constant pressure for air.

In order to link the convection coefficient with these dimensionless parameters, Whitaker's correlation for the Nusselt number of a sphere is utilized [45], presented as follows:

$$Nu = 2 + \left(0.4Re^{\frac{1}{2}} + 0.06Re^{\frac{2}{3}}\right)Pr^{0.4}\left(\frac{\mu}{\mu_r}\right)^{-\frac{1}{4}}, \quad (13)$$

where Re explicitly incorporates the sphere's velocity to address its relationship with convective heat transfer. The Sutherland formula [46] provides an accurate model for expressing air's dynamic viscosity, denoted as μ , in relation to temperature variations:

$$\frac{\mu}{\mu_r} = \left(\frac{\theta_b}{\theta_r}\right)^{\frac{3}{2}} \left(\frac{\theta_r + S_\mu}{\theta_b + S_\mu}\right), \quad (14)$$

where θ_b represents the milling ball temperature, θ_r signifies the reference temperature, μ_r denotes the viscosity at θ_r , and S_μ is the Sutherland constant associated with viscosity.

Whitaker's model essentially relies on the concept of a stationary sphere located within an infinite-flow field characterized by uniform incoming velocity. However, this assumption is invalid within the confined airflow conditions in a shaker mill, as shown in Figure 1. In confined environments, the effectiveness of convective heat transfer diminishes as thermal energy builds up in ambient air. To rectify this oversimplification, a calibration factor β is used to modify the Nusselt number, which is dependent on the velocity, thus improving the accuracy of the convective heat transfer coefficient.

The heat transfer rate from the sphere to the internal air via convection, represented as $\dot{U}_b^{\text{conv}}$, following the required adjustments, can be expressed by:

$$\dot{U}_b^{\text{conv}} = 4\pi R^2 \beta h (\theta_b - \theta_a), \quad (15)$$

where θ_a denotes the temperature of the internal air. It should be noted that the convection coefficient h is determined using Equations (12)–(14) in each simulation time step. The inclusion of the calibration factor β fine-tunes the model to account for the specific conditions within the vial, thus improving the precision of the convective heat transfer simulation. Unlike previous research [33] that considered the surrounding air temperature θ_a as constant in Equation (15), this study addresses air temperature as a variable of lumped parameters. This distinction is essential to precisely depict the thermal dynamics within the air on the oscillating plate.

To account for the temperature fluctuations within the vial, supplementary heat transfer equations are developed that incorporate interactions with other simplified components. In this investigation, three lumped thermal reservoirs are used as state variables: the milling ball, the vial, and the internal air. Equation (15) quantifies the rate of convective heat transfer between the grinding ball and the internal air in the system. Heat exchange between the milling ball and the vial is assumed to occur due to the generation of heat from collisions at contact points, as indicated by $\dot{U}^{\text{irr}}$ in Equation (11).

Moreover, the thermal interactions between the vial and the surrounding air, both internally and externally, are characterized by Newton's law of cooling, formulated as linear convective heat transfer equations:

$$\dot{U}_v^{\text{conv},i} = h_{a,i}A_i(\theta_v - \theta_a), \quad (16)$$

$$\dot{U}_v^{\text{conv},o} = h_{a,o}A_o(\theta_v - \theta_\infty), \quad (17)$$

where $\dot{U}_v^{\text{conv},i}$ signifies the heat transferred to the internal air from the vial, while $\dot{U}_v^{\text{conv},o}$ denotes the heat expelled from the vial to the external air. A_i is the surface area of contact between the internal air and the interior of the vial, and A_o is the surface area of contact with the external environment. $h_{a,i}$ and $h_{a,o}$ are the inner and outer convective heat coefficients, respectively. The temperature of the surrounding external air, θ_∞ , is assumed to be constant.

In Equations (16) and (17), the heat transfer coefficients $h_{a,i}$ and $h_{a,o}$ are treated as constants. This approach deviates from the intricate, non-linear dynamics shown by the convective heat transfer coefficient between the ball and air, assessed using Equations (12)–(14). The constancy assumption for $h_{a,i}$ and $h_{a,o}$ is based on fairly stable conditions for convective heat transfer at the boundaries of the vial, in contrast to the fluctuating interaction between the milling ball and the air.

3.4. Internal Energy Time Evolution

The rate of change in internal energies of the milling ball, the vial, and the internal air can be determined by applying the power form of the first law of thermodynamics, which is expressed as:

$$\dot{U}_b = \lambda \dot{U}^{\text{irr}} - \dot{U}_b^{\text{conv}}, \quad (18)$$

$$\dot{U}_v = (1 - \lambda) \dot{U}^{\text{irr}} - \dot{U}_v^{\text{conv},i} - \dot{U}_v^{\text{conv},o}, \quad (19)$$

$$\dot{U}_a = \dot{U}_b^{\text{conv}} + \dot{U}_v^{\text{conv},i}, \quad (20)$$

where λ describes the proportion of thermal energy transferred to the milling ball compared to the total rate of heat produced during collisions. These equations indicate that internal energy change rates, denoted $\dot{U}_b$, $\dot{U}_v$, and $\dot{U}_a$, are governed by the balance between the rate of irreversible heat generation, $\dot{U}^{\text{irr}}$, and the heat dissipation rates by convection, that is, $\dot{U}_b^{\text{conv}}$, $\dot{U}_v^{\text{conv},i}$, and $\dot{U}_v^{\text{conv},o}$.

To establish the connection between internal energy and temperature for each thermal reservoir model, the concept of heat capacity is applied as defined in [46]. This relationship is represented by the following equations:

$$\dot{U}_b = m_b C_{v,b} \dot{\theta}_b, \quad (21)$$

$$\dot{U}_v = m_v C_{v,v} \dot{\theta}_v, \quad (22)$$

$$\dot{U}_a = m_a C_{v,a} \dot{\theta}_a, \quad (23)$$

where $C_{v,b}$, $C_{v,v}$, and $C_{v,a}$ denote the specific heat capacities at constant volume for the ball material, vial, and air, respectively. The terms m_b , m_v , and m_a correspond to the masses of

the milling ball, the vial, and the air, respectively, while $\dot{\theta}_b$, $\dot{\theta}_v$, and $\dot{\theta}_a$ signify the rates of change in temperature for the milling ball, the vial, and the air, respectively.

This study presumes that the milling ball experiences a constant-volume process during the analysis. Therefore, variations in internal energy due to changes in volume are omitted in Equations (21) to (23). This simplification removes the requirement to incorporate a constraint force induced by volume changes in the momentum evolution equation of the Hamiltonian framework. Hence, when solving the governing equations numerically, there is no need to implement an additional equation of state that correlates the density, pressure, and internal energy of the material of the milling ball.

This assumption is especially applicable to the solid phase, as density variations and volume changes are insignificant under the operating conditions of the shaker mill. By focusing solely on temperature-dependent energy changes, the model reduces computational complexity while maintaining accuracy in representing the thermodynamic behavior of the milling ball.

3.5. Hamilton's Equations

The configuration space related to the one-dimensional collision scenario illustrated in Figure 1 is defined using five generalized coordinates: the position and linear momentum of the milling ball, along with the internal energies of the milling ball, the vial, and the air. These coordinates effectively characterize the kinematic and thermodynamic conditions of a one-dimensional shaker mill system. The thermomechanical Hamiltonian [47], which encompasses the total energy associated with the spherical milling ball, the vial, and the air inside the shaker mill, incorporates elements from kinetic, potential, and internal energies:

$$H(x, p, U_b, U_v, U_a) = V(x) + T(p) + U_b + U_v + U_a, \quad (24)$$

where $V(x)$ represents the elastic potential energy during contact, $T(p)$ corresponds to the kinetic energy as described by the linear momentum p , and U_b , U_v , and U_a signify the internal energy contributions of the ball, the vial, and the air inside, respectively.

The kinetic energy T and the co-energy T^* can be established via a Legendre transformation [47] and are specified by the following expressions:

$$T = \frac{p^2}{2m}, \quad T^* = \frac{1}{2}mv^2, \quad (25)$$

where m represents the mass of the milling ball, v signifies its velocity, and p is the linear momentum defined in Lagrangian mechanics as $p = \partial T^* / \partial v = mv$.

The time-dependent evolution of the generalized coordinates is represented by Hamilton's canonical equations, which are formulated from the thermomechanical Hamiltonian [48]:

$$\dot{x} = \frac{\partial H}{\partial p}, \quad (26)$$

$$\dot{p} = -\frac{\partial H}{\partial x} + Q_x, \quad (27)$$

$$\frac{\partial H}{\partial U_b} = Q_{U_b}, \quad (28)$$

$$\frac{\partial H}{\partial U_v} = Q_{U_v}, \quad (29)$$

$$\frac{\partial H}{\partial U_a} = Q_{U_a}. \quad (30)$$

Equation (27) denotes Q_x as the generalized non-conservative force related to changes in position x . The associated work and power can be derived by considering these variations:

$$\delta W^{\text{nc}} = Q_x \delta x, \quad \delta \dot{W}^{\text{nc}} = Q_x \delta v, \quad (31)$$

where δ denotes the variation operator. For the milling ball, the only non-conservative force is the damping force F_d , such that $Q_x = F_d$ as derived from Equation (10).

The partial derivatives of H with respect to U_b , U_v , and U_a in Equation (24) produce $Q_{U_b} = 1$, $Q_{U_v} = 1$, and $Q_{U_a} = 1$, respectively [49]. Because Equations (28) through (30) lead to such trivial generalized forces associated with internal energies, the non-trivial evolution of internal energies must instead be derived from the internal energy evolution equations expressed in Equations (18) through (20).

The equations governing the thermomechanical variables x , p , U_b , U_v , and U_a are obtained by integrating Hamilton's canonical equations, given in Equations (26) to (30), together with the internal energy evolution equations stated in Equations (18) to (20), and their representation is as follows:

$$\dot{x} = \frac{1}{m_b} p, \quad (32)$$

$$\dot{p} = \frac{4}{3} \sqrt{RE_{\text{eff}}^2 \xi^{\frac{3}{2}} n_w} - \sqrt{\frac{20}{3}} \left(\frac{\ln e}{\ln^2 e + \pi^2} \right) \left(m_b^2 RE_{\text{eff}}^2 \xi \right)^{\frac{1}{4}} \xi n_w, \quad (33)$$

$$\dot{U}_b = \frac{\lambda \eta F_d}{m_b} p - 4\pi R^2 \beta h (\theta_b - \theta_a), \quad (34)$$

$$\dot{U}_v = \frac{(1 - \lambda) \eta F_d}{m_b} p - h_{a,i} A_i (\theta_v - \theta_a) - h_{a,o} A_o (\theta_v - \theta_\infty), \quad (35)$$

$$\dot{U}_a = 4\pi R^2 \beta h (\theta_b - \theta_a) + h_{a,i} A_i (\theta_v - \theta_a). \quad (36)$$

These governing equations form a system of non-linear first-order ordinary differential equations (ODEs) that delineate the coupled kinematic and thermodynamic behavior of the milling ball, the vial, and the internal air. Solving these equations requires numerical integration, using specified initial conditions.

Temperatures θ_b , θ_v , and θ_a , which are important output variables, are not considered generalized coordinates. Instead, they are calculated from the changes in internal energy by using the heat capacity formula:

$$\theta_b = \int_0^t \frac{\dot{U}_b}{m_b C_{v,b}} dt, \quad (37)$$

$$\theta_v = \int_0^t \frac{\dot{U}_v}{m_v C_{v,v}} dt, \quad (38)$$

$$\theta_a = \int_0^t \frac{\dot{U}_a}{m_a C_{v,a}} dt. \quad (39)$$

Within the Hamiltonian framework, these equations reveal that the temperatures θ_b , θ_v , and θ_a are variables that vary over time, shaped by changes in internal energy in accordance with the first law of thermodynamics. This approach encapsulates the interaction between mechanical and thermal processes in the shaker mill system.

4. Numerical Results and Discussion

An in-house computational algorithm was developed using Matlab (version 2024a, MathWorks Inc., Natick, MI, USA) to numerically solve the governing Equations (32) through (36). Figure 3 illustrates the computational procedure. Initially, input datasets are

entered, comprising simulation parameters, vial operating conditions, material properties, and initial conditions. In each increment in computational time, the governing equations are formulated by calculating contact force, collisional heat generation, and convective heat transfer. These equations are solved numerically to iteratively refine the state variables until the designated simulation duration is met. Upon completion of the simulation, a regression analysis is performed alongside a graphical presentation of the data to aid in effectively interpreting the results.

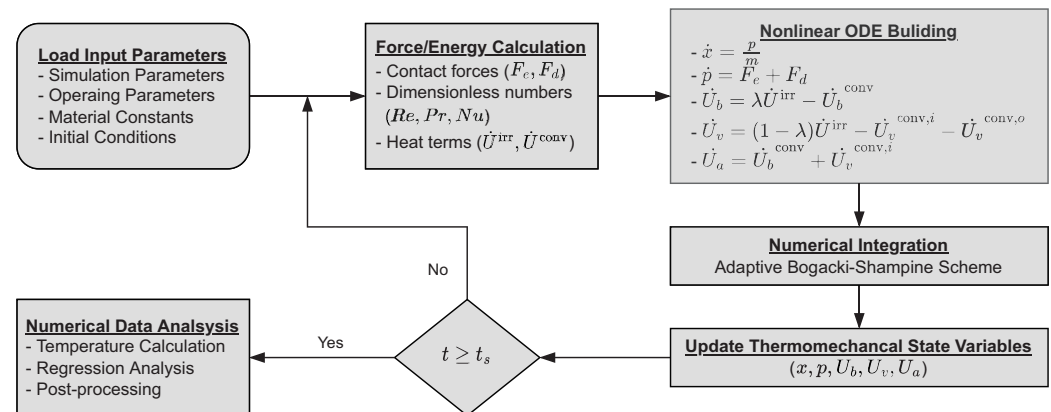


Figure 3. Flow diagram of the numerical method for addressing the one-dimensional collisional heating issue in a shaker mill.

The initial step in numerical integration involves identifying all relevant material properties and model parameters. Table 2 lists the fundamental physical attributes of the steel milling ball, crucial for assessing the contact force and internal energy.

Table 2. Physical properties of steel vial and milling ball.

Property	Symbol	Value	Unit
Density	ρ_s	7800	kg/m ³
Elastic modulus	E	200	GPa
Poisson's ratio	ν	0.3	-
Specific heat capacity	C_v	461	J/kg · K

Table 3 lists the physical and thermal properties of the internal and ambient air. These properties are essential for assessing the convective heat transfer coefficient and the resulting temperature variations. The Nusselt number is determined for an ambient temperature of 20 °C, as described in Equation (12). In parallel, the dynamic viscosity is calculated using the Sutherland equation, with a reference temperature set at 0 °C.

Table 3. Physical and thermal properties of air.

Property	Symbol ¹	Value	Unit
Density	ρ	1.225	kg/m ³
Dynamic viscosity	μ_r	1.716×10^{-5}	Pa · s
Thermal conductivity	k	0.0241	W/m · K
Specific heat capacity	C_p	1003.5	J/kg · K
Sutherland constant	S_μ	111	K
Inward convection coefficient	$h_{a,i}$	200	W/m ² · K
Outward convection coefficient	$h_{a,o}$	45	W/m ² · K

¹ The subscript r indicates the reference temperature of 0 °C, while ambient conditions are evaluated at 20 °C.

Table 4 provides a comprehensive summary of the simulation parameters, which include contact force, heat generation due to collisions, and the convection calibration factor. The duration of the simulation was set to 60 min in order to align with the empirical findings reported by Takacs in [17]. Given that approximately 90% of the energy loss in metallic systems is converted to thermal energy [50], the collision-induced heat production ratio, denoted η , was determined to be 0.9. The convection calibration factor β is a parameter that modulates the heat transfer from the milling ball to the surrounding air. An increase in this factor leads to a monotonic decrease in the steady-state temperature of the ball. In this analysis, no optimization algorithm was employed for calibration. Instead, a manual method was utilized. The factor value was iteratively modified until the discrepancy between the simulation results and the experimental data was minimized. This technique provided an optimal balance between accuracy and computational efficiency. Through this method, β was determined to be 0.3, allowing the steady-state numerical temperature and the time constant to maintain an error of less than 0.1% compared to the experimental data.

Table 4. Simulation parameters for numerical analysis.

Parameter	Symbol	Value	Unit
Simulation time	t	60	min
Coefficient of restitution	e	0.7	-
Collision heat generation ratio	η	0.9	-
Heat division ratio	λ	0.368	-
Convection calibration factor	β	0.3	-

The inherent non-linearity in the governing equations, mainly attributed to F_d , F_e , and h , makes it impossible to find an analytical solution. To tackle this challenge, the Bogacki–Shampine algorithm [51] was employed using Matlab’s ode23 solver for numerical integration. This solver employs an explicit Bogacki–Shampine method that balances computational efficiency with moderate accuracy. It handles local truncation errors via adaptive step size adjustment, using relative and absolute tolerances to maintain errors within acceptable limits. This approach dynamically alters the step size throughout the integration process to ensure the desired accuracy and boost computational efficiency. This adaptive step-size method decreases the time step when sharp contact forces induce stiffness and increases it during steady non-contact phases, thereby optimizing computational precision and efficiency.

To ensure numerical stability during collision phenomena, the time step must remain below the critical Rayleigh time step. This condition is elaborated upon by [38,52] and can be expressed as follows:

$$t_c = \frac{\pi R}{0.1631\nu + 0.8766} \sqrt{\frac{\rho}{G}}, \quad (40)$$

where G represents the shear modulus of the milling sphere. The Rayleigh time describes the duration necessary for elastic shear waves to traverse a spherical surface. Exceeding this time step results in inaccurate computation of contact overlap, causing unrealistic outcomes such as exaggerated elastic forces or inconsistencies in post-collision momentum. In this investigation, the Rayleigh time, identified as crucial, was calculated to be 6.745 μ s. To ensure stability, the integration timestep during the contact phases was kept consistently at a minimum of 10% below this critical value.

In the course of numerical integration of the system, a total of approximately 4,265,455 temporal solution data points were produced. These calculations were executed sequentially on an Intel® Xeon® Gold 6136 CPU, operating at 3.0 GHz in Santa Clara, CA, USA, with the entire process lasting 41.3 min.

Figure 4 displays the position and momentum curves for the milling ball during the initial 1.0 s, illustrating its kinematics. Consistent with collision dynamics principles, the position exhibits a ramp-like path, while the velocity presents a step-like pattern due to the impulsive characteristics of contact forces. These observations confirm the stability of the numerical integration method, with both the position and velocity remaining within realistic boundaries. This stability is crucial to avoid numerical artifacts, such as overestimated contact forces, which could lead to divergence in the solution. The adaptive time step mechanism within the ODE solver improved numerical stability by keeping the computational time step size sufficiently small to prevent excessive contact overlap. The precise control of step size prevents numerical problems, such as excessive elastic forces or particles that penetrate the boundary walls, thereby ensuring the precision of the simulation. Moreover, the velocity graph's step-like pattern signifies the impulsive nature of high-speed collisions. Swift changes in velocity result from rapid momentum transfers at the vial walls, while constant velocity segments indicate the uninterrupted motion of the grinding ball between impacts. The position graph's ramp-like pattern emphasizes the ball's oscillatory movement, driven by alternating collisions and flights within the vial. These patterns are consistent with theoretical predictions for collision-driven systems, affirming the ability of numerical results to accurately reflect the dynamics of the shaker mill.

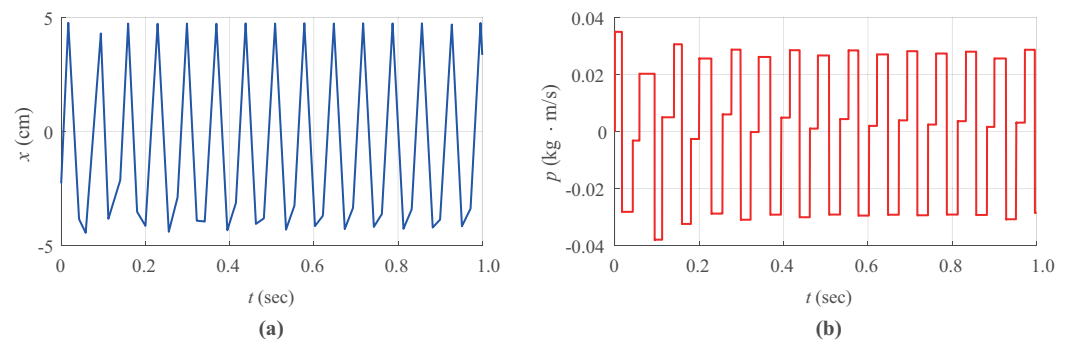


Figure 4. Numerical results: (a) position-time graph, (b) momentum-time graph.

The thermodynamic characteristics of the milling ball, the vial and the internal air, particularly in terms of their temperature changes, are identified by solving the internal energy equations given in Equations (21) to (23). The experimental data presented in [17], combined with the numerical findings from this study, indicate that the temperature increases following a concave upward trajectory, eventually stabilizing at equilibrium. This trend can be analytically approximated by an exponential function with an added constant:

$$\theta(t) = (\theta_0 - \theta_\infty)e^{-\frac{t}{\tau}} + \theta_\infty, \quad (41)$$

where θ_0 is the initial temperature, θ_∞ indicates the steady-state value, and τ is the time constant that defines the rate at which temperature equilibrium is reached. These variables act as performance indicators for assessing the thermal efficiency of the milling operation. Non-linear regression analysis using Matlab's `fit` function was conducted to estimate θ_∞ and τ .

Figure 5 depicts the temperature progression of the milling ball throughout the 60-min simulation interval. In Figure 5a, the fitted curve is presented along with the numerical solution, with the curve fitting applied to more than 4.27 million data entries in the time step. For better clarity, only 20 data points are shown in the graph. Figure 5b offers a magnified view of a 100 ms segment at the 10-min mark, highlighting the alternating thermal effects. A rapid temperature increase is observed when the ball impacts the vial due to collisional

heating, while a slower temperature decrease occurs during the non-contact phase as a result of convective cooling.

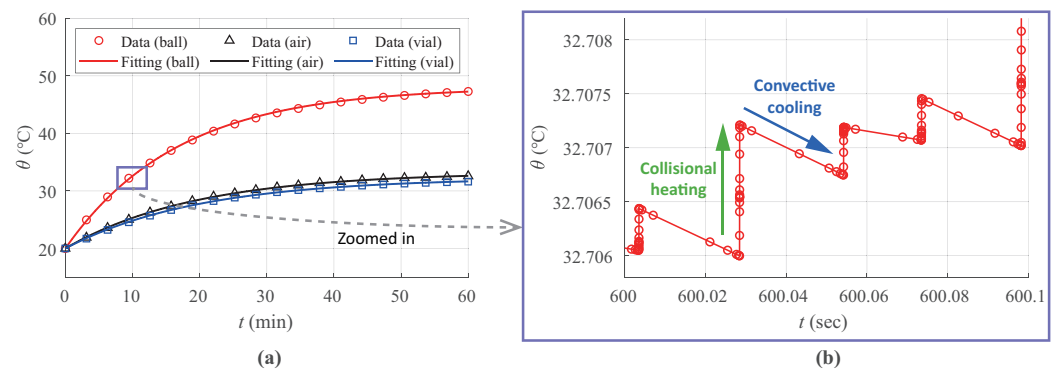


Figure 5. Numerical results: (a) temperature-time plot for the milling ball, air, and vial, (b) detailed view showing the periodic interaction of collisional heating and convective cooling in the milling ball.

The observed temperature increase depicted in Figure 5a is attributed to two alternating mechanisms: collisional heat generation at contact and convective heat dissipation during flight. Initially, collisional heating is predominant because of frequent high-energy collisions. However, as the ball temperature increases, the temperature gradient between the ball and the surrounding air becomes more pronounced. This enhanced gradient increases the rate of convective heat transfer, as described by the last term in Equation (34). Ultimately, the thermal equilibrium is achieved when the rate of heat generation equals the rate of heat dissipation. Equation (18) provides the mathematical representation of this state of equilibrium. At this point, the internal energy change rate ($\dot{U}_b$) is zero, as the heat generation rate, as denoted by the first term ($\lambda \dot{U}^{\text{irr}}$), equals the convective heat dissipation rate, as indicated by the second term ($\dot{U}_b^{\text{conv}}$). This condition indicates that the milling ball has achieved thermal equilibrium, with its temperature attaining a steady-state.

To conduct a more in-depth examination of the thermal properties, the initial rate of temperature change $\dot{\theta}_0$ can be calculated from the regression coefficients θ_∞ and τ via the equation:

$$\dot{\theta}_0 = \frac{\theta_\infty - \theta_0}{\tau}. \quad (42)$$

This formula offers an understanding of the initial energy gain rate within the system and acts as a measure of the efficiency of collisional heating.

Table 5 compares the numerical results obtained in this study with the experimental data reported in [17]. The steady-state temperature θ_∞ , the time constant τ , and the initial temperature change rate $\dot{\theta}_0$ were evaluated. The numerical discrepancies for θ_∞ and τ are 0.24% and 0.03%, respectively, reflecting the high precision of the model. Moreover, the error for $\dot{\theta}_0$ is 0.58%, which underscores the reliability of the numerical method.

Table 5. Comparison of experimental and numerical analysis results for temperatures of milling balls.

Performance Metrics ¹	Experiment	Analysis	Error
Steady-state temperature θ_∞ (°C)	48.0	47.89	−0.24%
Time constant τ (min)	16.7	16.70	−0.03%
Initial temperature evolution rate $\dot{\theta}_0$ (°C/min)	1.6766	1.6702	−0.58%

¹ The parameters θ_∞ and τ were derived via regression analysis employing Equation (41), whereas $\dot{\theta}_0$ was determined with the help of Equation (42).

The research reported in [17] presented experimental data on the correlation between temperature and time for the milling ball in a shaker mill, considering variables such as the number of balls and the presence of powder. However, temperature information for the vial was provided exclusively for scenarios involving five milling balls, which precludes direct comparisons with the numerical findings of this study for the one-ball case. To provide a point of reference, the experimental results for the five-ball case were utilized. For scenarios with five milling balls, the milling ball's temperature rose by 46 °C over one hour, whereas the vial's temperature climbed by 21 °C. This resulted in a vial-to-ball temperature increment ratio of 0.46, indicating the fraction of collision-induced thermal energy transferred to and stored in the vial. Assuming that this ratio remains similar for the single-ball case, the computational results of this study were indirectly evaluated against the experimental data in [17]. The lumped parameter model used in this study, represented by the equivalent circuit model in Figure 2, maintains the system configuration even when the number of milling balls increases, as energy is distributed across the same three reservoirs (milling ball, vial, and air). For the single-ball scenario, the numerical model predicted a vial-to-ball temperature increment ratio of 0.44. The associated simulation yielded an error of −4.35%, indicating considerable accuracy with a numerical error of less than 5%. It should be noted, however, that this comparison is not direct but serves as a reference point for assessing the model's validity under different conditions.

In summary, the numerical results exhibit substantial agreement with the experimental observations, thereby verifying the credibility of the suggested thermomechanical model. The minor numerical deviations observed can probably be attributed to approximations in the viscoelastic contact model and to the assumption of constant material properties. However, the overall accuracy highlights the robustness of the computational framework in predicting collisional heating and thermal behaviors in high-energy milling systems.

5. Conclusions

This paper presents an advanced mathematical model to examine the thermomechanical behavior of high-energy shaker mill systems, which are widely utilized in cutting-edge mechanochemical applications. The purpose of the study is to numerically analyze the dynamic and thermodynamic state variables of a system comprising a milling ball, the enclosing vial, and the internal air. Unlike previous studies that focused solely on the milling ball's thermodynamics, this research integrates the thermal dynamics of the vial and the internal air, significantly expanding the scope of analysis. Within this framework, the milling ball experiences repeated high-energy impacts within a harmonically oscillating vial. The vial and the internal air are treated as lumped thermal reservoirs, characterized by their respective internal energy states. The model employs Hamiltonian mechanics to couple system dynamics and thermodynamics, with generalized coordinates such as position, linear momentum, and internal energy defining the configuration space. Hamilton's canonical equations provided the basis for the derivation of the kinematic equations, while the first law of thermodynamics in its rate form served as a nonholonomic constraint for the evolution of internal energy. To achieve accurate predictions, the governing equations incorporated a viscoelastic contact force model, a collision-induced heat generation model, and a convective heat transfer model, with calibration factors ensuring alignment with experimental data. Numerical simulations demonstrated the capacity of the model to predict the evolution of the temperature of the grinding ball, vial, and air with exceptional precision, achieving steady-state temperature and constant time errors below 0.1%. Furthermore, the temperature evolution of the milling ball displayed a concave upward trajectory, asymptotically stabilizing at a steady-state value. This pattern aligns with experimental observations, thereby validating the robustness of the model.

A notable advancement of this study is the extension of the modeling framework to include the thermal behavior of the vial and internal air, allowing a more comprehensive representation of multiphysics in the shaker mill system. Despite these achievements, the study has certain limitations. It assumes a one-dimensional motion of the milling ball, excluding the more complex three-dimensional dynamics and rotational effects. Additionally, the model simplifies the heating mechanisms by considering only viscoelastic energy dissipation and convective cooling, neglecting other contributors such as Coulomb and rolling friction. These constraints should be taken into account when employing the model in situations involving significant three-dimensional dynamics or noticeable frictional effects. Future research should aim to develop a more sophisticated mathematical model incorporating three-dimensional discrete element methods to simulate translational and rotational kinematics. This would enable a more detailed exploration of additional heating mechanisms and enhance the applicability of the model to broader high-energy ball milling scenarios. These advancements would lead to greater precision in the model and expand its use in various milling processes. Such developments could optimize milling parameters, decrease energy use, and increase the efficiency of material synthesis in high-energy milling contexts.

In conclusion, this study provides a robust and accurate mathematical model for high-energy shaker mill systems, offering key insights into the thermomechanical behavior of the milling ball, vial, and internal air. By addressing significant gaps in existing models and delivering precise numerical results, this work lays a solid foundation for future investigations into high-energy milling processes.

Funding: This research was supported by the Basic Science Research Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education (No. RS-2022-NR075787).

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

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