Thermal rectification of thermal diode based on $\mathrm{VO_2}$ under transient Dirichlet conditions

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Abstract - In this study, we focused on the main thermal control element, which is the thermal diode and considered its operation in the conductive heat transfer regime. The thermal rectification of a thermal diode made of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$, is investigated by changing various parameters under Dirichlet boundary conditions. We found that the thermal rectification factor can rise to very high values during the transient process before reaching steady-state conditions. Thus, the study of the thermal diode behaviour under transient conditions is very promising for a better control of practical thermal systems.

1. Introduction

Thermal management is becoming one of the most important engineering endeavours and it is essential to keep the temperature within a certain level for various applications for both performance and safety such as photovoltaic panels [1], batteries [2], thermal storage systems [3]. The thermal diode, which is analogous to the electronic diode, is an encouraging device to generate thermal rectification for thermal management. It is a two-terminal system that rectifies the heat flux depending on the direction of the temperature gradient between the boundaries of the two terminals [4]. Thermal rectification is a process that occurs when the heat flux depends on the direction of the temperature gradient [5]. The topic was firstly studied in 1936 by Starr [6]. Among thermal rectification devices, researches on thermal diodes have dramatically increased in the past decade [4]. Thermal diodes based on phase change materials (PCM) are a beneficial alternative to obtain efficient thermal rectification. Among PCMs, $\mathrm{VO_2}$, which is one of the most popular PCMs, has recently drawn great attention thanks to its close critical transition temperature to room temperature. $\mathrm{VO_2}$ shows monoclinic and tetragonal-rutile crystalline structures below and above the critical temperature, T_c = 341 K, respectively [7]. Metallic phase results in high thermal conductivity above T_c, whereas dielectric phase results in low thermal conductivity below it [8].

In the literature, available studies mostly focused on exploring conductive thermal rectification under steady-state conditions. Yang et al. [9] modelled a thermal diode that consists of two materials with linear temperature-dependent thermal conductivities based on Fourier's law of heat conduction and carried out a study to optimize the thermal rectification. They obtained a maximum rectification ratio of 0.5 [9]. However, reaching this high rectification ratio is difficult and costly, because there is a need for a high temperature difference more than 100 K to obtain it [9]. As a practical advantage of PCMs, this drawback can be overcome thanks to their thermal conductivity alteration to some extent. Thus, there are detailed investigations especially on $\mathrm{VO_2}$ to use in thermal diodes as a single PCM or combination with another PCM [10, 11, 12]. Ordonez-Miranda et al. [11] examined a thermal diode with a single PCM, they examined $\mathrm{VO_2}$ and nitinol under steady-state conditions. They reached 19.7% of thermal rectification and concluded that a higher thermal conductivity contrast, smaller thermal hysteresis and faster phase

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transition can generate higher thermal rectification. Moreover, Kasali et al. [10] theoretically investigated the thermal diode that was made by two PCMs as the combination of $\mathrm{VO_2}$ and Polyethylene. In their study, they reached a thermal rectification of 60%. Later, they analysed the diode geometry. They obtained a thermal rectification of 63.5% and 63.2% for spherical and cylindrical thermal diodes, respectively, that were made by $\mathrm{VO_2}$ and Polyethylene [12].

Nevertheless, not much effort has been devoted to the study of conductive thermal rectification under transient conditions. The latter needs to be well understood to be able to utilize thermal components practically and efficiently. Herrera et al. [13] published the first study related to thermal diodes under transient conditions. They calculated the thermal rectification of thermal diodes whose thermal conductivity varies linearly with temperature by applying finite difference method. Also, they introduced time-dependent thermal rectification factor and observed a higher rectification factor under transient conditions [13]. Klinar et al. [14] carried out a numerical study to investigate the influence of a thermal diode in a magnetocaloric refrigeration device. They analyzed various temperature dependent thermal conductivity profiles and observed that the thermal rectification reaches higher values under transient conditions than steady-state conditions.

There are many studies that examine the thermal rectification of thermal diodes in steady-state conditions and the interest for transient analysis is increasing. However, we have not encountered any prior work that studied thermal diodes while considering properties of $\mathrm{VO_2}$ in full aspects under transient conditions. Therefore, the objective as well as the novelty of this study is to investigate a thermal diode based on a single PCM, under transient conditions. The thermal diode is made of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$ and we consider Dirichlet boundary conditions to be applied. The thermal conductivity and specific heat of $\mathrm{VO_2}$ depend strongly on temperature, mainly in the vicinity of the critical transition temperature. On the other hand, the thermal conductivity and specific heat of $\mathrm{SiO_2}$ are constant. The thermal rectification of the thermal diode is investigated in detail by changing different parameters.

2. Theoretical modelling

We consider a thermal diode that is made of a PCM and non-PCM in this study as stated before. There is a heat exchange between the two thermal baths due to their temperature difference $T_h - T_c$, as illustrated in Fig.1. The heat flux flows from the PCM to the non-PCM in the forward configuration. Conversely, it flows in the opposite direction in the backward configuration. Heat fluxes in forward and backward configurations are driven by the thermal conductivities of the PCM and non-PCM. The total length of the model is $2l$ and both materials have equal lengths, which mean half of the total length, as shown in Fig.1.

2.1. Nondimensionalization of the transient process

The nonlinear heat diffusion equation for $\mathrm{VO_2}$ is given by:

$$\rho_v c_p(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[k(T)\frac{\partial T}{\partial x}\right] \tag{1}$$

The thermal conductivity, $k(T)$, and specific heat capacity, $c_p(T)$, of $\mathrm{VO_2}$ vary with temperature. The thermal conductivity of $\mathrm{VO_2}$ can be described using the following equation [11]:

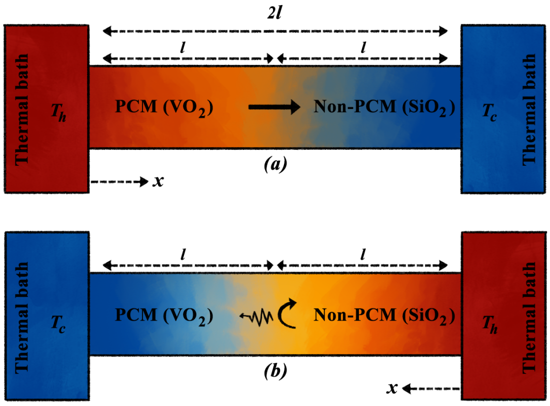

Figure 1 : *Schematic representation of the studied thermal diode in the forward and backward configurations*

$$k(T) = k_d + \frac{k_m - k_d}{1 + e^{-\beta(T - T_o)}} \tag{2}$$

where k_d and k_m represent the thermal conductivity of VO$_2$ in the dielectric and metallic phases, respectively. T_o is the phase transition temperature and β is the phase transition slope. The values of these parameters are as follows: 3.6 $\mathrm{W.m^{-1}.K^{-1}}$ for k_d, 6 $\mathrm{W.m^{-1}.K^{-1}}$ for k_m and 1.6 $\mathrm{K^{-1}}$ for β. In addition, T_0 takes the values 342.9 K and 334.9 K during the heating and cooling processes respectively due to 8 K hysteresis effect of VO$_2$ between these processes [11].

As reported in Ref [15], the expression of the specific heat capacity of VO$_2$ is given by:

$$c_p(T) = c_d(T) + T\frac{\alpha^2}{\rho_v \kappa} + L_n \frac{\partial f}{\partial T} \tag{3}$$

where c_d, ρ_v, α, κ, L_n represent the specific heat capacity predicted by Debye Model, density of VO$_2$, coefficient of thermal expansion, isothermal compressibility and latent heat, respectively. Since the variation of c_d within the range of BCs is negligibly small, we assume it to be constant and we take the average of the values of c_d at the BC temperatures as 0.704 $\mathrm{kJ.kg^{-1}.K^{-1}}$. Moreover, ρ_v of VO$_2$ changes according to its crystalline structure. However, for simplicity sake throughout the study, we assume ρ_v to be also constant and we take the average of the values of the dielectric monoclinic and metallic tetragonal-rutile crystalline structures as 4612 $\mathrm{kg.m^{-3}}$. L_n equals 51.45 $\mathrm{kJ.kg^{-1}}$ for the heating process of VO$_2$ [16] and we assume the same value for the cooling process. As explained in the study of Ordonez-Miranda et al. [15], the second term in the right side of Eq.3 can be neglected, because the values of this term are much smaller than the values of c_d within the phase transition temperatures. Thus, its contribution is neglected throughout the study. The temperature behaviours of the thermal conductivity and specific heat capacity of VO$_2$ are reported in Figs.2(a) and 2(b), respectively.

Eq.1 can be nondimensionalized as

$$\frac{\overline{\alpha}}{\alpha_d}\left[1 + \frac{L_n}{c_d \Delta T_o}\frac{\partial f}{\partial \theta}\right]\frac{\partial \theta}{\partial t^*} = \frac{\partial}{\partial x^*}\left\{\left[1 + (k_r - 1)\, f(\theta)\right]\frac{\partial \theta}{\partial x^*}\right\} \tag{4}$$

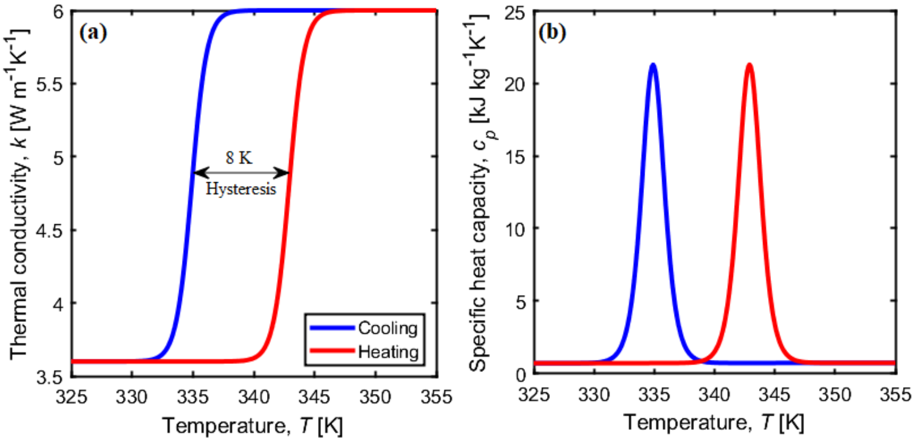

Figure 2 : *Computed behaviours of the (a) thermal conductivity and (b) specific heat capacity of* $\mathrm{VO_2}$ *as functions of temperature*

where the dimensionless temperature is defined by $\theta = (T - T_o)/\Delta T_o$, the dimensionless length by $x^* = x/l$ and the dimensionless time by $t^* = \overline{\alpha}t/l^2$. ΔT_o is the difference between the transition temperatures of heating and cooling processes: $\Delta T_o = T_{oh} - T_{oc}$. $\overline{\alpha}$ is the average thermal diffusivity between the one of the dielectric structure of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$, which is $\overline{\alpha} = (\alpha_d + \alpha_s)/2$. α_d and α_s represent the thermal diffusivity of the dielectric structure of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$, respectively. They are given by $\alpha_d = k_d/(\rho_v c_d)$ and $\alpha_s = k_s/(\rho_s c_s)$. ρ_v and ρ_s are the densities of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$ in order. The thermal conductivity, k_s, specific heat capacity, c_s, and density, ρ_s, of $\mathrm{SiO_2}$ are 1.5 $\mathrm{W.m^{-1}.K^{-1}}$, 0.73 $\mathrm{kJ.kg^{-1}.K^{-1}}$ and 2650 $\mathrm{kg.m^{-3}}$, respectively. k_r=k_m/k_d and $f(\theta)$ is expressed as $f(\theta) = \left[1 + e^{-\beta\Delta T_o\theta}\right]^{-1}$.

Moreover, the heat diffusion equation in $\mathrm{SiO_2}$, whose thermal conductivity and specific heat capacity does not vary with temperature, can be nondimensionalized as

$$\frac{\overline{\alpha}}{\alpha_s}\frac{\partial\theta}{\partial t^*} = \frac{\partial^2\theta}{\partial x^{*2}} \tag{5}$$

Eq.(4-5) are numerically solved by using implicit finite difference method and discretized in time and space for many nodes. Finally, the nondimensional heat flux density can be evaluated by using Eq.6 and Eq.7 for forward and backward configurations.

$$\phi_+^* = -k_s\frac{\partial\theta}{\partial x^*} \tag{6}$$

$$\phi_-^* = -k_d\left[1 + (k_r - 1)\,f(\theta)\right]\frac{\partial\theta}{\partial x^*} \tag{7}$$

where + and - signs represent forward and backward fluxes, respectively.

2.2. Thermal rectification analysis

In the absence of an internal heat source, the heat flux remains constant throughout the system under steady-state conditions. Therefore, thermal rectification can be calculated using the ratio of the difference between forward and backward heat fluxes to the maximum heat flux between the two configurations. However, this is not valid for transient conditions as emphasized by Herrera et al. [13], because heat flux can vary throughout the system under these conditions. Thus, we analysed the thermal rectification on the basis of the heat flux density at the cold end by considering the fact that heat spontaneously moves from the hot side to the cold side according to the second law of thermodynamics. Consequently, we define the thermal rectification as

$$R(t^*) = \frac{\left|\phi_+^* - \phi_-^*\right|}{max(\phi_+^*, \phi_-^*)} \tag{8}$$

R_{max}, which is one of the metrics proposed by Herrera et al. [13] to evaluate the thermal rectification, is also investigated throughout the study and it represents the maximum thermal rectification factor.

3. Results and discussion

In our analysis of the time dependent thermal rectification behaviour of the suggested VO_2 based thermal diode under transient Dirichlet conditions, we assume $T_h = 354$ K and $T_c = 324$ K and we explore the consequences of two initial conditions: $T(t = 0) = T_c$ leading to a heating process of the full system and $T(t = 0) = T_h$ which leads to a cooling process. We investigate the impact of varying three different parameters; β, L_n and the ratio k_r. During the study, only one parameter is changed in each analysis and the rest is kept unchanged. We consider five different cases for each parameter as shown in Table 1.

	β	L_n	k_r
	K^{-1}	$kJ.kg^{-1}$	
(i)	0.5	$66.89(+30\%)$	1.2
(ii)	1	$59.17(+15\%)$	1.5
(iii)	1.6	51.45	1.667
(iv)	3	$43.73(-15\%)$	3
(v)	5	$36.02(-30\%)$	5

Table 1 : *Investigated parameters and cases*

As expressed by Eqs.2 and 3, the thermal conductivity k and specific heat capacity c_p of VO_2, depends strongly on the parameter β. The variation of this parameter affects considerably the temperature profile of these two properties. Indeed, by decreasing β, the jump from the dielectric value k_d to the metallic value k_m become less steep and the amplitude of c_p decreases. On other hand, sharper transition behaviour occurs in k and higher c_p are observed when β increases. We report in Figs.3, the computed time behaviours of the normalized heat flux density (ratio of the heat flux density to the quantity $\Delta T_o/l$) at the cold boundary [Figs.3(a) and 3(c)] and the thermal rectification factor [Figs.3(b) and 3(d)] in the forward and backward configurations for both the heating [Figs.3(a) and 3(b)] and cooling [Figs.3(c) and 3(d)] processes of the full thermal diode. The general trend is the same for the different values of β in each process and each configuration. In the heating process, the normalized heat flux density increases with time to saturate at the steady-state values for both forward and backward configuration, while there is a decreasing behaviour in the cooling process. The behaviour of the thermal rectification factor R shows interesting features, which are consequences of the behaviour of the normalized heat flux densities in the forward and backward configurations for each process.

In both the heating and cooling processes, R manifests a maximum R_{max}, goes to zero, then increases again to reach the steady-state value. R_{max} has a higher amplitude and occurs in early times in the cooling process in comparison to the heating process. The time at which R vanishes in the cooling process is almost double the one for the heating process. Interestingly also, is the fact that varying β affects more R_{max} in the heating process and the time of R vanishing in the cooling process, in comparison to the opposite process, respectively. The effect of β becomes less pronounced in the steady-state regime.

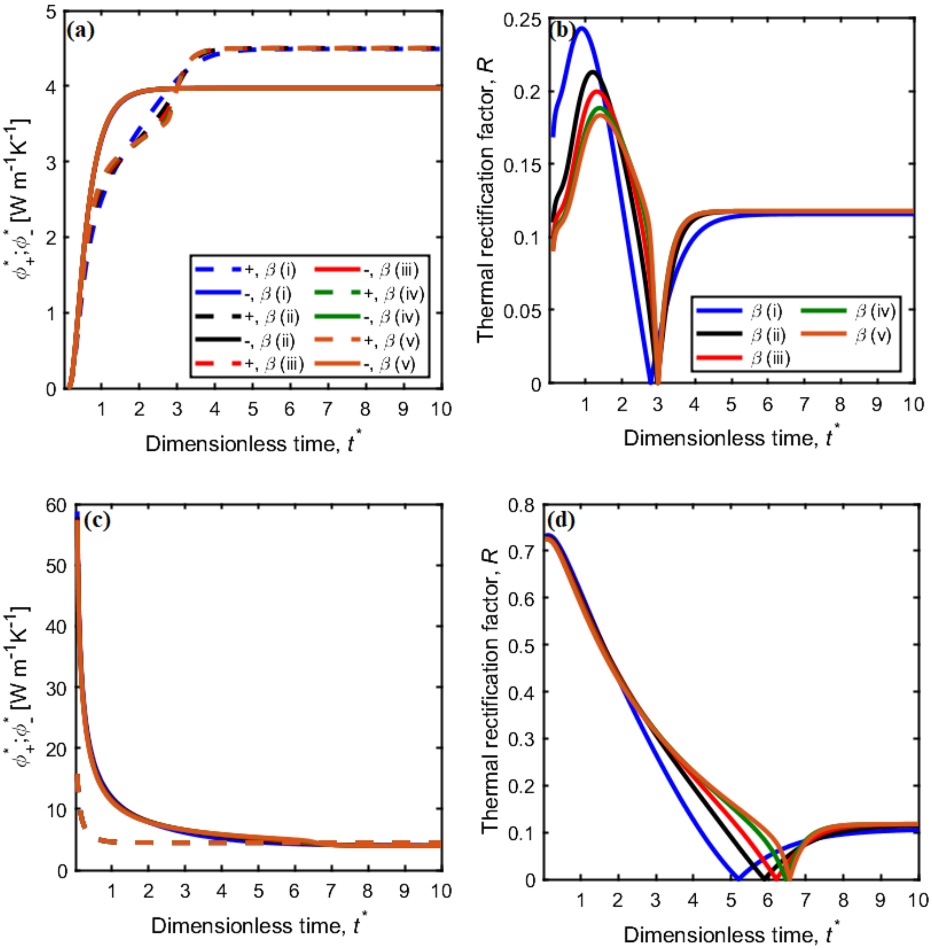

Figure 3 : *Computed time behaviours of the normalized heat flux density and thermal rectification factor in the heating [(a) and (b)] and cooling [(c) and (d)] processes, respectively, for different values of the parameter* β

The specific heat capacity c_p has a direct effect on heat transfer under transient conditions. In the case of VO_2 and as we discussed it above, the latent heat L_n plays a key role in the behaviour of c_p. We report in Figs.4(a) and 4(b), the computed time behaviours of the thermal rectification factor R in the heating and cooling processes, respectively, for different values of L_n. The main features in the time profile of R, are almost similar to the ones shown in Figs.3(b) and 3(d). While varying L_n affects more R_{max} in the heating process than in the cooling process similarly to the effect of β, it influences the time at which R vanishes in both processes. In the steady-state regime, the effect of L_n disappears and all the curves collapse on each other as expected. c_p has no impact on the heat transfer under steady-state conditions.

The third and last parameter we considered in our study is the ratio of the thermal conduc-

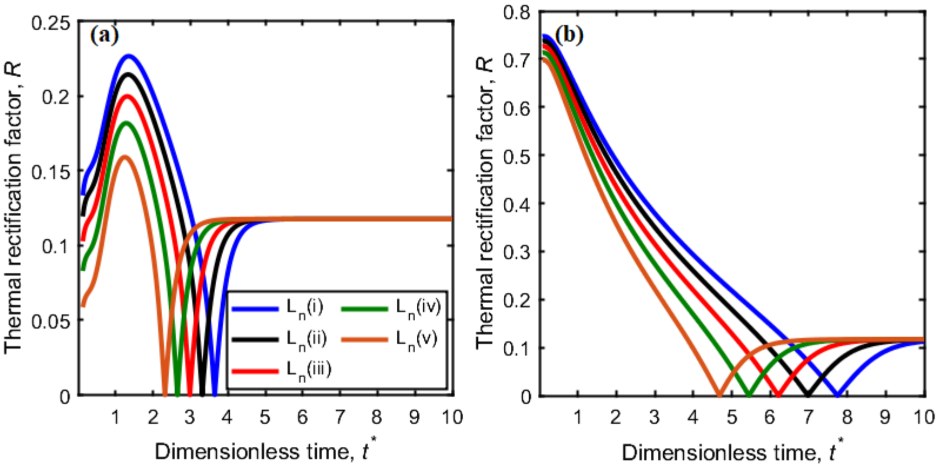

Figure 4 : *Computed time behaviours of the thermal rectification factor in the heating (a) and cooling (b) processes, for different value of the parameter* L_n

tivity of the metallic and dielectric phases of $\mathrm{VO_2}$, k_r. We show the computed time behaviours of the thermal rectification factor R in the heating and cooling processes, in Figs.5(a) and 5(b), respectively, for different values of k_r. While in the cooling process, the features remain similar to the case of varying β and L_n, the time profiles of R in the heating process manifest interesting additional features depending on the value of k_r. Varying k_r impacts strongly the entire time profile of R spanning from the transient regime to the steady-state regime.

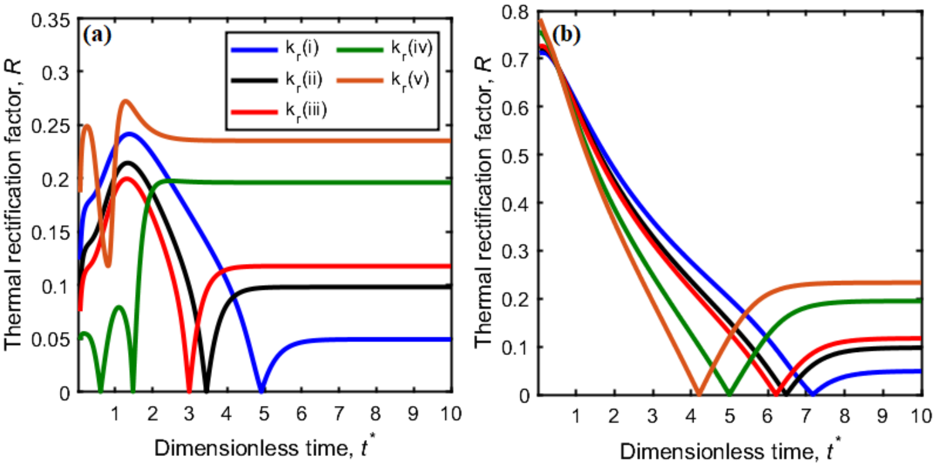

Figure 5 : *Computed time behaviours of the thermal rectification factor in the heating (a) and cooling (b) processes, for different value of the parameter* k_r

4. Conclusion

To summarize the merit of this study; we have not come across a study that examines thermal diodes with considering properties of $\mathrm{VO_2}$ in full aspects under transient conditions. The studies in the literature are generally made based on simplified assumptions regarding the temperature dependent behaviour of thermal conductivity and specific heat capacity or conducted under steady-state conditions. In this study, we have theoretically analyzed the thermal rectification factor of a thermal diode that is made of $\mathrm{VO_2}$ and $\mathrm{SiO_2}$ considering Dirichlet boundary conditions under transient conditions.

We have examined various parameters that affect the thermal rectification under transient conditions. It has been shown that thermal conductivity and specific heat capacity have a major impact on the behaviour of the thermal rectification under transient conditions. Moreover, although transient studies are not considered enough in the literature, we observed higher thermal rectification under transient conditions than steady-state conditions in almost all parameters. Considering the reasonable outcomes of this theoretical study, further research should be conducted on thermal diodes especially under transient conditions in order to demonstrate the full benefits of the transient analysis for a better control of practical thermal systems.

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