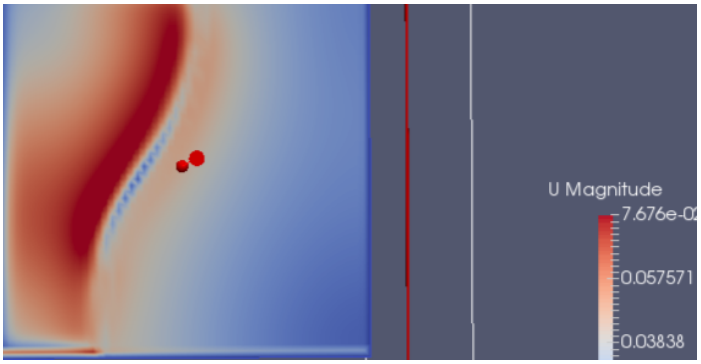
Numerical Simulation of Melt Zone Profiles for Thermal Energy Storage System Design

Report Prepared

by

BioCompScience



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Abstract

The reduction of material cost in energy storage devices is a critical aspect of efficient system design. This study investigates the interface between the melt pool and solid region in a thermal energy storage system using numerical simulation. A heat flux is applied from one side of the storage tank. Initially, heat transfer occurs through conduction; however, as the material melts, convection becomes the dominant mode of energy transfer.

The governing continuity, momentum, and energy equations are solved to analyze the phase change behavior. An enthalpy-based formulation, incorporating latent heat, is used to track the liquid–solid interface, while a momentum sink term is applied to enforce zero velocity in the solid region. The results indicate that optimized thermal behavior can enable a reduction in material usage in the design of energy storage systems.

Contributors

Table 1: List of Contributors for the Project

S.No.	**Name**	**Designation**	**Responsibility**
1	Avinash Kumar	CFD Engineer	Solver Design, Simulation, Pre-processing, post processing
2	Amit Kumar	Thermal Engineer	Simulation
3	Ajay Singh	Thermal Engineer	Provides strategic guidance and decision-making support
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Acknowledgments

BioCompScience and Technology sincerely acknowledges and appreciates the efforts of all employees involved in the successful execution and completion of this project. Their dedication, technical expertise, and continuous commitment played a vital role in achieving the desired outcomes of this work.

The company also extends its sincere gratitude to the client for placing their trust and confidence in BioCompScience and Technology, and for providing the opportunity to undertake and successfully deliver this project. Their valuable support and cooperation were instrumental throughout the course of this work.

We also express our appreciation to all individuals and stakeholders who contributed directly or indirectly to the successful completion of this project.

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Chapter 1

Problem Definition and Objectives

1.1 Introduction

The primary objective of this work is to reduce the cost of materials used in the design of an energy storage system. In this project, Numerical Simulation of Melting using OpenFOAM, the primary objective is to investigate the melting behaviour of a material by determining the evolution of the melting front, molten volume fraction, temperature distribution, and velocity field.

This problem lies at the intersection of heat transfer and fluid dynamics. Heat transfer occurs from a higher temperature region to a lower temperature region through three fundamental modes: conduction, convection, and radiation. When energy is supplied beyond the melting temperature of the material, it induces a phase change. During this process, the supplied thermal energy is absorbed as latent heat, enabling the transformation of solid material into its molten phase while maintaining a nearly constant temperature.

The molten volume fraction is directly governed by the latent heat of fusion. Once the energy input equals or exceeds the latent heat requirement, the material undergoes complete phase transition, resulting in a volume fraction of unity (fully molten state).

To analyze this complex phenomenon, a Computational Fluid Dynamics (CFD) approach is implemented using OpenFOAM. The computational domain is defined as a square block, where one boundary is maintained at a temperature above the melting point, another below the melting point, and the remaining boundaries are treated as adiabatic conditions.

The governing equations solved in this study include the energy equation, momentum equations, and continuity equation. The energy equation is formulated in

terms of enthalpy, which enables accurate tracking of phase change. By incorporating latent heat effects, the position and evolution of the melting front can be predicted, which is otherwise difficult to determine analytically.

This study provides valuable insights for the design and optimization of thermal energy storage systems and other heat-transfer-based engineering applications, where accurate prediction of phase change behaviour is critical.

1.2 Objective

The primary objective of this work is to reduce the cost of materials used in the design of an energy storage system. The following parameters have been investigated to develop an efficient and optimized energy storage system:

1. Determination of the melting zone profile, as the molten region is responsible for storing energy in the form of latent heat as well as sensible heat.
2. Analysis of velocity fields within the molten zone.
3. Evaluation of the temperature distribution.
4. Further relevant design parameters.

Chapter 2

Physical Model and Material Properties

2.1 Physical Model

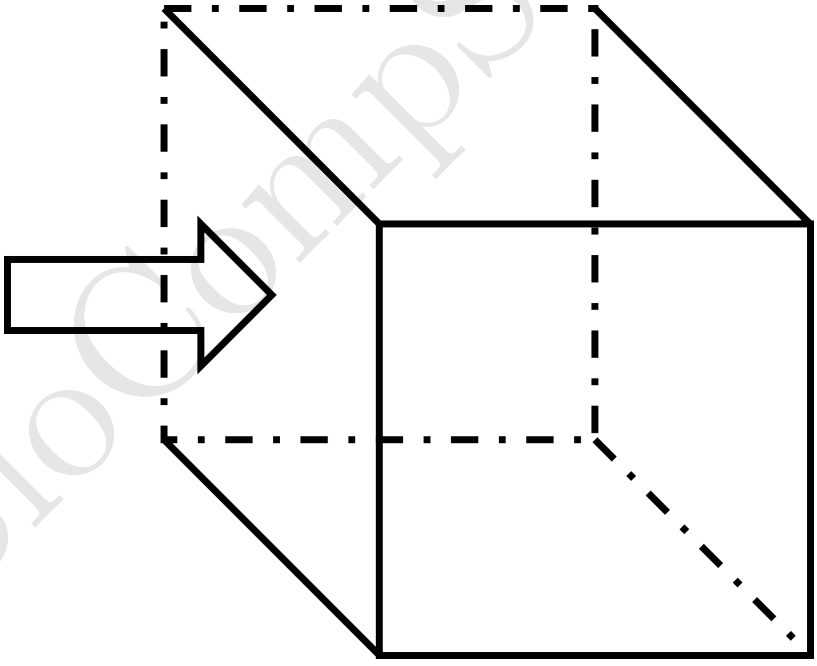


Figure 2.1: Physical domain of energy storage device

The configuration illustrated in Figure 2.1 represents the physical and computational domains used in the design of the energy storage device. The length, width, and height of the device are 50 cm, 50 cm, and 50 cm, respectively. The arrow shown in the physical domain indicates the direction of energy transfer from the energy source to the storage device.

2.2 Material Properties

The material used in this numerical simulation is *n*-octadecane ($C_{18}H_{38}$), an alkane belonging to the paraffin family. The relevant properties of the material are listed below:

1. Material: *n*-octadecane ($C_{18}H_{38}$), paraffin (alkane).
2. Melting temperature: 300 K.
3. Latent heat of fusion: 243,680 J.

Chapter 3

Numerical Model Setup

3.1 Computational Domain

In this study, the initial geometry is a cuboid; therefore, no geometric preprocessing is required, and the computational domain can be generated directly.

3.2 Mesh Generation

In Figure 3.1, the generated mesh used in the computational domain is presented. A highly refined mesh is employed in the region where energy is transferred from the source to the energy storage domain. This fine discretization is necessary to accurately capture the physics and the parameters that vary significantly over time and space.

3.3 Initial Conditions

The initial conditions used in this numerical simulation are listed below:

1. Initial temperature: 293.15 K.
2. Velocity at all nodes is zero.
3. Initial volume fraction of the melted zone is zero.

3.4 Boundary Conditions

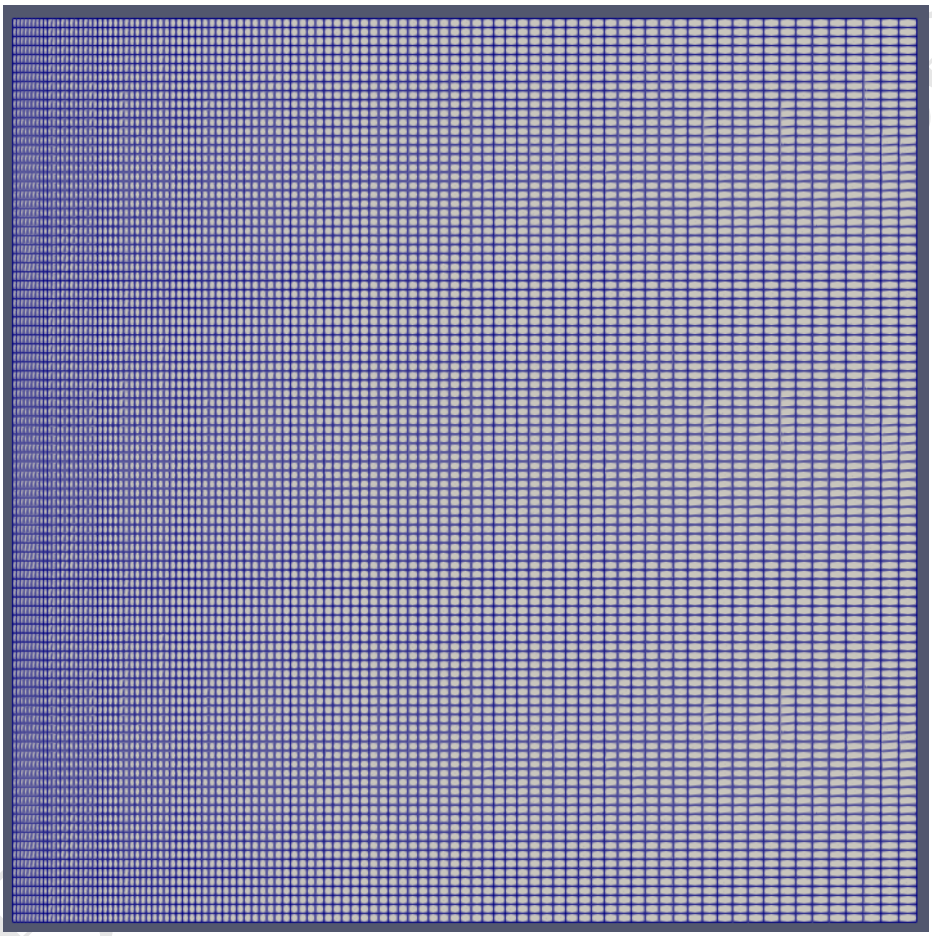


Figure 3.1: Mesh generated for computation.

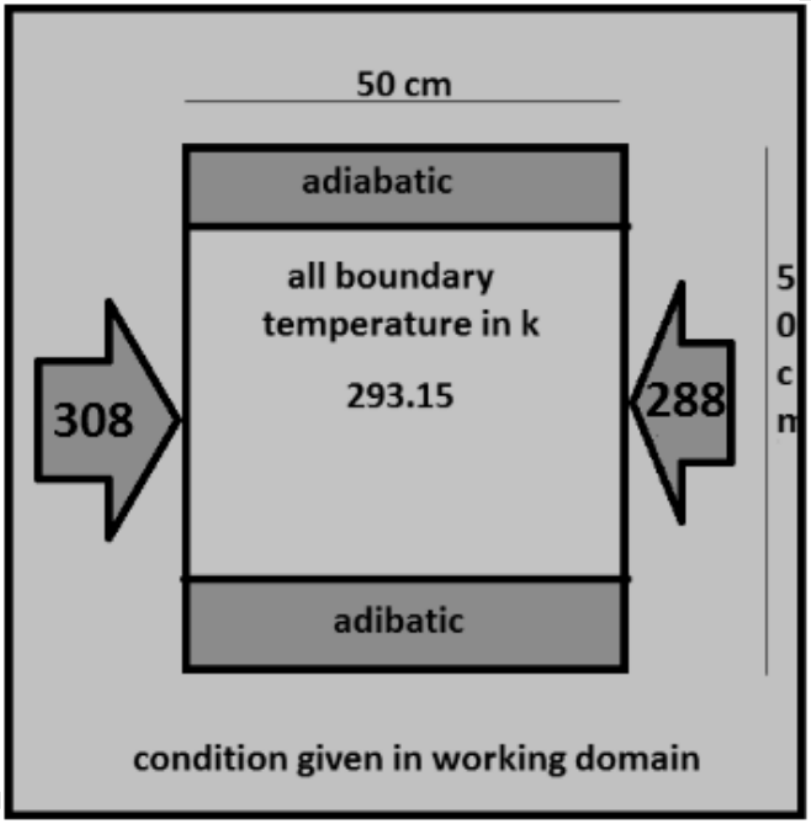


Figure 3.2: Boundary condition applied to computational domain.

Chapter 4

Mathematical Formulation and Numerical Methodology

4.1 Governing Equation

The physics involved in this problem is complex. Initially, heat is transferred within the energy storage device by conduction. Once the solid begins to melt, buoyancy effects generate a velocity field, and convective heat transfer becomes dominant. To determine the temperature and enthalpy distribution, the energy equation is solved, while the motion of the molten material is captured by solving the momentum and continuity equations.

4.1.1 Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{4.1}$$

1. ρ : density ($\mathrm{kg\,m^{-3}}$)
2. $\mathbf{u}$: velocity vector ($\mathrm{m\,s^{-1}}$)
3. $\frac{\partial \rho}{\partial t}$: transient density change
4. $\nabla \cdot (\rho \mathbf{u})$: mass flux divergence

4.1.2 Momentum Equation

In the momentum equation, a sink term is introduced whose value depends on the volume fraction. When the volume of fluid is equal to 1, the sink term becomes zero,

corresponding to free flow. Conversely, when the volume of fluid is 0, the sink term approaches a very large value, effectively restricting motion in the solid region.

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u} + (\rho - \rho_0)\mathbf{g} - S_m \tag{4.2}$$

$$S_m = A\frac{(1-f_l)^2}{f_l^3 + \epsilon}\mathbf{u} \tag{4.3}$$

1. ρ : local density ($\mathrm{kg\,m^{-3}}$)
2. ρ_0 : reference density ($\mathrm{kg\,m^{-3}}$)
3. $\mathbf{u}$: velocity vector ($\mathrm{m\,s^{-1}}$)
4. p : pressure (Pa)
5. μ : dynamic viscosity ($\mathrm{Pa\,s}$)
6. $\mathbf{g}$: gravitational acceleration ($\mathrm{m\,s^{-2}}$)
7. $(\rho - \rho_0)\mathbf{g}$: buoyancy force due to density difference
8. S_m : mushy zone momentum sink ($\mathrm{N\,m^{-3}}$)
9. A : mushy zone constant (typically 10^5–10^7)
10. f_l : liquid fraction (0 = solid, 1 = liquid)
11. ϵ : small number to avoid division by zero

$f_l = 1$ (liquid) $\rightarrow S_m \approx 0 \rightarrow$ free flow
$f_l = 0$ (solid) $\rightarrow S_m \rightarrow \infty \rightarrow$ velocity suppressed
$0 < f_l < 1 \rightarrow$ mushy zone (partial solidification)

4.1.3 Energy Equation

In this project, energy is transferred from the source to the energy storage device. Once the supplied energy exceeds the fusion (melting) threshold, the material begins to melt. To account for the latent heat during this phase change, an enthalpy-based formulation is used, in which the enthalpy depends on the melt fraction of the material.

The energy equation is expressed in terms of enthalpy as follows:

$$H = \begin{cases} c_s\, T, & \text{if } T < T_m \\ c_s\, T_m + c_l (T - T_m) + L, & \text{if } T > T_m \end{cases} \tag{4.4}$$

Here, H represents the enthalpy for both solid and liquid phases.

The transient heat conduction equation can be written in terms of enthalpy. The original equations of the Stefan problem reduce to:

$$\rho \frac{\partial H}{\partial t} = k \nabla^2 T \tag{4.5}$$

The liquid volume fraction is defined to distinguish between solid and liquid phases:

$$g_l = \begin{cases} 0, & \text{solid} \\ 1, & \text{liquid} \end{cases} \tag{4.6}$$

The fraction of melted material is determined based on the fusion energy. Specifically, the liquid volume fraction is calculated as the ratio of the total available enthalpy to the latent heat of fusion.

The total enthalpy of the material, including both phases and latent heat, is expressed as:

$$H = (1 - g_l) \int_{T_{\text{ref}}}^{T} \rho c_s \, dT + g_l \int_{T_{\text{ref}}}^{T} \rho c_l \, dT + \rho g_l L \tag{4.7}$$

Substituting Equation (4.7) into Equation (4.5), the energy equation in terms of temperature becomes:

$$\rho c \frac{\partial T}{\partial t} = k \nabla^2 T - L \frac{\partial (\rho g_l)}{\partial t} \tag{4.8}$$

In this formulation, latent heat is introduced as a source term. During phase change, the temperature remains constant while the material absorbs latent energy.

Initially, heat transfer occurs primarily by conduction. However, once the material begins to melt, a velocity field develops, leading to convective heat transfer. Therefore, the final form of the energy equation is:

$$\rho c \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla (\rho c T) = \nabla \cdot (k \nabla T) - L \frac{\partial (\rho g_l)}{\partial t} \tag{4.9}$$

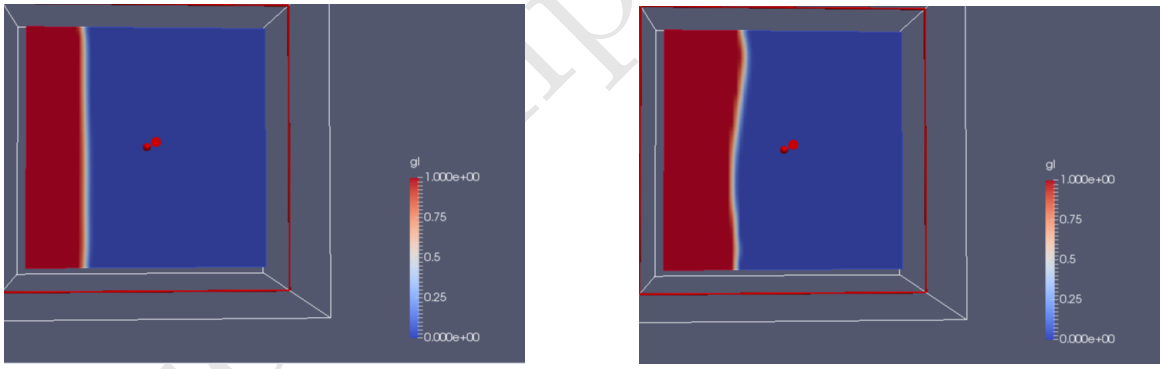
Here, the convective term is included to account for fluid motion in the liquid phase.

Chapter 5

Results and Discussion

5.1 Evolution of the Melt Region

Figure 5.1 illustrates that heat transfer initially occurs primarily through conduction. As the lower-density material begins to rise, fluid motion develops, leading to the formation of velocity fields and the onset of convective heat transfer. In Figure 5.2, convection becomes the dominant mode of heat transfer.

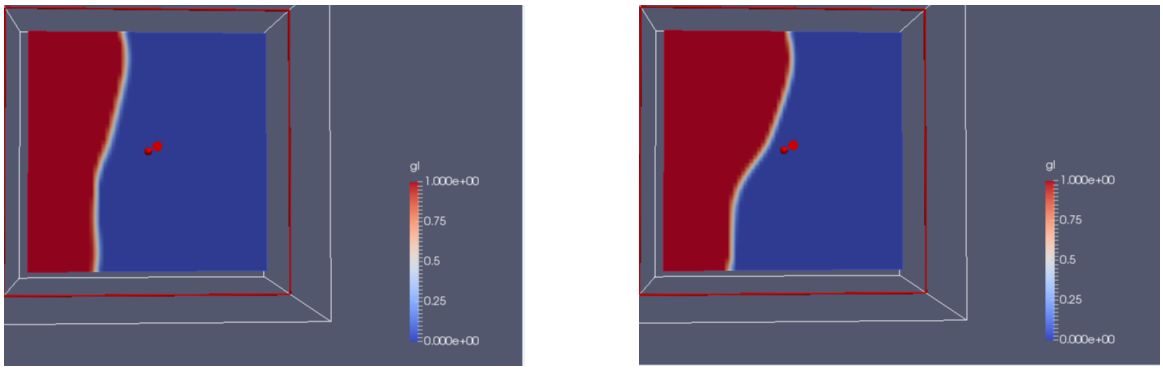


(a) Meltpool region at time t=6s (b) Meltpool region at time t=10s

Figure 5.1: Developed meltpool region at t = 6 s and t = 10 s.

The melt pool profile is a critical feature, as it defines the extent of the melted region and governs the system's energy storage capacity. It also influences the rate of heat transfer, offering insight into how efficiently energy is distributed within the material. Moreover, the profile serves as a valuable guide for designing optimal material configurations, particularly in the development of energy storage devices, where both performance and thermal behavior are key considerations.

The melt pool profile is a critical feature, as it defines the extent of the molten region and directly reflects the amount of energy absorbed and stored within the

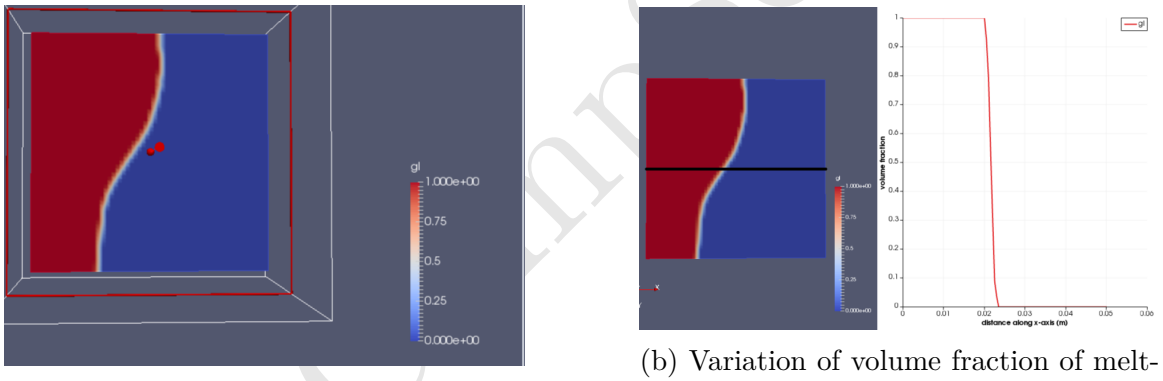


(a) Meltpool region at time t=25 s.

(b) Meltpool region at time t=40 s.

Figure 5.2: Developed meltpool region at t = 25 s and t = 40 s.

system. Its geometry—such as depth, width, and shape—plays a decisive role in determining how heat is distributed and retained over time. A well-formed melt pool indicates efficient energy utilization, while an irregular or unstable profile may lead to uneven thermal gradients and energy losses.



(a) Meltpool region at time t= 60s.

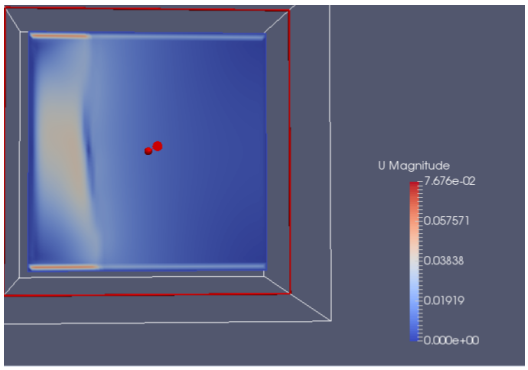
(b) Variation of volume fraction of meltpool region.

Figure 5.3: Developed meltpool region at t = 25 s and Graph to show variation of volume fraction of meltpool region.

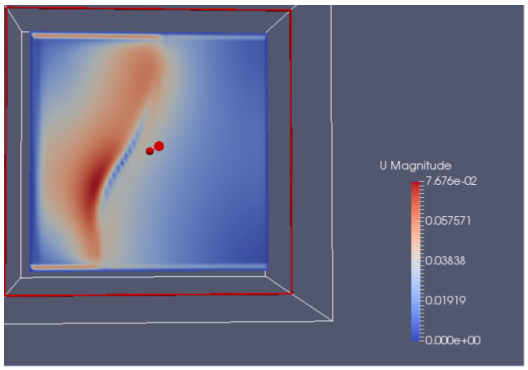
5.2 Flow Field Characteristics

In Figure 5.4, the velocity field is presented. It can be observed that at 8 s, the velocity magnitude is very low, which results in minimal heat transfer through convection.

In Figure 5.5, it can be observed that a well-developed velocity field emerges within the melt pool region. This strong fluid motion promotes the dominance of convective heat transfer, which in turn significantly influences the shape and evolution of the melt pool profile.



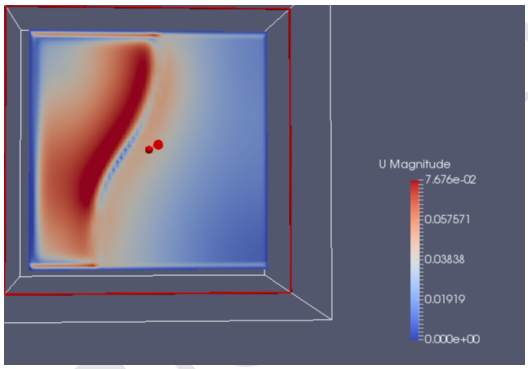
(a) Velocity fields at time t=8s.



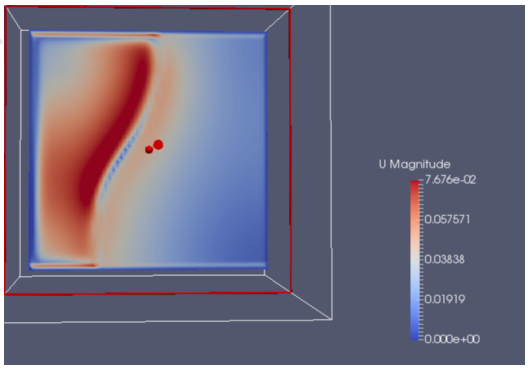
(b) Velocity field at time t=30s.

Figure 5.4: Development of velocity field inside meltpool region at time t= 8s and time t= 30s.

Furthermore, the dominance of convection at these later stages provides important insights for process control and material design. By understanding how fluid flow influences heat transfer and melt pool geometry, it becomes possible to optimize operating conditions for improved energy distribution, better structural integrity, and enhanced performance in applications such as thermal processing and energy storage systems.



(a) Velocity fields at time t= 50s.



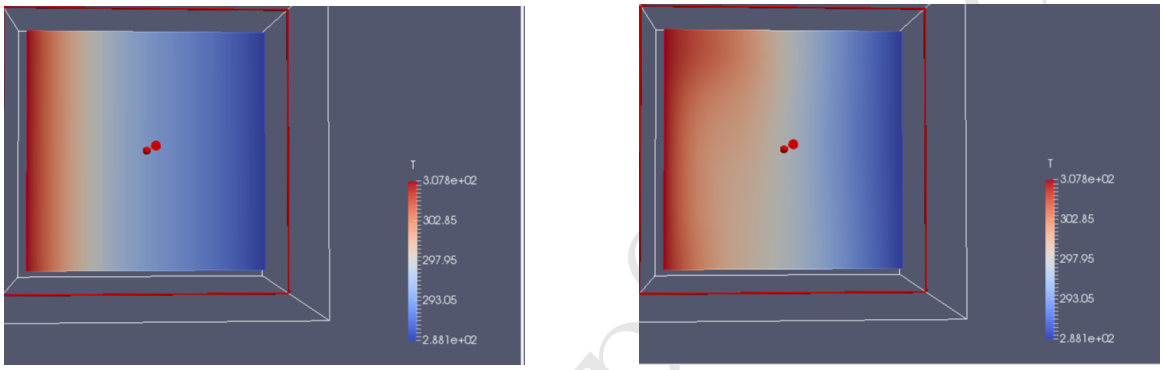
(b) Velocity fields at time t= 60s.

Figure 5.5: Development of velocity field inside meltpool region at time t= 50s and time t= 60s.

5.3 Thermal Field Distribution

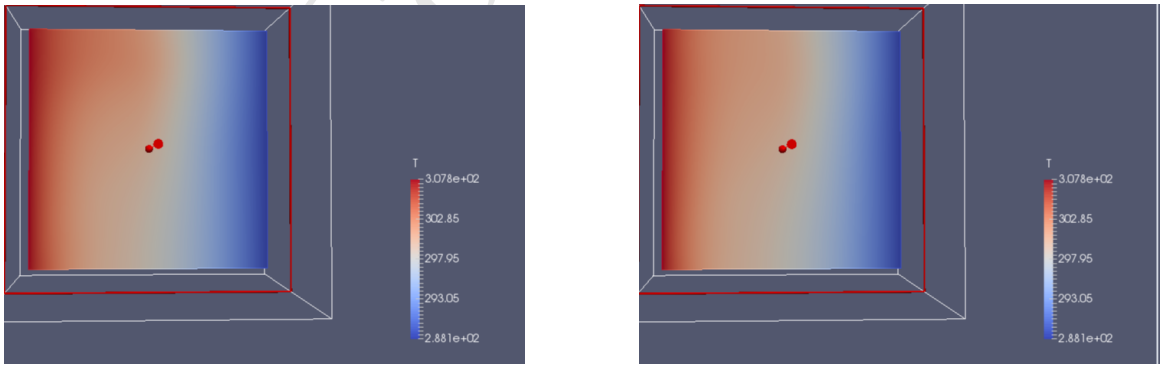
As discussed, the velocity field plays a crucial role in the formation and evolution of the melt pool, as it enhances convective heat transfer within the molten region. Strong fluid motion promotes efficient heat redistribution, which directly influences the size, shape, and stability of the melt pool.

In Figure 5.6, it can be observed that the temperature distribution near the wall is relatively uniform in depth. This indicates that heat transfer in this region is primarily governed by conduction, with limited influence from fluid motion at this early stage.



(a) Temperature field at t= 6s. (b) Temperature field at t=20 s.

Figure 5.6: Variation of temperature at time t= 6s and time t=20 s



(a) Temperature fields at t= 40s. (b) Temperature fields at t=60s.

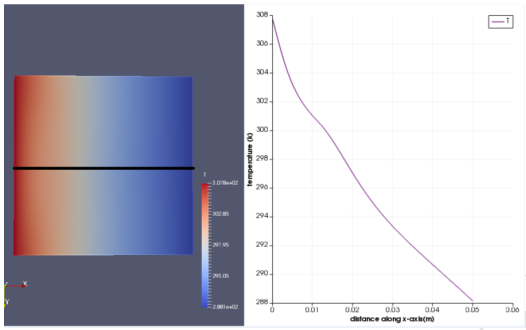
Figure 5.7: Variation of temperature at time t= 40s and time t=60 s

In Figure 5.7, it can be observed that the temperature variation along the vertical direction is no longer uniform. This non-uniformity indicates the increasing influence of fluid motion within the melt pool, leading to the dominance of convective heat transfer. Unlike earlier stages, where conduction governs a more uniform thermal

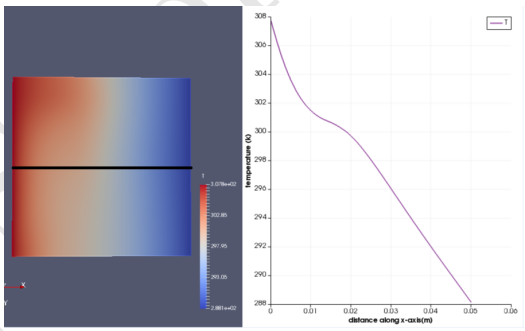
gradient, the presence of convection introduces localized temperature differences due to continuous mixing and circulation of the molten material.

This convective behavior plays a key role in shaping the melt pool region. The enhanced heat transport caused by fluid flow redistributes thermal energy more effectively, resulting in variations in melt depth and profile. Consequently, the melt pool becomes more dynamic and irregular in structure, reflecting the strong coupling between velocity fields and temperature distribution at this stage.

In the figure, the temperature variation has been plotted to illustrate the underlying heat transfer behavior. In Figure 5.8a, the temperature profile exhibits a nearly linear trend, which is characteristic of conduction-dominated heat transfer. This linearity indicates a steady and uniform temperature gradient, with minimal influence from fluid motion.



(a) Variation of temperature along meltpool region at t=10s.



(b) Variation of temperature along meltpool region at t=30s.

Figure 5.8: Variation of temperature along meltpool region at time t=10s and time t=30s.

In contrast, Figure 5.8b shows a clear deviation from this linear profile. The curvature and irregularity in the temperature distribution suggest the increasing influence of convective heat transfer. As fluid motion becomes significant, it disrupts the uniform gradient established by conduction, leading to enhanced mixing and non-uniform temperature distribution. This deviation highlights the transition from conduction-dominated to convection-dominated heat transfer, which plays a crucial role in altering the thermal characteristics and overall behavior of the system.

Chapter 6

Conclusions and Future Work

6.1 Conclusion

In conclusion, the analysis highlights the transition of heat transfer mechanisms and their strong influence on melt pool behavior. At the initial stage, heat transfer is primarily governed by conduction, resulting in uniform temperature gradients and a relatively stable melt region. As time progresses, the development of velocity fields within the molten material initiates and strengthens convective heat transfer.

This shift from conduction to convection significantly alters the thermal distribution, leading to non-uniform temperature profiles and enhanced heat transport. The presence of strong fluid motion not only accelerates energy redistribution but also affects the shape, depth, and stability of the melt pool. Consequently, the melt pool becomes more dynamic, with its geometry closely linked to the intensity of convection.

Overall, the study emphasizes that velocity-induced convection plays a dominant role in later stages, governing both thermal behavior and melt pool evolution. Understanding this interplay between conduction and convection is essential for optimizing material design, controlling process parameters, and improving the efficiency of systems involving melting and energy storage.

This project focuses on the numerical simulation of melting using OpenFOAM. It is highly relevant in engineering, particularly for the design of thermal energy storage systems. Such systems are increasingly important today because they enable the storage of solar energy, which is a clean and non-polluting energy source.

The numerical simulation of melting is a complex problem due to the involvement of phase change. One of the key challenges is tracking the moving solid–liquid interface, which cannot be predicted in advance. Various numerical methods, such as the Volume of Fluid method and front-tracking techniques, are commonly used to

address this issue.

In this study, adiabatic boundary conditions are applied to some walls. However, in practical applications, perfectly adiabatic conditions are not achievable, and some heat loss from these walls is inevitable.

At the initial stage of the simulation, heat transfer is dominated by conduction. As melting progresses and the liquid phase develops, fluid motion begins, leading to the dominance of convective heat transfer.

Mesh generation also plays a crucial role in the accuracy of the simulation. A finer mesh generally provides more accurate results but significantly increases computational time.

Additionally, a higher temperature difference between the hot and cold regions accelerates the melting process.

To model the solid phase, an additional term is introduced in the momentum equation to suppress velocity in solid regions. However, this approach is not perfectly accurate, as small non-zero velocities may still appear in the solid phase, introducing some error into the solution.

6.2 Future work

This project focuses on the numerical simulation of melting, which is inherently a complex problem due to the presence of phase change and the movement of the solid–liquid interface. Accurately tracking this moving interface remains a major challenge, and various numerical approaches have been developed for this purpose. Different methods can be implemented to capture the evolution of the interface effectively.

In this study, two phases are involved, each with distinct thermophysical properties. Moreover, these properties vary with temperature, which adds further complexity to the simulation. To address this, appropriate interpolation models can be used to represent the variation of thermophysical properties with temperature.

Additionally, a moving heat source can be implemented as a boundary condition to better represent realistic thermal processes. The model can also be extended by incorporating temperature-dependent thermophysical properties, improving the accuracy of the simulation.

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