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Analyzing Stability of Nano-Enhanced PCM via Control Volume Method

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Abstract: This work presents a rigorous numerical and theoretical investigation into the stability characteristics of nano-enhanced phase change materials (NEPCMs) subjected to control volume discretization. The governing energy conservation equation is discretized using a finite volume scheme, incorporating nonlinear thermophysical properties of NEPCMs, modeled via Maxwell-Garnett and mixture theory formulations for thermal conductivity and heat capacity, respectively. An explicit expression for the axial velocity component is derived from the energy balance, linking it to enthalpy evolution, spatial temperature gradients, and grid resolution. A generalized stability criterion is reformulated from the Courant-Friedrichs-Lewy (CFL) condition, parameterized by local thermophysical properties and mesh-dependent quantities. Stability number maps and phase-plane portraits are generated using MATLAB to define feasible computational domains under varying spatial variations. The impact of nanoparticle concentration, enthalpy flux, and thermal diffusion coefficients on the stability regime is systematically quantified. Results demonstrate that stability deteriorates nonlinearly with increasing nanoparticle concentration due to suppressed thermal diffusivity, and that finer spatial grids necessitate exponentially smaller time steps to maintain numerical fidelity. The analysis bridges the gap between physical modeling and numerical stability in NEPCM systems and establishes a robust framework for parameter selection in transient thermal simulations of latent heat storage media.

Keywords: Control Volume Discretization, Enthalpy Evolution, Grid Resolution, Finite Volume Scheme, Nano-Enhanced Phase Change Material; Stability Characteristics.

I. INTRODUCTION

The rising global energy demand, coupled with environmental concerns and the need for sustainable energy alternatives, has driven extensive research into efficient energy storage technologies [17]. Among these, Thermal Energy Storage (TES) systems have emerged as viable options for mitigating the mismatch between energy supply and demand, particularly in solar energy applications. Latent Heat Thermal Energy Storage (LHTES) systems utilizing Phase Change Materials (PCMs) are widely recognized due to their high energy density and the ability to store and release thermal energy at nearly constant temperatures.

PCMs have emerged as effective thermal energy storage media due to their high latent heat and isothermal energy absorption characteristics [28]. However, the inherently low thermal conductivity of PCMs limits their response time in transient thermal systems. To address this limitation, researchers have explored the incorporation of nanoparticles into PCMs, leading to the formation of nano-enhanced phase change materials (NEPCMs), which exhibit significantly improved thermal properties. NEPCMs combine the latent heat of fusion of PCMs with the enhanced thermal conductivity of dispersed nanoparticles, making them particularly suitable for applications such as thermal management in electronics, solar energy storage, and smart building materials.

Despite promising experimental advancements, the numerical modeling of NEPCMs poses challenges due to the complex interplay of conduction, convection, phase transition, and stability constraints. The stability of numerical schemes,

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particularly when solving the governing energy equations using the control volume method (CVM), is sensitive to parameters such as grid size, time step, and thermal properties. The Courant–Friedrichs–Lewy (CFL) condition places critical limits on the allowable spatial and temporal discretization for stable simulations [7]. Existing works largely overlook stability analysis in NEPCM simulations, especially in the context of coupled heat transfer processes within finite control volumes [22, 24].

This study addresses this gap by developing a comprehensive control volume-based stability framework for NEPCM systems. The formulation involves explicit discretization of the energy conservation equation using thermophysical models such as Maxwell's model for thermal conductivity and effective heat capacity relations. The stability criterion, $S = \frac{\Delta x \Delta y}{\Lambda t}$, is systematically evaluated across varying spatial and temporal grids, and its relationship with thermophysical parameters is explored. Furthermore, the study extracts an analytical expression for velocity u_i , derived from the discretized energy equation, and links it directly to energy gradients, thermal diffusivity, and grid resolution. The influence of grid size, time step, and volumetric nanoparticle fraction on the numerical behavior of NEPCMs is systematically analyzed. Phase-plane plots further elucidate the directionality of stability evolution under parametric variation.

II. RELATED WORKS

Several studies have investigated phase change materials (PCMs) in the context of thermal energy storage. [27] emphasized the mathematical modeling and numerical techniques applicable to phase change problems using finite element and control volume methods. [1] reviewed enhancement strategies for PCM performance and highlighted the role of nanoparticle inclusion in improving thermal conductivity.

[26] explored molecular-level enhancements in thermal conductivity due to nanoparticle dispersion and emphasized the Maxwell model as an effective approximation for bulk NEPCM behavior. Similarly, [2] demonstrated the applicability of control volume methods in modeling heat transfer during phase change but did not extend the study to nanoparticle enhancement or numerical stability.

[15] applied control volume discretization for NEPCMs in thermal regulation devices and proposed stability-aware meshing. However, a full analytical linkage between energy equation discretization, stability limits, and velocity evolution was absent. Furthermore, while some works have considered the CFL condition in pure conduction systems, there remains a lack of literature explicitly addressing its impact in the convective and conductive mixed domains of NEPCM systems.

The thermal conductivity model most widely used in NEPCM modeling is based on Maxwell's relation [19], which estimates the effective thermal conductivity of spherical nanoparticle dispersions. Combined with empirical expressions for specific heat capacity and density [16], this model serves as the foundation for control volume discretizations in this study.

[5] and [21] highlighted the need for improved computational models in NEPCM simulation, particularly those that account for enhanced conduction, convection, and latent heat interactions. These models often lack explicit criteria for stability, leading to simulation inaccuracies under certain mesh conditions.

The low thermal conductivity of conventional PCMs, typically in the range of 0.1-0.7 W/mK—remains a critical bottleneck limiting the rate of heat transfer and overall system efficiency. To overcome this drawback, recent studies have proposed the incorporation of thermally conductive nanoparticles into PCMs, creating NEPCMs. The rationale is that nanoparticles such as aluminum oxide (Al $_2O_3$), copper oxide (CuO), carbon nanotubes (CNTs), and graphene exhibit significantly higher thermal conductivities compared to the base PCM. For instance, multi-walled carbon nanotubes (MWCNTs) can have thermal conductivities exceeding 3000 W/mK, while graphene can reach values over 5000 W/mK. These enhancements are expected to facilitate more rapid melting and solidification, reduce thermal gradients, and improve the consistency of thermal cycles.

[18] developed a finite volume numerical model to simulate the melting behavior of NEPCMs within a horizontal cylindrical enclosure. Aluminum oxide (Al $_2O_3$) was selected as the nanoparticle additive. The authors discretized the governing equations for mass, momentum, and energy conservation, applying non-dimensionalization and enthalpy-based

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formulation to analyze thermal interactions during phase transition. The enclosure was heated from the inner cylindrical shell while maintaining adiabatic conditions elsewhere. The simulations accounted for fluid velocity, nanoparticle distribution, and thermophysical property variations using the Maxwell and Brinkman models for thermal conductivity and viscosity, respectively. The findings revealed a direct relationship between enthalpy and thermal energy, with improved energy storage capabilities resulting from the presence of nanoparticles. 3D plots of enthalpy, energy, and velocity demonstrated a strong positive correlation, indicating that increased velocity enhanced convective heat transfer and led to higher stored energy. The introduction of nanoparticles was shown to significantly increase the thermal conductivity and phase stability of the PCM, though at higher concentrations, issues such as agglomeration and sedimentation could reduce uniformity

[17] applied a control volume approach to evaluate the spatial energy distribution in NEPCMs under varying temperature gradients. The researchers modeled the PCM domain using two-dimensional cross-sections and discretized the thermal field using the Finite Volume Method (FVM). The primary focus was to examine how spatial coordinates (Δx , Δy) and temperature difference (ΔT) affected energy concentration and uniformity. The simulation employed characteristic scales and implemented a non-linear enthalpy-temperature relationship to represent the phase change process. The findings noted that energy distribution became more concentrated with higher temperature gradients. Spatial analysis indicated that energy storage was more uniform in regions near the heat source and deteriorated along the Δx and Δy directions, especially under lower thermal gradients. Surface plots further suggested non-linear dependencies between energy, spatial position, and thermal gradients, highlighting complex interactions during the phase change process.

[18, 17] studies concluded that NEPCMs substantially improve the thermal behavior of LHTES systems. The inclusion of nanoparticles not only increased thermal conductivity and energy storage capacity but also enhanced the uniformity of heat transfer and phase stability over multiple cycles.

A. Literature Gap

Despite growing scholarly attention on NEPCMs for thermal energy storage, stability analysis within control volumebased numerical frameworks remains insufficiently addressed. Foundational studies such as [27, 2] employed finite element and control volume methods to simulate classical PCM phase transitions but did not consider the altered thermophysical behavior introduced by nanoparticle inclusion. Critically, these studies omitted key aspects of numerical stability, including timestep sensitivity, mesh resolution, and CFL constraints—factors essential for ensuring the reliability of transient NEPCM simulations.

Subsequent contributions by [1, 26] focused on nanoparticle-driven thermal conductivity enhancements, providing empirical and molecular justification for materials such as Al ₂O ₃, CuO, and CNTs. However, these works did not extend their analysis to control volume discretizations or explore how such enhancements influence numerical stability or convergence.

More recently, [15] proposed meshing techniques for NEPCMs, yet fell short of establishing analytical connections between discretized energy equations, fluid velocities, and stability limits. Although numerical oscillations were acknowledged, explicit stability formulations, especially those based on the Courant number, were not provided.

Studies by [5, 21] highlighted the need for improved NEPCM modeling incorporating latent heat and mixed-mode heat transfer but did not assess the implications of spatial-temporal discretization on simulation robustness.

Closer to the current investigation, [18, 17] utilized finite volume methods to examine NEPCM thermal behavior and spatial energy distribution. While insightful, their studies were primarily empirical, lacking derived velocity expressions, CFL-based criteria, or visualized stability maps to guide mesh and timestep selection.

Across the literature, a clear methodological gap persists: the absence of an integrated framework linking NEPCM thermophysical properties, control volume discretization, and numerical stability. This study addresses that void by analytically deriving discretized energy expressions incorporating thermal conductivity, specific heat, and phase change effects; extracting velocity evolution equations; and formulating Courant-based stability criteria. The work further visualizes stability zones across mesh and material parameters, offering practical guidelines for robust NEPCM simulations.

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B. Contribution

While extensive research has been undertaken on enhancing the thermal performance of nano-enhanced phase change materials (NEPCMs), there remains a notable lack of focus on numerical stability within control volume-based simulation frameworks. Prior studies [27, 2, 1, 26, 15, 5, 21] have either emphasized material-level enhancements or employed discretization methods without systematically addressing mesh resolution, timestep effects, or Courant-Friedrichs-Lewy (CFL) conditions critical for stable and accurate NEPCM modeling. Recent works [18, 17] provided valuable empirical insights into energy behavior and flow dynamics but fell short of developing analytical stability formulations or simulation design maps grounded in discretization theory.

This study addresses this methodological gap by contributing a comprehensive stability-oriented modeling framework for NEPCMs under control volume discretization. The key contributions are as follows:

- i. Analytical derivation of a discretized energy equation that incorporates nanoparticle-dependent thermal conductivity, specific heat, and latent heat effects relevant to NEPCM behavior.
- ii. Formulation of an explicit expression for velocity u_i as a function of enthalpy gradients and grid resolution, linking thermofluid behavior to numerical structure.
- iii. Development of Courant-number-based stability criteria that integrate spatial and temporal discretization scales with material parameters.
- iv. Visualization of stability domains through 3D surface plots, contour maps, and vector field representations across varying spatial steps (Δx , Δy), timestep (Δt), and nanoparticle volume fraction (ϕ).
- v. Proposal of quantitative guidelines for selecting optimal mesh sizes and timesteps to ensure simulation stability and convergence in NEPCM applications.

By bridging the gap between thermophysical modeling and numerical stability analysis, this study offers a robust framework for simulating NEPCMs with high fidelity, thereby supporting the design of reliable, efficient, and scalable thermal energy storage systems.

III. PROPOSED METHOD

In physical geometry and thermal energy systems, solar irradiation represents a fundamental source of heat, which is conveyed through gravitationally driven hot water circulation and stored within a phase change material (PCM) during the melting phase as latent heat. This stored energy is subsequently recovered during the solidification phase when thermal demand arises. To enhance the thermal conductivity and overall energy transfer characteristics of the PCM, a controlled incorporation of aluminum oxide (Al_2O_3) nanoparticles is implemented. These nanoparticles are introduced at low volume fractions and dispersed within a eutectic salt blend comprising sodium nitrate and potassium nitrate in a mass ratio of 3:2. The selection of spherical nanoparticles with diameters approximating 100 nm is deliberate, as their morphology provides a high surface area-to-volume ratio, which significantly augments conductive heat transfer at the microstructural level.

The development of the governing mathematical models for this system is predicated on the assumption of a smooth interfacial boundary, where both the thermal conductivity and latent heat of fusion are modeled as continuous and differentiable functions of temperature. Nevertheless, the modeling of phase change processes is inherently complex due to the presence of a mushy or transition region. This region encompasses a coexisting mixture of solid and liquid phases in which the transformation occurs, inducing non-linear variations in critical thermophysical properties such as density, specific heat capacity, thermal conductivity, and latent heat. These parameters exhibit strong temperature dependency, further complicating the accurate resolution of energy transport mechanisms within the domain. As the phase boundary evolves temporally and spatially, the resultant mathematical formulation assumes the structure of an initial value problem characterized by singularities at the moving interface. This introduces significant numerical challenges in simulation, particularly in maintaining stability and accuracy at the phase front.

As highlighted in [25], three principal modeling strategies are employed to capture the physics of phase change: the sharpinterface model, the enthalpy method, and the phase-field model. The sharp-interface approach conceptualizes the solid and liquid phases as being distinctly separated by an infinitesimally thin boundary [9]. Within this formulation,

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discontinuities are introduced in transport properties such as density, thermal conductivity, and specific heat at the interface. Furthermore, the latent heat of fusion is assumed to be either absorbed or released instantaneously at this boundary, leading to discontinuous (step) changes in thermal properties. Consequently, the governing equations for the solid and liquid domains are derived independently. While this method provides a structured framework for theoretical analysis, it suffers from critical drawbacks: the presence of interface singularities in the mathematical formulation and the need for sophisticated front-tracking algorithms to accurately capture the dynamic evolution of the moving boundary.

A. Boundary Conditions

The physical model representing PCM under consideration is enclosed within an annular cavity formed between two concentric horizontal cylindrical shells with the inner wall considered to be very thin and subjected to a constant heat of 235 °C (1°C higher than the melting point of the PCM) at Γ_1 . The walls Γ_2 , Γ_3 and Γ_4 are under adiabatic conditions, enclosing the domain within which simulation of storing of thermal energy takes place during charging. The source of heat triggers melting of the PCM causing it to move upwards within the domain at an initial velocity of 0.03 m/s. Elementary cross-section of the domain within x and y, is illustrated in Fig. 1.



Fig. 1: Cross-sectional cavity for modelling the phase change process.

The length of the boundaries (x and y) enclosing the domain are in the ratio 1:1 and the boundary conditions are presented in Fig. 2.



Fig. 2: Illustration of the boundary conditions.

$$\Gamma_1 = \{0,1\} \times \{0\}, \ \frac{\partial T}{\partial n} = \varphi \tag{1}$$

This is the bottom wall, Neumann boundary condition specifying heat flux.

$$\Gamma_2 = \{0,1\} \times \{d\}, \ \frac{\partial T}{\partial n} = 0 \tag{2}$$

This is the right vertical wall, adiabatic condition with no heat flux.

$$\Gamma_3 = \{1\} \times \{0, d\}, \frac{\partial T}{\partial n} = 0 \tag{3}$$

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This is the top wall, adiabatic condition with no heat flux.

$$\Gamma_4 = \{0\} \times \{0, d\}, \frac{\partial T}{\partial n} = 0 \tag{4}$$

This is left vertical wall, adiabatic condition with no heat flux.

B. Governing Equations

Under the assumption that the nanofluid constitutes a continuum medium in which thermal equilibrium is maintained between the base fluid and the suspended nanoparticles, the governing equations are systematically derived through the integration of the fundamental conservation principles of mass, linear momentum, and energy. This coupled framework forms the basis for characterizing the thermofluidic behavior and dynamic evolution of the nanofluid system.

i). Conservation of mass

The conservation of mass, formally represented by the continuity equation, stipulates that the temporal variation of mass contained within a control volume VVV must be balanced by the net mass flux across the control surface S

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V} \right) = 0 \tag{5}$$

where ρ is the fluid density and \vec{V} is the fluid velocity vector. Due to incompressibility of the fluid flow after melting process, $\frac{\partial \rho}{\partial t}$ reduces to zero since the density is assumed to be constant and hence the equation becomes

$$\nabla \cdot \vec{V} = 0 \tag{6}$$

However, for problems with moving grids, which involve continuous changes of control volume, this term might be considered depending on the numerical method employed.

ii). Conservation of momentum

A second fundamental formulation emerges from the application of Newton's Second Law of Motion, which establishes a relationship between the net forces exerted on a fluid element and its resulting acceleration. The momentum conservation equation posits that the total change in momentum, comprising both the temporal rate of momentum accumulation within the control volume and the convective (or advective) transport of momentum across its boundaries, is governed by the sum of all external forces acting upon the fluid contained within the control volume. This principle is mathematically expressed as:

$$\left[\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{V}}{\partial t} + \left(\vec{V} \cdot \nabla\right)\vec{V}\right] = -\nabla p + \mu \nabla^2 \vec{U} + \mu \nabla^2 \vec{V} + \rho \vec{g}(T - T_0) + S,\tag{7}$$

The momentum equation in x direction is given by

$$\rho\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right),\tag{8}$$

and momentum equation in y direction

$$\rho\left(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}\right) - \frac{\partial p}{\partial y} + \mu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + \beta\rho g(T - T_r)(9)$$

where ρ is the density, p is the pressure, μ is the dynamic viscosity, t is the time, β is the thermal expansion coefficient of the PCM, g is the gravitational acceleration, T is the temperature, T_r is the reference temperature. Assumptions to be made in phase change process are: the liquid phase of PCM is Newtonian and laminar, incompressible fluid with transient state of flow, all thermophysical properties of the PCM are assumed to be constant, the Boussinesq model is used in the buoyancy force term. In the energy equations, the internal heat generation and the viscous dissipation effect are neglected. The pressure inside the domain is constant and hence $\frac{\partial P}{\partial y}$ and $\frac{\partial P}{\partial x}$ reduce to 0 leaving the momentum equations in x and y direction as:

$$\rho(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y}) = \mu(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})$$
(10)

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$$\rho(\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y}) = \mu(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}) + \beta \rho g(T - T_r)$$
(11)

iii). Conservation of energy

In fluid flow rate of increase in energy of the fluid particles is equal to the sum of net rate of energy gained by fluid particles and net rate of work done on the particles, given below as:

$$\frac{\partial(\rho H)}{\partial t} + \rho c_p \left[u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right] = k \left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right]$$
(12)

The derivation of the energy equation is fundamentally based on the First Law of Thermodynamics, which asserts that the temporal change in the total energy contained within a control volume arises from the mechanical work performed by external forces and the net heat transfer into the system. The Finite Volume Method (FVM) is formulated from the integral form of the conservation laws. Rather than applying differential approximations at discrete points, FVM operates by subdividing the computational domain into a finite number of control volumes and computing the total flux across each volume's boundaries. During each time step, these fluxes are updated based on the flow across the edges of individual control volumes.

The discretization process in FVM involves three primary stages: domain discretization, temporal discretization, and the discretization of the governing equations. Domain discretization refers to the numerical subdivision of the physical domain into discrete elements, typically referred to as control volumes, with each volume associated with a computational point, often located at its centroid—where the dependent variables are evaluated. This procedure is known as grid generation. Time discretization entails the segmentation of the entire simulation period into a finite sequence of small time steps, ensuring numerical convergence and stability. Finally, discretization of the governing equations involves substituting the continuous differential terms with algebraic approximations that relate variable values at adjacent computational nodes within the grid, as schematically illustrated in Fig. 3.



Fig. 3: 2-dimensional control Volume

The following variables are used to non dimensionlize the parameters: time, distance, velocity, temperature and pressure as:

$$t^{*} = \frac{t}{L/U_{\infty}}, x^{*} = \frac{x}{L}, y^{*} = \frac{y}{L}, z^{*} = \frac{z}{L}, u^{*} = \frac{u}{U_{\infty}}, v^{*} = \frac{v}{U_{\infty}}, w^{*} = \frac{w}{U_{\infty}}, p^{*} = \frac{p - p_{\infty}}{\rho/U_{\infty}^{2}}, T^{*} = \frac{T - T_{\infty}}{\Lambda T}, T = T^{*} \bigtriangleup T + T_{\infty}.$$

The flow of molten PCM is governed by continuity equation and momentum equations expressed in cartesian coordinates. Non dimesionalizing (5), yields

$$\nabla = i\frac{\partial}{\partial x} + j\frac{\partial}{\partial y} + k\frac{\partial}{\partial z}$$
(13)

$$\vec{V} = ui + vj + wk \tag{14}$$

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$$\nabla \cdot \vec{V} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}$$
(15)

In 2-Dimensional, (12) becomes,

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \mathbf{0},\tag{16}$$

which upon Non-Dimesionlizing (15), yields

$$\frac{\partial u^* U_{\infty}}{\partial x^* L} + \frac{\partial v^* U_{\infty}}{\partial y^* L} = 0 \tag{17}$$

Factorizing and simplifying (17) results in:

$$\frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0 \tag{18}$$

Discretization of the normalized conservation of mass (18) from an infinitesimal control volume enclosure at the point P = (i, j) results in

$$\int_{t_{k}}^{t_{k+1}} \int_{y_{(j-\frac{1}{2})}}^{y_{(j+\frac{1}{2})}} \int_{x_{(i-\frac{1}{2})}}^{x_{(i+\frac{1}{2})}} \frac{\partial u^{*}}{\partial x^{*}} dx^{*} dy^{*} dt^{*} + \int_{t_{k}}^{t_{k+1}} \int_{y_{(j-\frac{1}{2})}}^{y_{(j+\frac{1}{2})}} \int_{x_{(i-\frac{1}{2})}}^{x_{(i+\frac{1}{2})}} \frac{\partial v^{*}}{\partial y^{*}} dx^{*} dy^{*} dt^{*}$$

$$\tag{19}$$

Integration with respect to time and y yields

$$\Delta t^* \Delta y^* \int_{x_{(i-\frac{1}{2})}}^{x_{(i+\frac{1}{2})}} \frac{\partial u^*}{\partial x^*} dx^* + \Delta t^* \Delta x^* \int_{y_{(j-\frac{1}{2})}}^{y_{(j+\frac{1}{2})}} \frac{\partial v^*}{\partial y^*} dy^*$$
(20)

Discretised equation is then obtained as

$$\Delta t^* \Delta y^* (u^*_{(i+\frac{1}{2})} - u^*_{(i-\frac{1}{2})}) + \Delta t^* \Delta x^* (v^*_{(j+\frac{1}{2})} - v^*_{(j-\frac{1}{2})}) = 0$$
(21)

Re-expressing yields,

$$\Delta y^* \Delta t^* \{ \left(\frac{u_{i+1}^* + u_i^*}{2} \right) - \left(\frac{u_{i-1}^* + u_i^*}{2} \right) \} + \Delta x^* \Delta t^* \{ \left(\frac{v_{j+1}^* + v_j^*}{2} \right) - \left(\frac{v_{j-1}^* + v_j^*}{2} \right) \} = 0$$
(22)

Followed by

$$\frac{\Delta t^* \Delta y^*}{2} \left(u_{i+1}^* - u_{i-1}^* \right) + \frac{\Delta x^* \Delta t^*}{2} \left(v_{j+1}^* - v_{j-1}^* \right) = 0$$
(23)

Simplifying further yields,

$$\Delta y^*(u_{i+1}^* - u_{i-1}^*) + \Delta x^*(v_{j+1}^* - v_{j-1}^*) = 0$$
⁽²⁴⁾

Non-dimensionlizing (8), momentum equation in x-direction using, the non-dimensionalization variables, we get

$$\frac{\partial u}{\partial t} = \frac{U_{\infty}^2}{L} \frac{\partial u^*}{\partial t^*}$$
(25)

Similarly the other partial derivatives are obtained as:

$$\frac{\partial u}{\partial x} = \frac{\partial (u^* U_{\infty})}{\partial x^*} \frac{\partial x^*}{\partial x} = \frac{U_{\infty}}{L} \frac{\partial u^*}{\partial x^*}$$

$$\frac{\partial u}{\partial u} = \frac{\partial (u^* U_{\infty})}{\partial y^*} \frac{\partial y^*}{\partial y^*} = \frac{U_{\infty}}{U_{\infty}} \frac{\partial u^*}{\partial x^*}$$
(26)

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x^*} \frac{\partial x^*}{\partial x} \left(\frac{U_{\infty}}{L} \frac{\partial u^*}{\partial x^*} \right) = \frac{U_{\infty}}{L^2} \frac{\partial^2 u^*}{\partial x^{*2}}$$
(27)

and

$$\frac{\partial^2 u}{\partial y^2} = \left(\frac{U_{\infty}}{L}\frac{\partial u^*}{\partial y^*}\right) = \frac{U_{\infty}}{L^2}\frac{\partial^2 u^*}{\partial y^{*2}}$$
(29)

Substituting (25)-(29) in the momentum (8), yields,

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$$\rho\left(\frac{U_{\infty}^{2}}{L}\frac{\partial u^{*}}{\partial t^{*}} + u^{*}U_{\infty}\frac{U_{\infty}}{L}\frac{\partial u^{*}}{\partial x^{*}} + v^{*}U_{\infty}\frac{U_{\infty}}{L}\frac{\partial u^{*}}{\partial y^{*}}\right) = \mu\left(\frac{U_{\infty}}{L^{2}}\frac{\partial^{2}u^{*}}{\partial x^{*2}} + \frac{U_{\infty}}{L^{2}}\frac{\partial^{2}u^{*}}{\partial y^{*2}}\right)$$
(30)

Multiplying (30) with $\frac{L}{\rho U_{\infty}^2}$ yields:

$$\left(\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*}\right) = \frac{\mu}{\rho L U_{\infty}} \left(\frac{\partial^2 u^*}{\partial x^{*2}} + \frac{\partial^2 u^*}{\partial y^{*2}}\right)$$
(31)

Re-expressing (31) to 0, yields

$$\left(\frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*}\right) - \frac{\mu}{\rho L U_m} \left(\frac{\partial^2 u^*}{\partial x^{*2}} + \frac{\partial^2 u^*}{\partial y^{*2}}\right) = 0$$
(32)

resulting into Non-dimensionlised momentum equation in x direction with Reynolds number $\frac{\mu}{\rho L U_{\infty}} = \frac{1}{Re}$, $Re = \frac{\rho L U_{\infty}}{\mu}$. Refer to Conservation of energy (12), the enthalpy H of PCMs is defined as,

$$H = C_p (T - T_r) + f_l L \tag{33}$$

where f_l is the PCM liquid fraction and L is the latent heat of the PCMs. By caculating the enthalpy H of PCMs, the liquid fraction and temperature can be updated by the following equations

$$f_{1} = \begin{cases} 0, & H \le H_{s} \\ \frac{H - H_{s}}{H_{l} - H_{s}}, & H_{s} \le H < H_{l} \\ 1, & H \ge H_{l} \end{cases}$$
(34)

$$T = \begin{cases} T = \frac{H_s - H}{c_p}, & H \le H_s \\ T_m, & H_s < H < H \\ T + \frac{H_s - H}{c_p}, & H \le H_l \end{cases}$$
(35)

Non-dimensionalizing (12) using the non-dimensionalization variables, yields,

$$\frac{U_{\infty}}{L}\frac{\partial(\rho H)}{\partial t^{*}} + \rho C_{p} \left[u^{*} \frac{U_{\infty}}{L} \frac{\partial(T^{*} \triangle T + T_{\infty})}{\partial x^{*}} + v^{*} \frac{U_{\infty}}{L} \frac{(T^{*} \triangle T + T_{\infty})}{\partial y^{*}} \right]
= \frac{k}{L} \left[\frac{\partial^{2} (T^{*} \triangle T + T_{\infty})}{\partial x^{*2}} + \frac{\partial^{2} (T^{*} \triangle T + T_{\infty})}{\partial y^{*2}} \right]$$
(36)

Multiplying (36) by $\frac{L}{U_{infty}}$ and taking $T_{\infty} = 0$, yields

$$\frac{\partial(\rho H)}{\partial t^*} + \rho C_p \left[u^* \frac{\partial(T^* \Delta T)}{\partial x^*} + v^* \frac{\partial(T^* \Delta T)}{\partial y^*} \right] = \frac{k}{U_m} \left[\frac{\partial^2(T^* \Delta T)}{\partial x^{*2}} + \frac{\partial^2(T^* \Delta T)}{\partial y^{*2}} \right]$$
(37)

Further simplification of (37) as we multiply by $\frac{1}{\Lambda \tau}$ yields,

$$\frac{1}{\Delta T}\frac{\partial(\rho H)}{\partial t^*} + \rho C_p \left[u^* \frac{\partial T^*}{\partial x^*} + v^* \frac{\partial T^*}{\partial y^*} \right] = \frac{k}{U_{\infty}} \left[\frac{\partial^2 T^*}{\partial x^{*2}} + \frac{\partial^2 T^*}{\partial y^{*2}} \right]$$
(38)

Discretizing conservation of energy (38)

$$\begin{split} &\int_{t_{(k)}}^{t_{(k+1)}} \int_{y_{(j-\frac{1}{2})}}^{y_{(j+\frac{1}{2})}} \int_{x_{(i-\frac{1}{2})}}^{x_{(i+\frac{1}{2})}} \left[\frac{1}{\Delta T} \frac{\partial H^{*}}{\partial t^{*}} + \rho C_{p} u^{*} \frac{\partial T^{*}}{\partial x^{*}} \right] \\ &+ \rho C_{p} v^{*} \frac{\partial T^{*}}{\partial y^{*}} dx dy dt \\ &- \frac{k}{U_{\infty}} \int_{t_{(k)}}^{t_{(k+1)}} \int_{y_{(j-\frac{1}{2})}}^{y_{(j+\frac{1}{2})}} \int_{x_{(i-\frac{1}{2})}}^{x_{(i+\frac{1}{2})}} \left[\frac{\partial^{2} T^{*}}{\partial x^{*2}} + \frac{\partial^{2} T^{*}}{\partial y^{*2}}\right] dx dy dt \end{split}$$

(39)

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Integrating the components of (39) yields,

$$\frac{\Delta x^* \Delta y^*}{\Delta T^*} \{H_{k+1} - H_k\} + C_p \frac{\Delta y^* \Delta t^*}{2} u_i^* \left(T_{(i+1)}^* - T_{(i-1)}^*\right) + C_p \frac{\Delta x^* \Delta t^*}{2} v_j^* \left(T_{(j+1)}^* - T_{(j-1)}^*\right) \\ = \Delta y^* \Delta t^* \left(\frac{T_{i+1}^* - 2T_i^* + T_{i-1}^*}{\Delta x}\right) + \Delta x^* \Delta t^* \left(\frac{T_{j+1}^* - 2T_j^* + T_{j-1}^*}{\Delta y}\right)$$
(40)

Hence discretised energy equation is given by

$$S\{H_{k+1} - H_k\} + 0.5A\rho(C_p)u_i^*(T_{(i+1)}^* - T_{(i-1)}^*) + 0.5B\rho(C_p)v_j^*(v_{(j+1)}^* - T_{(j-1)}^*)$$

$$= \frac{k}{U_{\infty}} \{Q(T_{i+1}^* - 2T_i^* + T_{i-1}^*) + R(T_{j+1}^* - 2T_j^* + T_{j-1}^*)\}$$
(41)

where $S = \frac{\Delta x \Delta y}{\Delta T}$, the simplified discretised energy equation after dropping * yields,

$$S(H_{k+1} - H_k) + 0.5A\rho(C_p)u_i(T_{(i+1)} - T_{(i-1)}) + 0.5B\rho(C_p)v_j(T_{(j+1)} - T_{(j-1)}) = \frac{k_{nf}}{U_{\infty}} \{Q(T_{i+1} - 2T_i + T_{i-1}) + R'(T_{j+1} - 2T_j + T_{j-1})\}$$

$$(42)$$

The thermal conductivity of NEPCM is calculated according to the Maxwell model as

$$k_{nf} = k_{PCM} \frac{k_p + 2k_{PCM} - 2(k_{PCM} - k_p)\phi}{k_p + 2k_{PCM} + (k_{PCM} - k_p)\phi}$$
(43)

where k_{PCM} , k_p , and k_{nf} are thermal conductivities of pure PCMs, nanoparticles and NEPCMs respectively.

The density of nanofluid ρ_{nf} is calculated as

$$\rho_{nf} = (1 - \phi)\rho_{PCM} + \phi\rho_p \tag{44}$$

where ρ_{PCM} , and ρ_p are densities of pure PCM and nanoparticles. The heat capacitance of NEPCMs $(\rho c_p)_{nf}$ is defined as

$$(\rho c_p)_{nf} = (1 - \phi)(\rho c_p)_{PCM} + \phi(\rho c_p)_p \tag{45}$$

where $(\rho c_p)_{PCM}$ is the heat capacitance of the PCM, and $(\rho c_p)_p$ is the heat capacitance of nanoparticles. Thermal expansion volume of NEPCMs $(\rho\beta)_{nf}$ is given as

$$(\rho\beta)_{nf} = (1-\phi)(\rho\beta)_{PCM} + \phi(\rho\beta)_p \tag{46}$$

where $(\rho\beta)_{PCM}$ and $(\rho\beta)_p$ are thermal expansion volume of pure PCM and nanoparticles, respectively. The latent heat of NEPCMs is computed as

$$(\rho L)_{nf} = (1 - \phi)(\rho L)_{PCM}$$
(47)

where $(\rho L)_{PCM}$ is the latent heat of pure PCM. Then the corresponding enthalpy of NEPCM H_{nf} is given as

$$H_{nf} = Cp_{nf}(T - T_r) + f_l L_{nf}$$
(48)

C. Stability Criterion

Applying the Von Neumann stability analysis requires that we discretize (42) in both time and space. Let Δt be the time step, and Δx and Δy be the spatial steps in the *x*- and *y*-directions, respectively. The Courant-Friedrichs-Lewy (CFL) condition provides a necessary criterion for stability in numerical solutions of PDEs. For (42) and is attained as outlined in the following steps

1. Step 1: Discretize the equation

To apply the CFL condition, we first discretize each term in both time and space. Let Δt be the time step, Δx be the spatial step in the *x*-direction, Δy be the spatial step in the *y*-direction.

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- 2. Discretizing each term
- (a) Time Derivative Term: Approximating $H_{k+1} H_k$ in the time domain as:

$$H_{k+1} - H_k \approx \frac{\partial H}{\partial t} \Delta t. \tag{49}$$

- (b) Convective Terms: For the convective terms
 - $T_{i+1} T_{i-1}$ and $T_{i+1} T_{i-1}$, we use central differences:

$$T_{i+1} - T_{i-1} \approx 2 \frac{\partial T}{\partial x} \Delta x, \ T_{j+1} - T_{j-1} \approx 2 \frac{\partial T}{\partial y} \Delta y.$$
(50)

(c) Diffusive Terms: For the diffusive terms $T_{i+1} - 2T_i + T_{i-1}$ and $T_{j+1} - 2T_j + T_{j-1}$, we approximate as:

$$T_{i+1} - 2T_i + T_{i-1} \approx \frac{\partial^2 T}{\partial x^2} \Delta x^2,$$

$$T_{j+1} - 2T_j + T_{j-1} \approx \frac{\partial^2 T}{\partial y^2} \Delta y^2.$$
(51)

3. Step 2: Construct the discretized form

Inserting these approximations in (51) into (42) gives a discretized form of the original PDE. Ignoring coefficients for simplicity, the equation can be written in a simplified form as follows:

$$\frac{\partial H}{\partial t}\Delta t$$
 + (Convective Terms) + (Diffusive Terms).

4. Step 3: Apply Von Neumann stability analysis

Von Neumann stability analysis assumes that the solution can be expressed in terms of Fourier modes. Let's assume a Fourier mode solution of the form:

$$T_i^n = \xi^n e^{i\omega x_i}$$

where ξ is the amplification factor and ω is the wavenumber. For stability, we require $|\xi| \le 1$ for all ω .

5. Step 4: Apply the CFL Condition to the Diffusive Term

The CFL condition primarily affects the diffusive term. For stability in two dimensions, the time step Δt must satisfy:

$$\Delta t \le \frac{1}{2} \left(\frac{\Delta x^2}{\alpha_x} + \frac{\Delta y^2}{\alpha_y} \right),\tag{52}$$

where $\alpha_x = \frac{k}{\rho c_p}$ and $\alpha_y = \frac{k}{\rho c_p}$ are the thermal diffusivities in the *x*- and *y*-directions, respectively. Inserting the thermal diffusivity values for this problem, we get:

$$S \le \frac{1}{2} \left(\frac{k}{\rho C_p} \frac{1}{\Delta x^2} + \frac{k}{\rho C_p} \frac{1}{\Delta y^2} \right),\tag{53}$$

which is the final stability criterion derived using the CFL condition. This inequality must hold for the discretized equation to be stable under the CFL condition.

6. Step 5: Interpretation of the CFL Condition

The CFL condition derived above provides a limit on *S* to ensure stability: *S* is limited by a factor that depends on the thermal diffusivity $(\frac{k}{\rho c_p})$, as well as the spatial resolution in both directions (Δx and Δy). – This condition ensures that the numerical solution remains bounded over time.

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IV. RESULTS

A. Numerical Computation

To explicitly extract velocity u_i from (42) (or its discretized form), we isolate it from the full energy balance equation to obtain

$$u_{i} = \frac{1}{0.5A\rho C_{p}(T_{i+1}-T_{i-1})} \left[\frac{k}{U_{\infty}} \left(Q\Delta_{x}^{2} + R\Delta_{y}^{2} \right) - S(H_{k+1} - H_{k}) - 0.5B\rho C_{p} v_{j}(T_{j+1} - T_{j-1}) \right]$$
(54)

where $\Delta_x^2 = T_{i+1} - 2T_i + T_{i-1}$, $\Delta_y^2 = T_{j+1} - 2T_j + T_{j-1}$. Thus, the final expression becomes,

$$u_{i} = \frac{1}{0.5A\rho C_{p}(T_{i+1}-T_{i-1})} \left[\frac{k}{v_{\infty}} \begin{pmatrix} Q(T_{i+1}-2T_{i}+T_{i-1}) + \\ R'(T_{j+1}-2T_{j}+T_{j-1}) \end{pmatrix} - S(H_{k+1}-H_{k}) - 0.5B\rho C_{p}v_{j}(T_{j+1}-T_{j-1}) \right]$$
(55)

Substituting S in (53) into (55) yields

$$u_{i} = \frac{1}{0.5A\rho C_{p}(T_{i+1}-T_{i-1})} \left[\frac{k}{U_{\infty}} \left(Q \Delta_{x}^{2} + R \Delta_{y}^{2} \right) - \frac{k}{2\rho C_{p}} \left(\frac{1}{\Delta x^{2}} + \frac{1}{\Delta y^{2}} \right) \left(H_{k+1} - H_{k} \right) - 0.5B\rho C_{p} v_{j} (T_{j+1} - T_{j-1}) \right]$$
(56)

B. Parameter estimation

The numerical simulations depends on the following parameters estimated in TABLE I.

Parameter	Description	Value range	Value used	Value Computed	Units	Source
ρ_p	Density of Al_2O_3	4 - 4.95	4.5		g/cm ³	[13]
ρ _{ΡCM}	Density of NaNO ₃	2.26	-	2.17		[11]
	Density of <i>KNO</i> ₃	2.11	-	-		[12]
Ср	Heat capacity of <i>Al</i> ₂ <i>O</i> ₃	0.849 - 0.9	0.88	-	J/K	[4]
Ср _{РСМ}	Heat capacity of NaNO ₃	0.072 - 0.298	0.129	0.137		[3]
	Heat capacity of KNO ₃	0.142	-			[10]
β _p	Coefficient of Thermal expansion volume of Al_2O_3	75×10^{-6}	-	75×10^{-6}	/K	[20]
β _{ΡCM}	Coefficient of Thermal expansion volume of <i>NaNO</i> ₃	83×10^{-6}	-	57.2		[6]
	Coefficient of Thermal expansion volume of <i>KNO</i> ₃	$30 - 100 \times 10^{-6}$	40	-		[8]
k _P	Thermal conductivity of Al_2O_3	237	-	-	W/mK	[29]
k _{PCM}	Thermal conductivity of NaNO ₃	0.5 - 0.512	0.512	0.58		[14]
	Thermal conductivity of KNO ₃	0.62	-			[23]

TABLE I: Parameter estimation (Estimation is based on Aluminum Oxide (Al₂O₃) as nano particles) and PCM.

C. Numerical simulation

This section presents the stability and energy response of a NEPCM system using the finite volume discretization of the energy equation. The governing relationships are based on (42), (43),(46), (53) and (56) and Fig. 1 and Fig. 2 from the study. Stability, energy distribution, and velocity behavior are examined across varying spatial and thermal configurations. Fig. 3 illustrate the relationship between nanoparticle volume fraction ϕ , maximum stability criterion S_{max} and the corresponding energy behavior of nano-enhanced phase change materials (NEPCM) when analyzed under the control volume method.

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Fig. 3: Relationship between nanoparticle volume fraction ϕ , maximum stability criterion S_{max} : (a) S_{max} as a function of nanoparticle volume fraction ϕ . (b) Energy content ΔH as a function of nanoparticle volume fraction ϕ . (c) Relationship between Energy and Stability Number S_{max} .

Fig. 3 demonstrates the variation of S_{max} with nanoparticle volume fraction ϕ . Initially, as ϕ increases, S_{max} decreases sharply. This behavior is due to the dominance of the increase in effective density and specific heat $(\rho_{nf}C_{p,nf})$ over the increase in thermal conductivity (k_{nf}) , resulting in reduced thermal diffusivity $\alpha_{nf} = \frac{k_{nf}}{\rho_{nf}C_{p,nf}}$ and hence a lower stability threshold. However, beyond a critical concentration near $\phi = 0.3$, a slight recovery in S_{max} is observed. This rebound suggests a nonlinear interaction governed by the Maxwell-Garnett model and thermophysical balance, indicating an optimal range of nanoparticle loading for numerical stability in simulations.

In Fig. 3, the energy requirement ΔH to achieve a given thermal state is plotted against ϕ . As expected, ΔH increases with ϕ due to the increasing effective heat capacity of the NEPCM. However, after peaking around $\phi = 0.3$, further increases in ϕ contribute less significantly to energy gain. This saturation arises from diminishing returns in heat capacity enhancement and increased thermal resistance due to higher particle loading.

Fig.3 visualizes the relationship between energy and S_{max} . The inverse correlation is evident: as S_{max} decreases, the required energy ΔH to maintain thermal balance increases. This reflects a fundamental trade-off in NEPCM optimization, while higher ϕ enhances energy storage, it also reduces the permissible stability range for numerical schemes. Consequently, achieving thermal efficiency via nanoparticle addition must be balanced against numerical constraints imposed by the stability criterion.

A higher volume fraction improves thermal storage but narrows the stability margin, potentially destabilizing the computation unless finer spatial or temporal discretization is adopted. Therefore, selecting $\phi \approx 0.3$ appears optimal, maximizing energy gain without significantly compromising numerical stability.

D. Stability Analysis of NEPCM in Control Volume Framework

Fig. 4 explore the variation of the maximum stability number S_{max} with respect to discretization parameters Δx , Δy , and the time step Δt . These parameters are critical in defining the numerical stability of the finite volume scheme applied to the simulation of nano-enhanced phase change materials (NEPCM).



Fig. 4: Relationship between nanoparticle volume fraction ϕ , maximum stability criterion S_{max} : (a) Effect of S_{max} on Δx and Δt . (b) Effect of S_{max} on Δx and Δy . (c) Effect of S_{max} on Δy and Δt .

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Fig. 4 reveals that S_{max} decreases nonlinearly with increasing Δt for fixed spatial resolution, while it increases with larger Δx . This indicates that as the spatial resolution becomes finer (i.e., smaller Δx), the numerical scheme becomes more restrictive in terms of allowable time steps, reducing S_{max} . This highlights the trade-off between accuracy and stability in the simulation.

Fig. 4 shows a symmetrical behavior of S_{max} , which is evident when plotted against Δx and Δy . As both spatial steps decrease, S_{max} also decreases significantly, emphasizing the sensitivity of the stability criterion to spatial discretization. The curvature of the surface suggests a quadratic dependence. For practical modeling of NEPCM, it is essential to avoid excessive spatial refinement unless compensated by extremely small time steps.

Fig. 4 extends the insight by focusing on Δy and Δt while fixing Δx . Similar to the previous cases, increasing Δt leads to a sharp decrease in S_{max} , while increasing Δy results in a corresponding rise in stability threshold. This relationship emphasizes the importance of maintaining a proper ratio between temporal and spatial resolutions for achieving stable simulations.

These stability characteristics become particularly significant when simulating NEPCM systems due to their temperaturedependent properties and enhanced thermal conductivity. The use of high-resolution grids to capture phase change fronts or sharp gradients must be carefully balanced against the imposed time step to avoid violating stability constraints. Failure to do so may result in spurious oscillations or divergence in the numerical solution. Thus, optimizing Δx , Δy , and Δt based on local S_{max} profiles is a crucial step in developing a robust and accurate control volume framework for modeling thermal storage in NEPCM systems.

E. Stability Variation with Grid Size, Time Step, Velocity, and Volume Fraction

The stability criterion for numerical schemes such as the FVM is significantly influenced by discretization parameters and thermophysical properties of NEPCMs. Fig. 5 demonstrate how the maximum allowable stability number S_{max} varies with the spatial step Δx , the temporal step Δt , fluid velocity u, and nanoparticle volume fraction ϕ .



Fig. 5: Stability Variation with Grid Size, Time Step, Velocity, and Volume Fraction: (a) Effect of S_{max} on Δt and u, (b) Effect of S_{max} on Δx and ϕ . And (c) Effect of S_{max} on Δx and u.

Fig. 5 shows that increasing the spatial discretization Δx generally increases the maximum stability number S_{max} , especially at lower fluid velocities. However, as velocity increases, S_{max} sharply declines for a given Δx , indicating that finer spatial resolutions become more unstable under high convective conditions. This trend highlights the sensitivity of numerical stability to the advective term, which scales with u_i .

In Fig. 5, S_{max} increases with time step Δt for a fixed velocity. This is expected since larger time steps ease the restrictive nature of explicit schemes; however, for small time steps and high velocities, the stability condition tightens considerably. The vertical gradient in the color map underscores the dominance of convective effects in destabilizing the scheme.

Fig. 5 analyzes the role of nano-enhancement via ϕ on numerical stability. At low values of ϕ , increasing Δx significantly raises S_{max} . However, as ϕ increases, the gain in S_{max} becomes subdued. This phenomenon is linked to the thermal diffusivity $\alpha_{\text{nf}} = k_{\text{nf}}/(\rho_{\text{nf}}C_{p,\text{nf}})$: although k_{nf} increases with ϕ , the rise in heat capacity and density is more substantial,

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leading to a reduction in α_{nf} and thus in S_{max} . The non-linear rise of k_{nf} modeled via the Maxwell equation contributes to a slight rebound in S_{max} at high ϕ , though the effect is minimal. These stability contours are critical for selecting appropriate numerical parameters in control volume simulations. For optimal performance: Use moderate ϕ (typically $\phi < 0.3$) to prevent excessive damping of thermal diffusivity; avoid large u or reduce Δx to maintain stability; and employ adaptive time-stepping to balance between accuracy and convergence when velocity or ϕ increases.

F. Energy-Stability-Velocity Interaction in NEPCM

The relationship between energy, stability, velocity interaction in NEPCM is presented in Fig. 6.



Fig. 6: Stability Variation with Grid Size, Time Step, Velocity, and Volume Fraction for Energy vs. S_{max} vs. velocity u_i and Energy H vs. volume fraction ϕ vs. initial temperature T_i .

Fig. 6 illustrates the relationship between energy, maximum stability number (S_{max}), and inlet velocity (u_i). It is evident that the energy content increases sharply with decreasing S_{max} , especially at lower velocities. This trend highlights the inverse proportionality between numerical stability and energy uptake; as S_{max} decreases (implying reduced stability margins), the system permits higher energy storage. However, this comes at a computational cost, necessitating finer discretization or smaller time steps to maintain accuracy and convergence.

Fig. 6 further expands the energy landscape by plotting enthalpy H as a function of the nanoparticle volume fraction (ϕ) and initial temperature (T_i). The energy rises consistently with both increasing ϕ and T_i , reinforcing the thermophysical enhancement provided by the nanoparticles. Specifically, the increased specific heat and thermal conductivity of the nano-enhanced PCM (NEPCM) contribute to improved heat absorption capacity. However, the shape of the surface suggests nonlinearity in response—likely due to changes in effective thermal diffusivity α_{nf} and its impact on transient heat transport.

These results imply that while increasing ϕ and reducing S_{\max} (e.g., via finer spatial/temporal resolution or slower velocities) improve thermal performance, they also impose stricter numerical stability constraints. For effective control volume simulations, this trade-off must be optimized by selecting ϕ and u_i combinations that maximize energy benefits without violating the S_{\max} threshold. The control volume method's sensitivity to both flow and material parameters is evident, underscoring the need for a coupled thermal-hydrodynamic optimization framework in NEPCM design.

G. Effect of Time Step on Stability

Fig. 7 presents four plots depicting the stability surface S_{max} in the Δx - Δy plane at different time steps Δt (0.10 s, 0.38 s, 0.72 s, 1.00 s), with phase plane representations (quiver plots showing gradient directions) depicting the numerical stability behavior of the finite-volume discretization scheme applied to NEPCM.



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Fig.7 indicate that increasing Δt leads to a proportional decrease in the computed stability values. Specifically, as Δt increases from 0.10 s to 1.00 s, the color gradients in the plots shift toward lower values, and the upper limits of the colorbars reduce from approximately 4×10^{-3} to less than 4×10^{-4} . This inverse relationship highlights the importance of small time steps in maintaining higher numerical stability limits for a given spatial discretization. Fig. 7 indicates that the contour shapes are consistent, with maximum S_{max} values located at the upper-right corner of the phase plane, where both Δx and Δy are large. These phase-plane plots offer a valuable design tool: for any selected Δt , the permissible combinations of Δx and Δy that ensure stability can be readily identified. Moreover, this visualization aids in optimizing computational efficiency by enabling the largest stable time step for a given grid resolution. Therefore, balancing time and space discretization is essential in control volume simulations of NEPCMs, particularly when resolving steep gradients during phase transitions.

Despite the change in magnitude, the gradient directions (red arrows) are consistent:

- Arrows point toward increasing Δx and Δy
- This implies stability improves with coarser grids, reinforcing the idea that small spatial steps reduce the stability margin for a given time step.
- At lower Δt , contour levels are spaced wider, indicating higher stability potential.
- At higher Δt , contours become compressed near the origin, indicating narrower zones of acceptable stability.

This reflects the CFL) condition: as Δt increases, allowable Δx and Δy for stable simulations decrease. In NEPCMs, accurate and stable simulations require proper tuning of time and space steps due to enhanced thermal conductivity and density and coupled heat and fluid flow effects. For finer grid simulations ($\Delta x, \Delta y \rightarrow small$), one must use smaller Δt to remain within the stable envelope. At higher Δt , stability drops rapidly, necessitating more robust schemes or adaptive time stepping. Fig. 7 confirm that stability is directionally governed by increases in both Δx and Δy . Maintaining control over Δt is critical in high relationship with NEPCM simulation equations to avoid numerical divergence.

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V. CONCLUSION

This study establishes a stability-centric numerical modeling framework for NEPCMs using the control volume method. The derived discretized energy equation incorporates thermophysical dependencies including nanoparticle-induced variations in thermal conductivity, specific heat, and density. A novel velocity expression, directly linked to enthalpy gradients and grid resolution, enables quantitative analysis of flow behavior in the melting domain. Key findings indicate that while increasing nanoparticle volume fraction (ϕ) enhances energy storage capacity, it concurrently reduces thermal diffusivity and, by extension, the numerical stability margin. The Courant-number-based stability criterion, expressed as $S = \frac{\Delta x \Delta y}{\Delta t}$ emerges as a pivotal parameter, governing the permissible combinations of spatial and temporal discretization for stable simulations.

Simulations reveal that coarser spatial grids and shorter time steps promote numerical stability, while fine discretization and high nanoparticle loadings necessitate adaptive schemes or tighter CFL control. Phase-plane and contour analyses illustrate directional trends in stability, with arrows consistently favoring larger Δx and Δy , reaffirming the benefits of grid coarsening in maintaining computational robustness. The proposed methodology addresses a critical gap in NEPCM modeling by linking physical parameters to numerical stability via analytical and visual tools. These insights offer practical guidance for the selection of simulation parameters in energy systems design, ensuring accurate, efficient, and stable numerical representations of thermally enhanced PCM domain.

REFERENCES

- [1] B. K. Choure, T. Alam, and R. Kumar. A review on heat transfer enhancement techniques for pcm based thermal energy storage system. *Journal of Energy Storage*, 72:108161, 2023.
- [2] B. K. Choure, T. Alam, and R. Kumar. A review on heat transfer enhancement techniques for pcm based thermal energy storage system. *Journal of Energy Storage*, 72:108161, 2023.
- [3] O. Enea, P. P. Singh, E. M. Woolley, K. G. McCurdy, and L. G. Hepler. Heat capacities of aqueous nitric acid, sodium nitrate, and potassium nitrate at 298.15 k: *cpo of ionization of water*. *The Journal of Chemical Thermodynamics*, 9(8):731–734, 1977.
- [4] T. Engel. The heat capacities of al2o3, uo2 and puo2 from 300 to 1100 k. Journal of Nuclear Materials, 31(2):211– 214, 1969.
- [5] N. Ferroudj, H. Köten, and S. Boudebous. Mixed convection heat transfer and entropy generation in a water-filled square cavity partially heated from below: The effects of richardson and prandtl numbers. *Journal of Applied and Computational Mechanics*, 8(1):282–297, 2022.
- [6] M. M. Ibrahim, V. Ramachandran, K. Sarangapani, and R. Srinivasan. Thermal expansion of sodium nitrate (i). *Journal of Physics and Chemistry of Solids*, 47(5):517–520, 1986.
- [7] B. E. Jebasingh and A. V. Arasu. A detailed review on heat transfer rate, supercooling, thermal stability and reliability of nanoparticle dispersed organic phase change material for low-temperature applications. *Materials Today Energy*, 16:100408, 2020.
- [8] M. Ji, L. Lv, J. Liu, Y. Rong, and H. Zhou. Nano3-kno3/eg/al2o3 shape-stable phase change materials for thermal energy storage over a wide temperature range: Sintering temperature study. *Solar Energy*, 258:325–338, 2023.
- [9] J. Kaiser, S. Adami, I. Akhatov, and N. Adams. A semi-implicit conservative sharp-interface method for liquid-solid phase transition. *International Journal of Heat and Mass Transfer*, 155:119800, 2020.
- [10] M. Kawakami, K. Suzuki, S. Yokoyama, and T. Takenaka. Heat capacity measurement of molten nano3-nano2-kno3 by drop calorimetry. In VII International Conference on Molten Slags Fluxes and Salts, The South African Institute of Mining and Metallurgy, pages 201–208, 2004.
- [11] M. A. Kedzierski. Viscosity and density of aluminum oxide nanolubricant. *international journal of refrigeration*, 36(4):1333–1340, 2013.

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- [12] W. Laue, M. Thiemann, E. Scheibler, and K. W. Wiegand. Nitrates and nitrites. Ullmann's Encyclopedia of Industrial Chemistry, 2000.
- [13] M. Liu, P. Masset, and A. Gray-Weale. Solubility of sodium in sodium chloride: a density functional theory molecular dynamics study. *Journal of The Electrochemical Society*, 161(8):E3042, 2014.
- [14] R. Li, J. Zhu, W. Zhou, X. Cheng, and Y. Li. Thermal properties of sodium nitrate-expanded vermiculite form-stable composite phase change materials. *Materials & design*, 104:190–196, 2016.
- [15] F. Mebarek-Oudina and I. Chabani. Review on nano enhanced pcms: insight on nepcm application in thermal management/storage systems. *Energies*, 16(3):1066, 2023.
- [16] B. Mehta, D. Subhedar, H. Panchal, and Z. Said. Synthesis, stability, thermophysical properties and heat transfer applications of nanofluid–a review. *Journal of Molecular Liquids*, 364:120034, 2022.
- [17] F. A. Misawo, T. T. O. Onyango, and F. O. Nyamwala. A control volume analysis of energy distribution on nanoenhanced phase change material. *International Journal of Recent Research in Interdisciplinary Sciences (IJRRIS)*, 12(2):1–10, 2025.
- [18] F. A. Misawo, T. T. O. Onyango, and F. O. Nyamwala. Heat transfer-based on nano-particles for thermal energy storage in phase change material. *International Journal of Recent Research in Physics and Chemical Sciences* (*IJRRPCS*), 12(1):1–10, 2025.
- [19] S. M. Mousavi, F. Khanmohammadi, and A. A. R. Darzi. Magnetic influence on phase change materials for optimized thermal energy storage: A comprehensive review and prospective insights. *Journal of Energy Storage*, 89:111625, 2024.
- [20] H.-Y. Peng, Y.-A. Wei, K.-C. Lin, S.-F. Hsu, J.-C. Chen, C.-P. Cheng, and C.-S. Yang. Terahertz characterization of functional composite material based on abs mixed with ceramic powder. *Optical Materials Express*, 13(9):2622– 2632, 2023.
- [21] R. K. Rajamony, A. Pandey, M. Samykano, J. K. S. Paw, T. Kareri, I. A. Laghari, and V. Tyagi. Heat transfer and energy performance analysis of photovoltaic thermal system using functionalized carbon nanotubes enhanced phase change material. *Applied Thermal Engineering*, 243:122544, 2024.
- [22] M. K. Rathod and J. Banerjee. Thermal stability of phase change materials used in latent heat energy storage systems: A review. *Renewable and sustainable energy reviews*, 18:246–258, 2013.
- [23] M. Roshandell. Thermal Conductivity Enhancement of High Temperature Phase Change Materials for Concentrating Solar Power Plant Applications. PhD thesis, UC Riverside, 2013.
- [24] S. N. A. Shah, S. Shahabuddin, M. F. M. Sabri, M. F. M. Salleh, M. A. Ali, N. Hayat, N. A. C. Sidik, M. Samykano, and R. Saidur. Experimental investigation on stability, thermal conductivity and rheological properties of rgo/ethylene glycol based nanofluids. *International Journal of Heat and Mass Transfer*, 150:118981, 2020.
- [25] K. Surana, A. Joy, L. Quiros, and J. Reddy. Mathematical models and numerical solutions of liquid-solid and solidliquid phase change. *Journal of Thermal Engineering*, 1(2):61–98, 2015.
- [26] Q. Wang, L. Yang, and J. Song. Preparation, thermal conductivity, and applications of nano-enhanced phase change materials (nepcms) in solar heat collection: a review. *Journal of Energy Storage*, 63:107047, 2023.
- [27] W.-B. Ye and M. Arıcı. Redefined interface error, 2d verification and validation for pure solid-gallium phase change modeling by enthalpy-porosity methodology. *International Communications in Heat and Mass Transfer*, 147:106952, 2023.
- [28] M. M. Zaytoun, M. M. El-Bashouty, M. M. Sorour, and M. A. Alnakeeb. Heat transfer characteristics of pcm inside a modified design of shell and tube latent heat thermal energy storage unit. *Case Studies in Thermal Engineering*, 49:103372, 2023.
- [29] A. Zhang and Y. Li. Thermal conductivity of aluminum alloysâ€"a review. Materials, 16(8):2972, 2023.