



Influence of Natural Convection on Design of Thermal Diodes

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ABSTRACT

Thermal diode, analogous to the electrical diode, is an emerging field of interest due to its potential application in thermal management, thermal shielding, and thermal circuits. Application of Phase Change Material (PCM) is among the different approaches proposed and analyzed to achieve high thermal rectification. However, these studies often limit the analysis to conduction heat transfer and neglect advection. In the present study, the influence of natural convection on conventional single PCM-based thermal diodes' thermal rectification has been analyzed. Natural convection enhances heat transfer in the inverse direction of gravity, augmenting thermal rectification of diodes with preferential flow in the opposite direction of gravity, whereas adversely affecting the performance of thermal diodes with preferential flow in the direction of gravity. Therefore, the design of thermal diode with preferential flow in gravity direction is modified to limit natural convection via the use of metal foam and baffles. The non-phase change material in a thermal diode with preferential flow in the direction inverse to the gravity is replaced with phase change material augmenting the natural convection because of the increase in length. The modified designs led to a mean thermal rectification enhancement of approximately 85% and 1275% in thermal diodes with preferential towards gravity and inverse to the gravity directions, respectively. A thermal rectification of more than 50 is achieved in a modified thermal rectifier for preferential flow in the direction inverse to the gravity.

1. Introduction

Thermal diodes are devices that allow the flow of thermal energy in a preferred direction and limit the flow of thermal energy in the opposite direction. Thermal rectification, which is defined as the ratio of heat transfer rate in the preferred direction to that in the opposite direction under the same temperature bias, is used to quantify a thermal diode's potential. An ideal thermal diode will yield a thermal rectification of infinity, i.e., it does not allow the flow of thermal energy in the opposite direction. Starr et al. [1] in 1936 first observed thermal rectification in a composite of copper and copper oxide. The thermal diode has attracted the attention of several researchers due to its potential application for the development of thermal logic gates, thermal transistors, thermal memory, thermal shielding, and thermal management system.

Several approaches have been proposed and investigated in the literature to achieve thermal rectification. O'Callaghan et al. [2] proposed and analyzed a thermal rectifier made from a stack of thin disks with a smooth and another artificially roughened surface. Chang et al. [3] developed and analyzed thermal rectifiers based on non-homogeneous loading of highly conductive carbon and boron nitride

with heavy molecules. Schmotz et al. [4] fabricated a thermal rectifier by drilling holes of different shapes in a thin silicon membrane using a focused ion beam. Sawaki et al. [5] developed a thermal rectifier using two different composites with positive and negative dependence of thermal conductivity on temperature arranged in different asymmetric shapes. Recently, few researchers have studied PCM-based thermal diodes due to difference in PCM's thermal conductivity in its solid and liquid states [6–10]. However, the studies assume heat transfer to occur primarily through conduction and neglects advection [7–10]. Advection can be neglected in miniaturized and nano-scale systems; however, advection dominates conduction in micro and macro scale systems. The presence of advection leads to multi-fold enhancement in the heat transfer compare to conduction-based heat transfer. Therefore, it is essential to understand the influence of advection on thermal diodes and modify their design to optimize performance in the presence of natural convection.

The present study is categorized into three parts; in the first part, conventional single PCM based thermal diodes are introduced and analyzed assuming conduction based thermal transport. In the subsequent part, the influence of natural convection on thermal rectification is analyzed. The findings highlight the need to consider advection in

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Nomenclature		Greek symbols	
A	Area (m^2)	α	Thermal diffusivity ($m^2 \cdot s^{-1}$)
C_p	Specific heat capacity ($J \cdot kg^{-1} \cdot K^{-1}$)	β	Thermal expansion coefficient (K^{-1})
Gr	Grashof number	γ	Thermal rectification
g	Acceleration due to gravity ($m \cdot s^{-2}$)	ϑ	Kinematic Viscosity ($m^2 \cdot s^{-1}$)
h	Convective heat transfer coefficient ($W \cdot m^{-2} \cdot K^{-1}$)	μ	Dynamic Viscosity ($kg \cdot m^{-1} \cdot s^{-1}$)
k	Thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$)	Subscript	
K	Permeability (m^2)	c	Cold
L	Height of liquid layer (m)	f	Forward
Nu	Nusselt number	h	Hot
Pr	Prandtl number	l	Liquid
q	Heat transfer rate	m	Melting
Ra	Rayleigh number	r	Reverse
T	Temperature (K)		

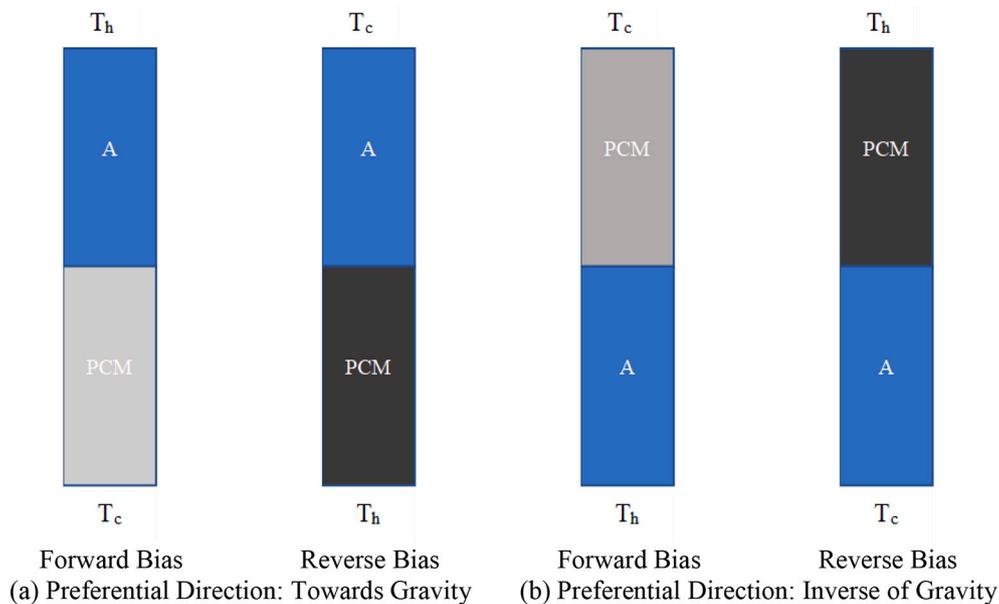


Fig. 1. Schematic of conventional single PCM based Thermal Diodes.

designing PCM based thermal diode. Furthermore, in the third part, modifications required in the design of thermal diode in the presence of natural convection has been discussed. Novel designs of thermal diodes have been proposed and analyzed in the presence of natural convection. These novel designs significantly augments the thermal rectification compared to conventional thermal diodes. *n*-octadecane is chosen as PCM for the present study because of stability, commercial availability, and its melting temperature being close to room temperature. A range of temperature biases has been analyzed with the hot side temperature varying from $T_m + 5$ to $T_m + 25$, and the cold side temperature varying from $T_m - 25$ to $T_m - 5$.

2. Conventional single PCM-based Thermal Diode

The difference in PCM's thermal conductivities in its solid and liquid states is primarily exploited for thermal rectification. In a single PCM based thermal diode, a combination of PCM and another material that does not undergo a phase transition in the operational range is utilized. PCM and non-phase change material are arranged such that PCM remains in a high thermal conductivity state when forward temperature bias is applied and in a low thermal conductivity state when a reverse

temperature bias is applied. In general, PCMs in the liquid state have lower thermal conductivity compared to their solid-state. Therefore, thermal diodes are designed such that the PCM is closer to cold boundary temperature under the forward bias, whereas vice-versa in reverse thermal bias. Figs. 1(a) and 1(b) shows the schematic diagrams of thermal diodes having preferential flow in the direction of gravity and inverse to the gravity, respectively. Non-phase change material has been placed on top in Fig. 1(a) such that PCM largely remains in the solid-state when the top surface is exposed to high temperature while maintaining a lower temperature on the bottom surface, whereas, in Fig. 1(b), orientation is inverted to keep PCM in the solid-state when bottom surface is exposed to a higher temperature. The Fourier law of conduction governs the heat transfer and is employed to calculate the heat transfer rate under a quasi-steady state, as given by

$$q = -kA \frac{dT}{dx}, \quad (1)$$

where q is the rate of heat transfer, and k is the thermal conductivity. Thermal rectification is calculated as the ratio of heat flow in the forward direction to that in the reverse direction in quasi-steady-state condition, as given by

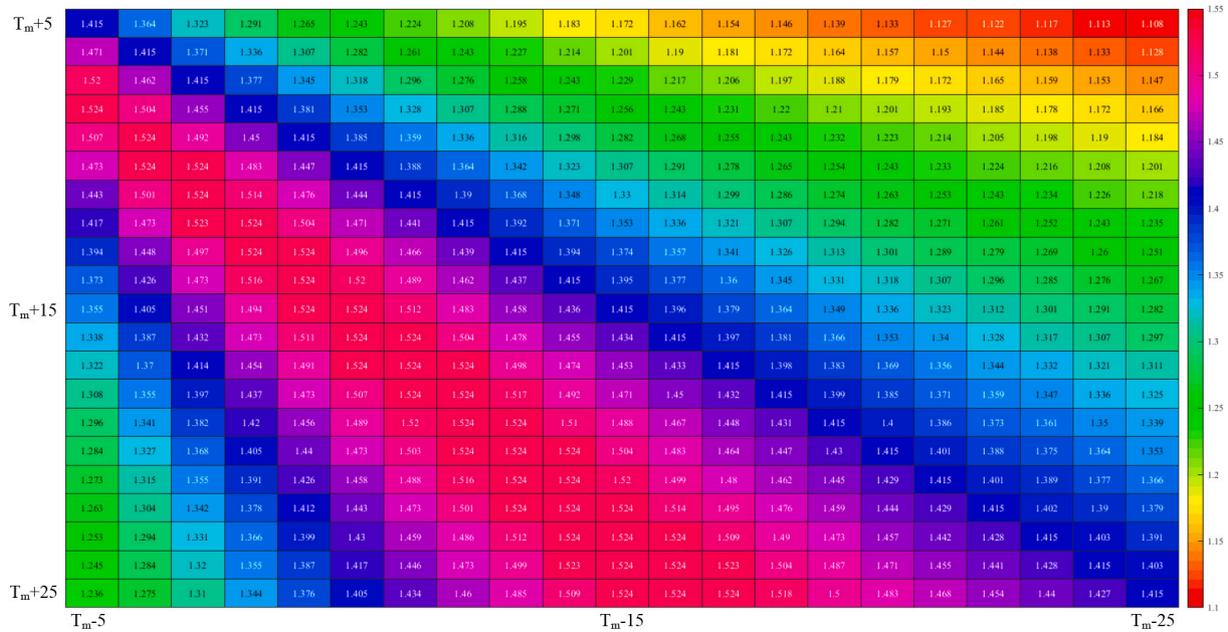


Fig. 2. Thermal Rectification obtained using conventional Thermal Diode assuming conduction to be dominant mode of heat transfer.

$$\gamma = \frac{q_f}{q_r}, \tag{2}$$

where q_f and q_r are the heat transfer in forward and reverse directions, respectively. Thermal rectification is calculated for thermal diodes shown in Fig. 1, with *n*-octadecane as PCM with boundary temperature on the hot side varying between $T_m + 5$ and $T_m + 25$ and on the cold side between $T_m - 25$ and $T_m - 5$. The thermal conductivity of non-phase change material is assumed to be the mean of PCM’s thermal conductivities in solid and liquid states. The length of both PCM and non-phase change material is assumed to be 5 cm each for the present study. The thermal rectification for both thermal diodes shown in Fig. 1 is the same under the assumption of pure conduction based thermal transport since the orientation of the thermal diode is inverted for reverse preferred thermal flow direction. Maple 18 and Octave 5.2 are employed to calculate thermal rectification using the correlations given by Eqs. (1) and (2). Fig. 2 shows the contour plot of thermal rectification of diodes shown in Fig. 1, assuming heat transfer to be predominantly through conduction. Thermal rectification varied between 1.1084 and 1.5237, with the mean thermal rectification being 1.3704. Higher thermal rectification has been achieved in literature upon optimizing the thermophysical properties of PCM, dimensions of the thermal diode, and selection of temperature bias [10]. However, the present study’s objective is to analyze the influence of natural convection and subsequently propose and validate the modification in the design of the thermal diode. Furthermore, from the thermal management/shielding applications perspective, such optimization has little relevance as the temperature bias experienced by the thermal diodes varies; hence, the thermal diode operation need not be restricted to a specific design point. Therefore, analysis has been conducted in the present study over a range of operating temperatures.

A higher thermal rectification is achieved when PCM is in the solid-state when exposed to a forward temperature bias and in the liquid state when exposed to reverse temperature bias, i.e., the phase-transition temperature of PCM lies in non-phase change material. Cottrill and Staro [10] showed that the highest thermal rectification is achieved when the phase-transition temperature coincides with the boundary between PCM and non-phase change material. Therefore, higher thermal rectification is achieved for specific combinations of temperature on hot and cold sides, which depends on PCM’s thermal conductivity in

solid and liquid states, as observed in Fig. 2. A higher temperature difference between the hot side and melting temperature compared to that between the cold and melting temperatures leads to PCM being largely in the liquid state even under forward temperature bias, resulting in an insignificant change in thermal resistance upon changing the direction of temperature bias. Similarly, a larger temperature difference between the cold side and melting temperature than that between hot and melting temperatures results in PCM being largely in the solid-state even in reverse temperature bias. The smaller change in the thermal resistance upon changing the direction of temperature leads to a marginal change in the forward and reverse the direction of heat flux. Hence, under large asymmetric temperature differences, thermal rectification is low, as observed in Fig. 2.

3. Influence of natural convection

The volume of materials varies with temperature based on their molecular arrangements, which results in the variation of their density with temperature. PCM in their liquid state generally expands with an increase in temperature, leading to decreased density with an increase in temperature. The presence of the high-temperature boundary on the bottom side increases the temperature of the PCM near the bottom side, reducing their density. In the liquid state at the bottom, PCM at higher temperature has lower density and experiences a buoyant force in the inverse gravity direction. The presence of viscous and inertia force limits the motion of fluid caused by buoyancy. Rayleigh number (*Ra*) is a dimensionless quantify which is used to characterize the flow associated with natural convection. Rayleigh number is defined as a product of two dimensionless numbers, i.e., Grashof number (*Gr*) and Prandtl number (*Pr*), as given by [11]:

$$Ra = GrPr = \left(\frac{g\beta(T_1 - T_2)L^3}{\nu^2} \right) \left(\frac{\nu}{\alpha} \right) = \frac{g\beta(T_1 - T_2)L^3}{\alpha\nu} = \frac{\rho^2 g\beta C_{pl}(T_1 - T_2)L^3}{k_l \rho}, \tag{3}$$

where, $(T_1 - T_2)$ is the temperature difference across which natural convection takes place, and L is the height of the liquid layer. As the higher temperature fluid moves upward, it carries thermal energy, resulting in advective thermal transport. Nusselt number (*Nu*) is a

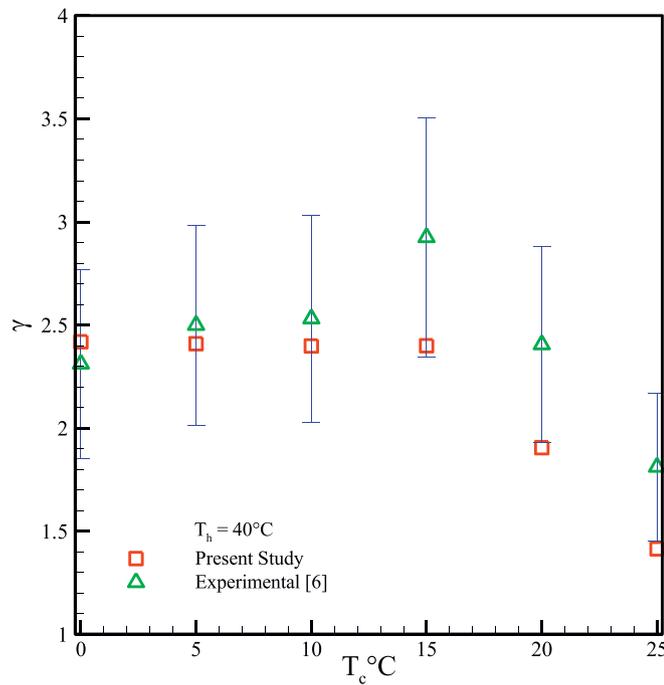


Fig. 3. Comparison of experimentally observed and numerically computed thermal rectification.

dimensionless quantity defined as the ratio of convective and diffusive thermal transport, as given by:

$$Nu = \frac{hL}{k_i} \tag{4}$$

where h is the convective heat transfer coefficient. The Nusselt number remains 1, i.e., thermal transport is purely through diffusion until a critical Ra is achieved. Critical Ra for heat transfer in an enclosure heated from the bottom is 1708. Nusselt varies with the Ra beyond critical Ra , depending upon the flow regime, i.e., laminar, transition, and turbulent flow. Nusselt for an enclosure with a heated bottom surface for different regimes is given by [11,12]:

$$Nu = \begin{cases} 1 & Ra < 1708 \\ 0.178Ra^{0.269} \left(\frac{Pr+1}{Pr}\right)^{0.02} & 1708 < Ra < 10^5 \\ 0.069Ra^{1/3} Pr^{0.074} & 3 \times 10^5 < Ra < 7 \times 10^9 \end{cases} \tag{5}$$

The heat transfer rate in the presence of natural convection is calculated as:

$$q = hA(T_1 - T_2) = \frac{Nuk_iA(T_1 - T_2)}{L} \tag{6}$$

whereas, heat transfer rate in non-phase change material and PCM in the solid state is calculated using Eq. (1). The convective heat transfer depends upon the isoflux surface temperature and height of liquid layer, which in turn depends upon the heat transfer rate. Therefore, an iterative approach is required to compute the heat transfer rate in the presence of natural convection.

The fluid motion is absent in the presence of a higher temperature boundary on top, as the low-density PCM remains on top. Therefore, Nusselt number remains 1 in the presence of a higher temperature boundary condition on the top side. The model is validated using experimental results published in literature [6]. Fig. 3 shows the thermal rectification computed and experimentally observed by Meng et al. [6]. Thermal rectification is found to be within the experimental uncertainty.

The influence of natural convection on thermal rectification of thermal diodes shown in Fig. 1 is analyzed in the following sub-sections. Thermal rectification is calculated using the same definition, i.e., given by Eq. (2).

3.1. Preferential direction: Gravity

The presence of natural convection augments heat transfer in the direction inverse to the gravity, adversely affecting the performance of thermal diodes with preferential heat flow in the direction of gravity. Fig. 4 shows the thermal rectification in the presence of natural convection for a range of temperature biases, for thermal diode shown in Fig. 1 (a). The thermal rectification varies from 0.50078 to 0.66191, with the mean thermal rectification being 0.62768. The thermal rectification of less than 1 signifies that the thermal resistance is higher in the preferred direction rather than in the reverse direction. Therefore, a

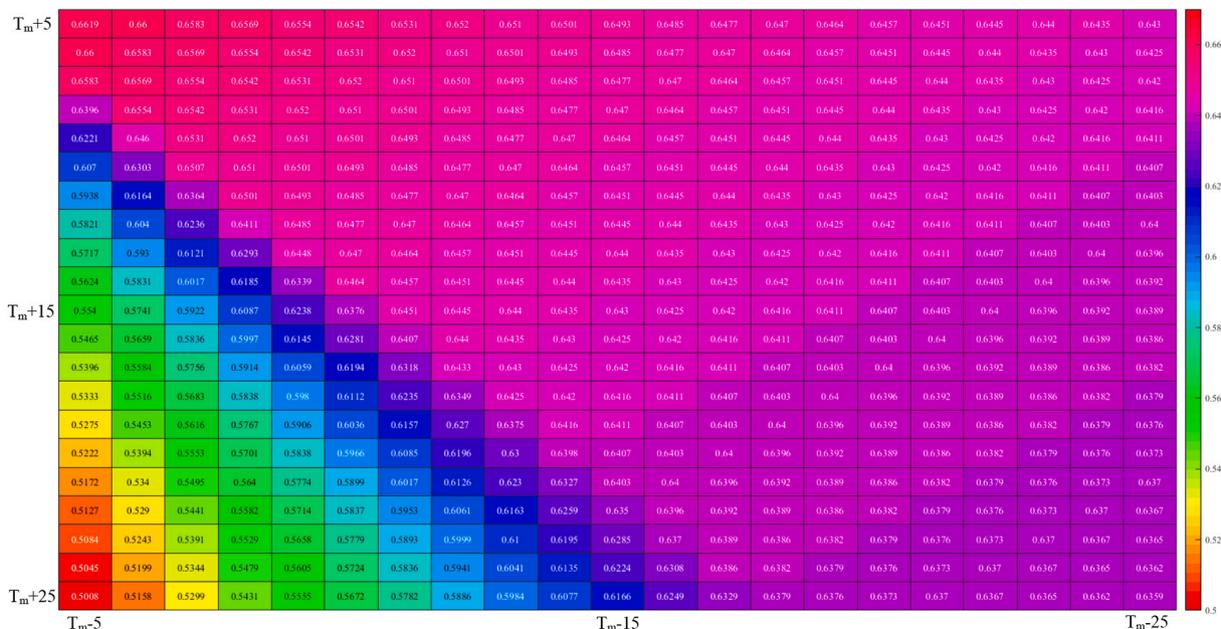


Fig. 4. Thermal Rectification obtained using conventional Thermal Diode for preferential heat transfer in the direction of gravity, in presence of natural convection.

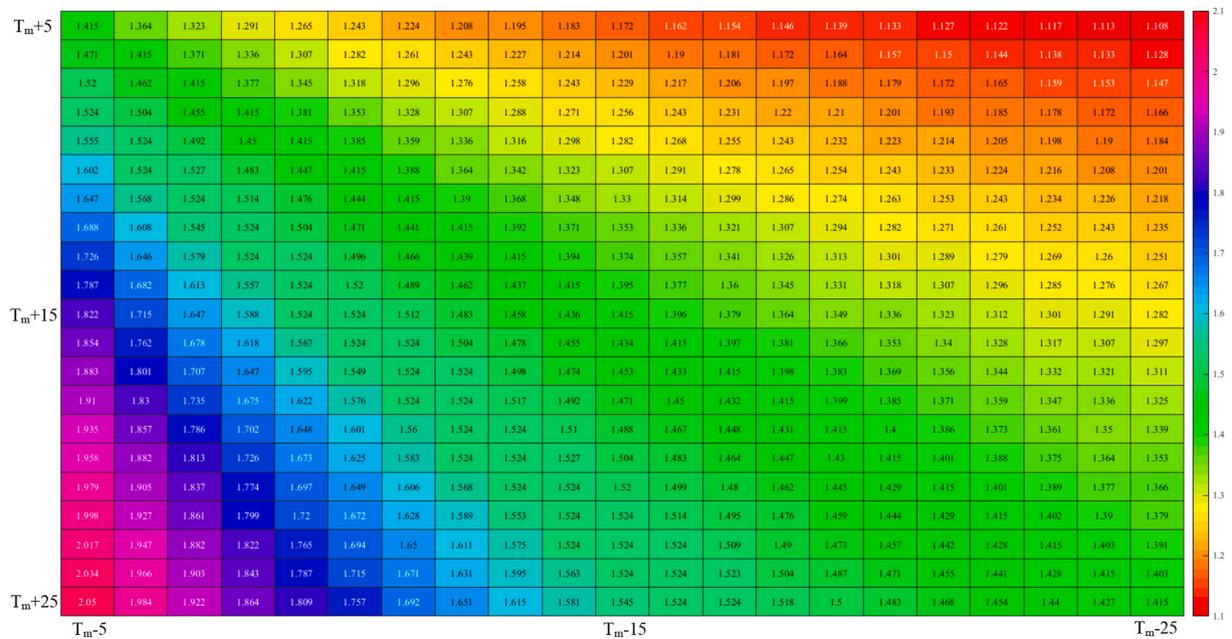


Fig. 5. Thermal Rectification obtained using conventional Thermal Diode for preferential heat transfer in the direction inverse of gravity, in presence of natural convection.

thermal rectification of less than 1 shows that the thermal diode fails to meet its operational objective. The same thermal diode under the assumption of diffusion-based thermal transport yields thermal rectification greater than one as shown in Fig. 2. Therefore, it is essential to consider the natural convection while designing and analyzing the performance of PCM based thermal diode.

Fig. 4 shows that thermal rectification in the presence of natural convection increases with a decrease in boundary temperature on both hot and cold sides. The increase in the surface temperature on the hot side adversely affects the thermal rectification due to an increase in the convective heat transfer coefficient under reverse temperature bias and potentially increases the liquid fraction under the forward bias. The increase in the convective heat transfer coefficient reduces the thermal resistance under reverse bias, which enhances heat transfer in the reverse direction. Moreover, the increase in the liquid fraction under a forward temperature bias increases thermal resistance as the thermal conductivity of *n*-octadecane in the liquid state is lower than in the solid-state, reducing the heat transfer rate in the forward direction. The lower surface temperature on the cold side helps maintain PCM in the solid-state under a forward bias and limit the convection heat transfer coefficient under reverse temperature bias. The lower temperature on the cold side reduces the liquid fraction height, directly influencing Nusselt number, as observed from Eq. (5). Therefore, a reduction in the liquid fraction height under reverse temperature bias increases thermal resistance via a decrease in convection coefficient and decreases thermal resistance in the forward bias. Therefore, a lower temperature on the cold side augments the performance of the thermal diode.

3.2. Preferential direction: Inverse to the Gravity

Fig. 5 shows the thermal rectification varies from 1.108 to 2.05 in the presence of natural convection for thermal diode designed to allow heat transfer in the direction inverse to the gravity, as shown in Fig. 1(b). The presence of natural convection augments the performance, as evident upon comparing Figs. 2 and 5, as natural convection augments heat transfer in the direction inverse to the gravity. The increase in the surface temperature on the hot side augments the performance due to an increase in convection coefficient and an increase in the thermal resistance under reverse temperature bias via an increase in liquid fraction,

as observed from Fig. 5. Moreover, it is evident from Fig. 5 that the decrease in surface temperature on the cold side adversely affects the performance of the thermal rectifier, as it augments the heat transfer in the reverse direction with an increase in solid fraction of PCM and adversely affects convective heat transfer in the forward direction.

4. Modified Design

The analysis in the previous section shows that the augmentation in the heat transfer in the direction inverse to the gravity adversely affects the performance of thermal diode designed to allow heat transfer in the direction of gravity and augments the performance of thermal diode designed to allow heat transfer in the direction inverse to the gravity. Therefore, it is pertinent to limit the natural convection in thermal diodes designed to allow heat transfer in the direction of gravity, whereas, enhance natural convection in thermal diodes designed to allow heat transfer in the direction inverse to the gravity.

4.1. Preferential direction: Gravity

One of the approaches to limit natural convection is the use of baffles. However, in order to eliminate natural convection, baffles need to be placed at small separations, such that *Ra* is less than the critical value (i.e., 1708). The theoretical spacing between baffles will need a large number of thin baffles, which will be challenging from manufacturing and economic perspectives. Furthermore, the presence of a large number of baffles will reduce the difference between the effective thermal conductivity of PCM in solid and liquid states. Another approach is the addition of nanoparticles to increase the viscosity of PCM to limit natural convection. However, the volume fraction of nanoparticles that needs to be added to limit natural convection is large, which presents two challenges, i.e., the stability of nanoparticles in PCM [13] and reduction in the difference in thermal conductivities in solid and liquid states. Another approach is the addition of porous media with lower permeability. The permeability of metal foam can reach an order of magnitude of 10^{-8} even at porosity greater than 0.9 [14]. However, the addition of metal foam of porosity greater than 0.9 does not suffice alone to limit natural convection, but baffles need to be added although at significantly larger distance compared when used alone. Although the

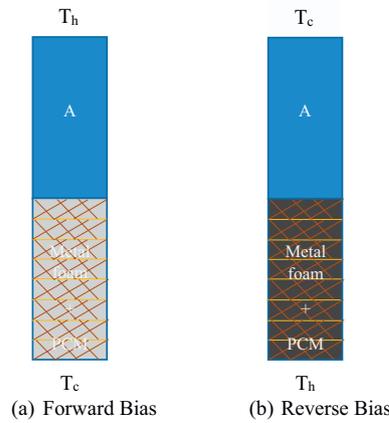


Fig. 6. Modified Design of Thermal Diode for preferential heat transfer in the direction of gravity.

use of lower porosity metal foam alone will eliminate natural convection, however, it will significantly diminish the difference in the effective thermal conductivity of PCM in solid and liquid states. Therefore, in the present study addition of stainless-steel metal foam and baffles made of the same material as non-phase change material is proposed, as shown in Fig. 6. It is significant to highlight that the thermal conductivity of non-phase change material is assumed to be mean of the effective thermal conductivity of PCM in solid and liquid states. The baffles are placed at separation, such that modified Ra remains below the critical limit. Ra for the presence of porous media is defined as [15]:

$$Ra = \frac{K\rho^2 g\beta C_{pl}(T_1 - T_2)L}{k_f\theta} \tag{7}$$

where K is the permeability of porous media. The critical modified Ra is approximately 40.

Fig. 7 shows the thermal rectification of the modified thermal diode for different temperature biases. The thermal rectification of the modified thermal diode is greater than 1, unlike the conventional thermal diode, as observed in Fig. 4, which implies the modified thermal diode can perform a desirable function as a thermal rectifier. The influence of boundary temperature is similar as observed for conventional thermal

diode under the assumption of pure conduction based thermal transport, as observed in Fig. 2, as heat transport in the presence of metal foam and baffle is primarily through conduction. However, the thermal rectification achieved is lower, compared to that observed in Fig. 2, due to a decrease in the difference in effective thermal conductivity of PCM in solid and liquid states upon addition of metal foam. The augmentation of thermal conductivity upon the addition of metal foam is higher in the state with lower thermal conductivity. Therefore, stainless steel has been used as material for metal foam rather than commonly employed aluminum and copper metal foam. The addition of metal foam of higher thermal conductivity further reduces the difference in the effective thermal conductivity of PCM and adversely affects the performance of thermal diode. Hence, it is recommended to employ porous media of lower thermal conductivity. However, the thermal conductivity of porous media should be greater than that of PCM in the solid-state; otherwise, the addition of porous media will reduce the effective thermal conductivity of PCM in the solid-state, significantly reducing the difference in effective thermal conductivity, and in turn degrading performance of thermal diode. Therefore, the addition of a combination of metal foam and baffles can augment the performance of single-PCM-based thermal diode compared to the conventional thermal single-PCM-based thermal diode. The performance can be further augmented by optimizing the material and porosity of metal foam and thermal properties of non-phase change material employed.

4.2. Preferential direction: Inverse to the Gravity

The presence of natural convection augments the performance of thermal diode designed to allow heat transfer in the direction inverse to the gravity. Therefore, it is preferred to augment natural convection. This implies that PCM needs to be close to the hot side under forward bias rather than away from the hot side as in conventional thermal diodes. The thermal rectification achieved in PCM-based thermal diode in the presence of natural convection is primarily contributed by the change in the mechanism for heat transfer (i.e., convection and conduction) rather than change in the thermal conductivity upon changing the direction of temperature bias. Therefore, the presence of another material in conjugate with PCM is not necessary, and the presence of a single PCM alone would suffice. Moreover, the presence of PCM alone would lead to an increase in the volume of PCM, which will augment the

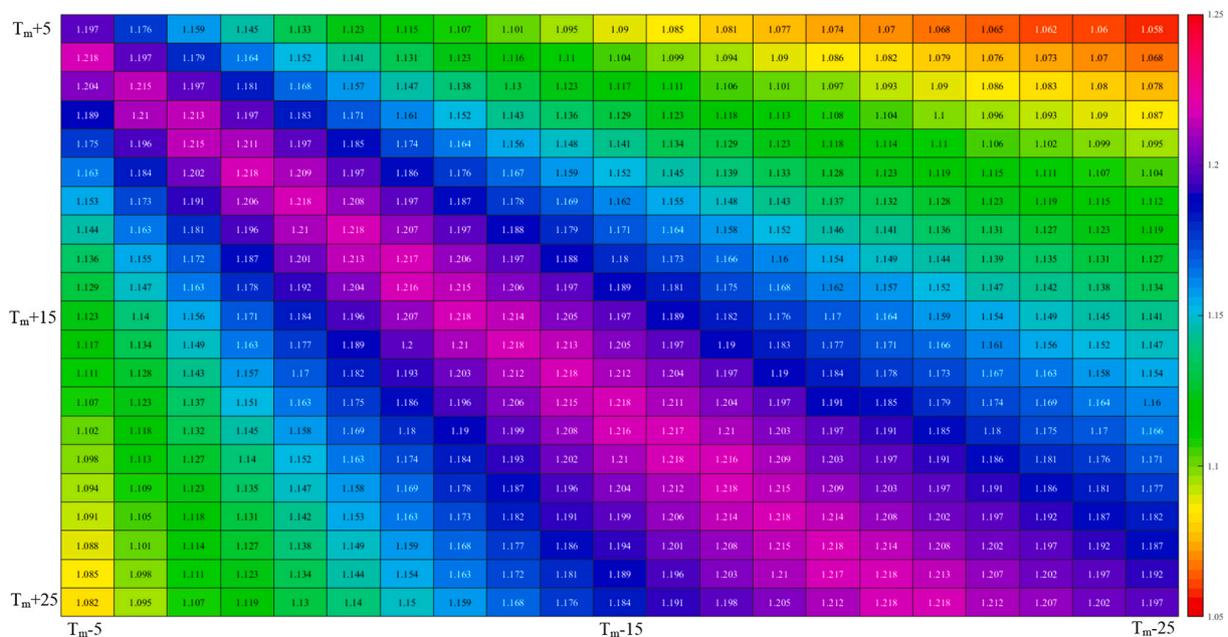


Fig. 7. Thermal Rectification obtained using modified Thermal Diode for preferential heat transfer in the direction of gravity, in presence of natural convection.

S Tasnim: Methodology, Instruction, Consultation, Review and Editing.

S A Gadsden: Project Management, Formal Analysis, Review and Editing.

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Declaration of Competing Interest

None.

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