Modeling of Heat Transfer and Dynamics in Phase Change Materials for Enhanced Thermoregulation and Energy Recovery

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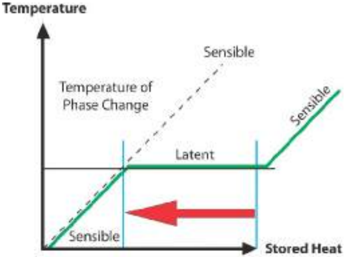
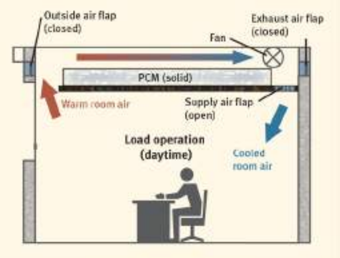
Phase Change Materials: PCMs

- Phase Change Materials exploit the Latent Heat of the solid/liquid phase transition to store or release a large amount of heat barely changing the temperature
- Example: melting $1\,kg$ *ice* at 0° : $\Delta H = 333k\,J$.
  Same energy to heat $1\,kg$ *water* from 0° to 80°
- Hundredths known: organic (paraffins, non-paraffins), inorganic (salt hydrates, metallics), eutectics
  - Paraffin waxes: stable with melting points within room temperatures



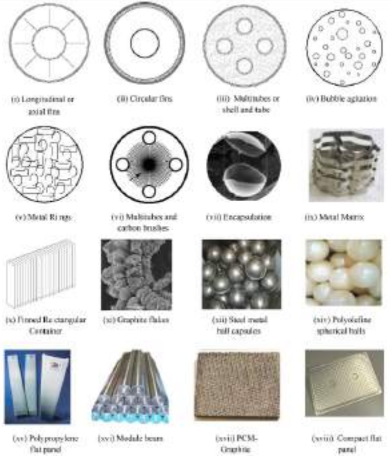
PCMs: applications

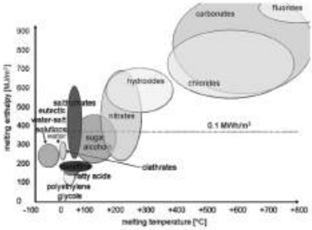


- Passive thermal control management
- Damping of extreme temperatures
- Heat storage
- Interior climate regulation in buildings
- Textiles: keeping body temperature
- Solar plants: buffering of energy

- Space applications
- Space suites
- Electronic thermal control
- Refrigeration of food
- Conservation of biological samples

PCMs: limitations





- Selection of a PCM for a given application
- Paraffins (and most of PCM) exhibit low conductivity: slow heat transfer

Goal: enhance heat transfer rate with minimum complexity

- Marangoni driving (microgravity)
- Dispersion of nanoparticles (high potential but no good modeling)

1. Nano-enhanced PCMs (NePCMs)

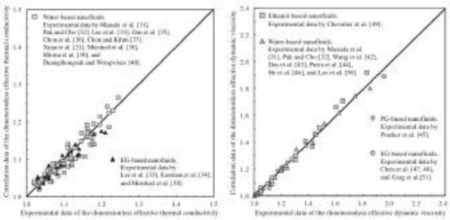
- Metallic nanoparticles increase conductivity and viscosity
- Modeled as an effective transport coefficients in NePCMs
- Ample experimental and theoretical work

Conductivity models

- Maxwell (spherical particles)
- Hamilton-Crosser
- Jeffrey
- Davis
- Lu-Lin

Viscosity model

- Brinkman
- Einstein
- Batchelor



Maxwell & Brinkman (mean field)

$$\frac{k_{eff}}{k_f} = \frac{k_{np} + 2k_f - 2\Phi(k_f - k_{np})}{k_{np} + 2k_f + \Phi(k_f - k_{np})}$$

$$\mu_{eff} = \frac{\mu_f}{(1-\Phi)^{2.5}}$$

Strong overestimation of heat transfer
Used in most of the studies

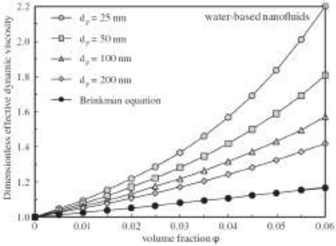
Corcione (empirical)

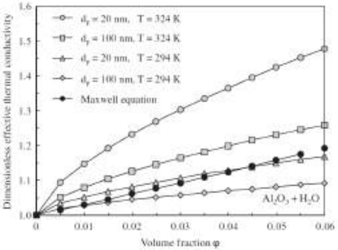
$$\frac{k_{eff}}{k_f} = 1 + 4.4\, Re^{0.4} Pr^{0.66} \left(\frac{T}{T_m}\right)^{10} \left(\frac{k_{np}}{k_f}\right)^{0.03} \Phi^{0.66}$$

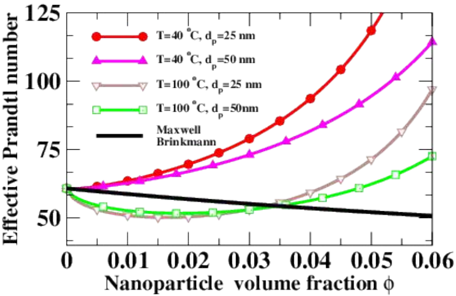
$$\frac{\mu_{eff}}{\mu_f} = \frac{1}{1 - 34.87(d_p/d_f)^{-0.3}\Phi^{1.03}}$$

Agreement with experiments
No used to study NePCM

1. NePCM: n-octadecane with dispersed alumina nanoparticles







- Liquid phase of PCM
  - Maxwell&Brinkman: continued decrease of Pr_{eff} with nanoparticle concentration
  - Empirical model: only some ranges of parameters decrease Pr_{eff}
- Solid phase of PCM
  - Maxwell's model for conductivity

1. NePCM: Enthalpy-porosity model with modified transport coefficients

Momentum equation with porous media term

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = -\nabla p + \nu_{eff} \Delta \mathbf{u} + C \frac{1 - f^2}{\epsilon + f^3} \mathbf{u} + \mathbf{g} \rho \beta (T - T_0)$$

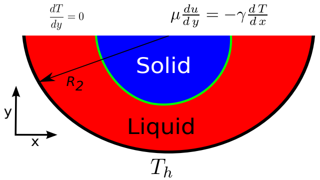
- Solid/liquid interface (Mushy region) behaves like a porous media
- Term $C \frac{1-f^2}{\epsilon+f^3} \mathbf{u}$ allows a common domain for NS and energy equations for liquid and solid phases

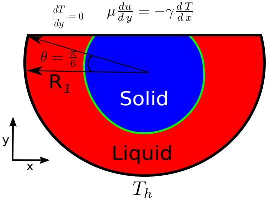
Energy equation with source term

$$\left[\frac{\partial}{\partial t} + \vec{u} \cdot \nabla\right] \left[\rho \left((1 - f_l - \phi) C_{pcm,s} + f_l C_{pcm,l}\right) + \rho_{np} \phi C_{np}\right] T$$
$$= \nabla(\kappa_{pcm,eff} \nabla T) - (1 - \phi) \rho L \frac{\partial f_l}{\partial t}$$

- Liquid phase of PCM: Maxwell&Brinkman and empirical fit for ν_{eff} and κ_{eff}
- Solid phase of PCM: Maxwell model for conductivity

Physical system: melting of n-octadecane with a free surface





- Curved boundary: conductive
- Flat boundary: adiabatic free surface with Marangoni driving

$R_1 = 1.577\,cm,\ R_2 = 2\,cm$

N-octadecane

$\rho\ (Kg\,m^{-3})$	776
$c_s \vert c_l\ (J\,Kg^{-1}\,K^{-1})$	1934|2196
$\kappa_s \vert \kappa_l\ (W\,m^{-1}\,K)$	0.358|0.13
$T_s \vert T_m\ (K)$	298.65|299.65
$L\ (J\,Kg^{-1})$	$243.5 \cdot 10^3$
$\alpha\ (K^{-1})$	$9.1 \cdot 10^{-4}$

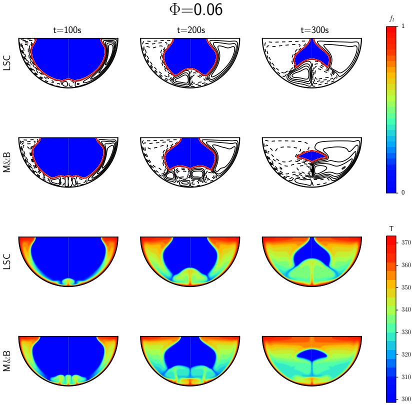
Adimensional numbers

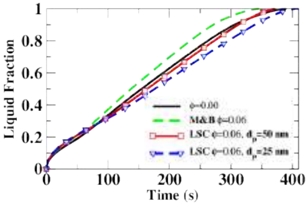
$$Pr = 60.8$$
$$Ste = 0.45(T_h = 50^\circ), 0.9(T_h = 100^\circ)$$

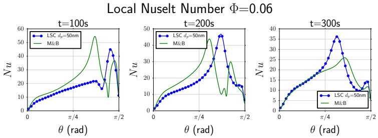
Numerics

- OpenSource FVs: *OpenFoam 2.31*
- Time integration: Cranck-Nicholson
- Momentum and continuity equation: PIMPLE (PISO&SIMPLE) algorithm
- $\sim$ 100000 hexahedral cells

1. NePCM: n-octadecane plus alumina nanoparticles

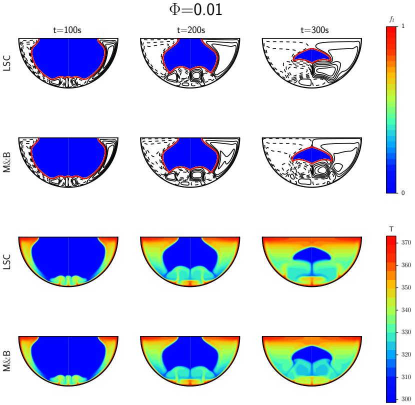


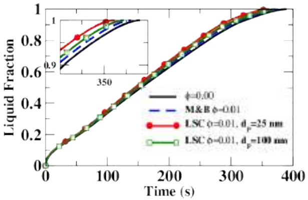


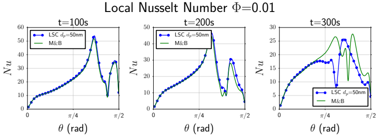


- Only Maxwell&Brinkman predicts faster melting
- Convective patterns between models differ since intermediate times

1. NePCM: n-octadecane plus alumina nanoparticles

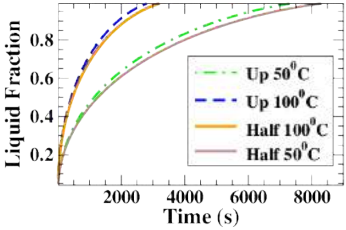


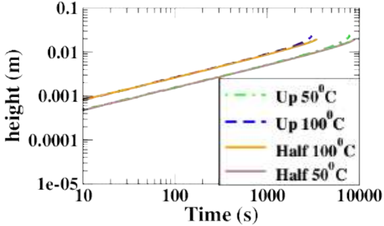




- Nanoparticles decrease the melting time
- Emprirical model predicts faster heat transfer rate (7.7%)
- Convective patterns between models differ at latter times

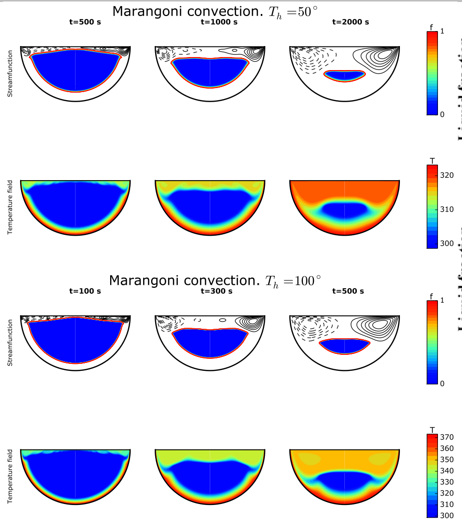
2. Melting of a paraffin wax in microgravity: conductive transport

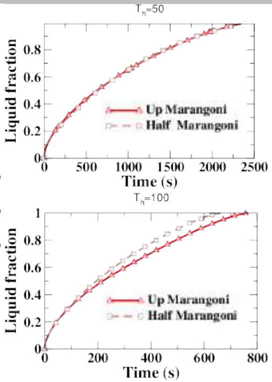




- Front propagation as $\sim t^{0.5}$ (Stefan problem)
- Higher conductivity of solid phase: quick advance at first stages
- 86% melting time to liquefy the remaining 50% of solid PCM
- Longer melting time for geometry *half*
- Differences of melting time increase with T_h

2. Melting of a paraffin wax in microgravity: Marangoni driving





- $Ma \sim 10^3$
- At $100°C$ melting is 5.2 (*half*), 4.18 (*up*) faster with thermocapillarity
- Average velocity at free surface double at $100°C$ w.r.t. $50°C$
- Enhance of heat transfer rate: long free surface
- $\sim 72\%$ time to melt remaining 50% of solid PCM

- Dept. of Mechanical and Systems Engineering, Faculty of Engineering, Okayama University
- Heat transfer laboratory (Chairman: Akihiko Horibe)
- Prof. Naoto Haruki (contact and collaborator)

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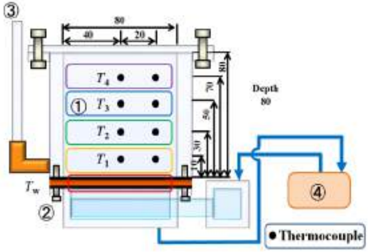
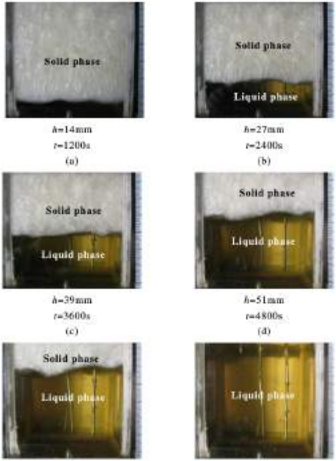
Melting in tetracosane within a cubic container

- Enough experimental data (Okayama)
- Appropriate model to fit experimental data (UPM)





h=14mm t=1200s (a)

h=27mm t=2400s (b)

h=39mm t=3600s (c)

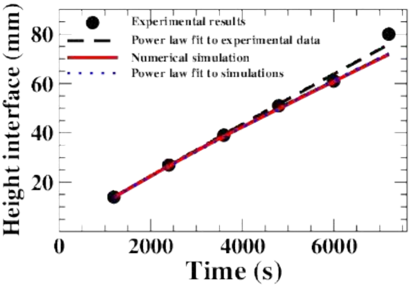
h=51mm t=4800s (d)

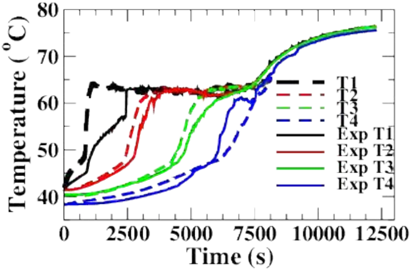
h=61mm t=6000s (e)

h=80mm t=7200s (f)

3. Collaboration with Okayama University: Tetracosane melting

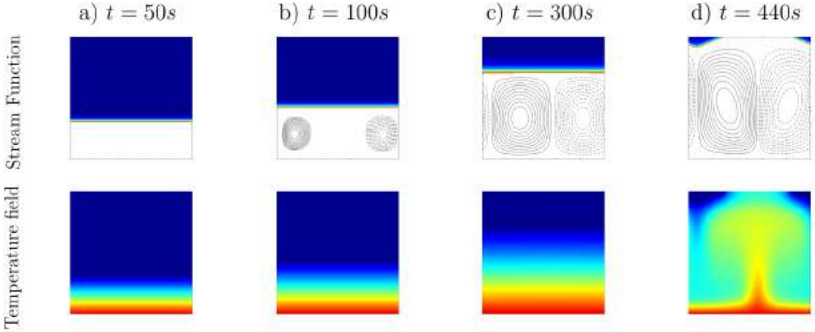
Melting in tetracosane within a cubic container





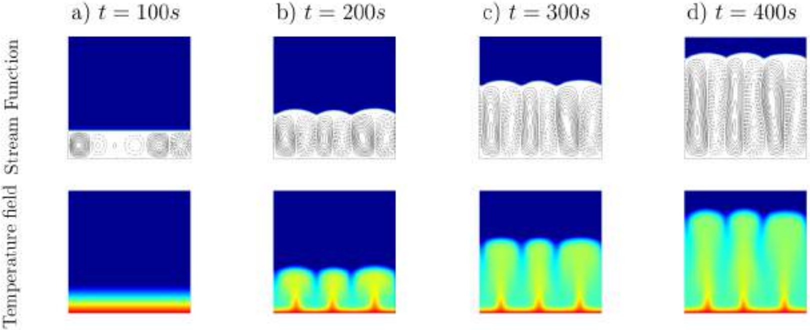
Good fit between experimental data y simulations.
Simulations with a finite volume code with 10^6 cells.

Conductive regime ⇒ Rayleigh-Bénard instability ⇒ Coarsening ⇒ Turbulence



$L = 0.5\,cm$

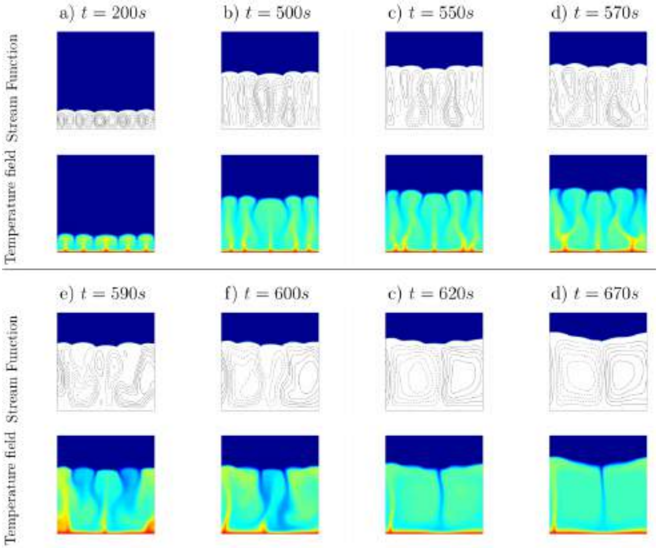
Conductive regime ⇒ Rayleigh-Bénard instability ⇒ Coarsening ⇒ Turbulence



$L = 1\,cm$

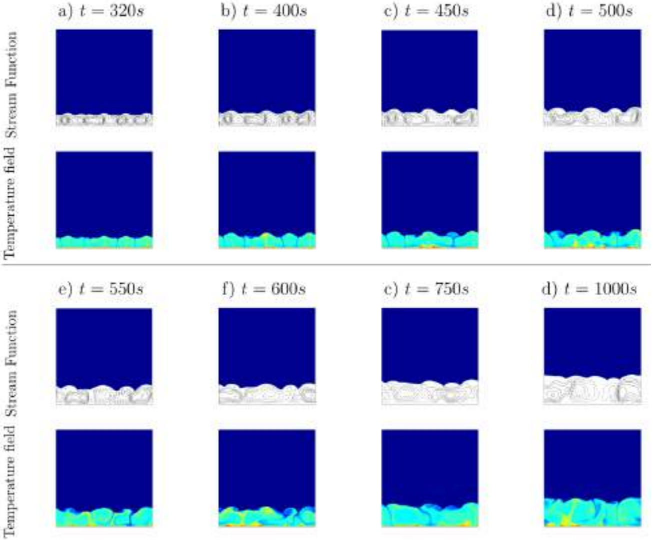
3. Melting stages: first coarsening

Conductive regime ⇒ Rayleigh-Bénard instability ⇒ Coarsening ⇒ Turbulence



$L = 2\,cm$

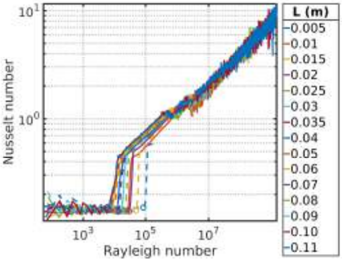
Conductive regime ⇒ Rayleigh-Bénard instability ⇒ Coarsening ⇒ Turbulence



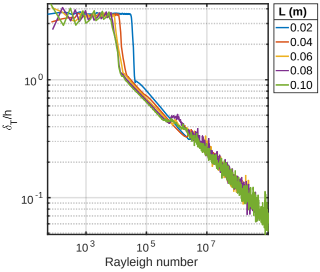
$L = 8\,cm$

- Turbulent regime: $Nu \sim Ra^{2/7}$, $\delta T/h \sim Ra^{-0.29}$
- Linear regime: $Nu \sim Ra^{0.28}$

Heat transfer at the bottom

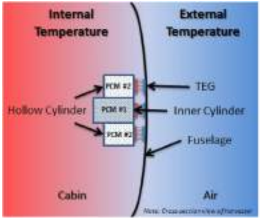


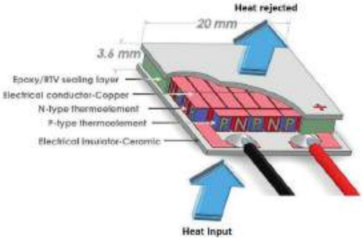
Thermal boundary layer



Coupling of thermoelectric modules with PCMs for sustained electricity generation with ambiental temperature gradients

Elefsiniotis et al. (2014)





Faraji et al. (2014)

New project: leverage our modeling/simulation capabilities on PCM to enhance the electric output of micro-energy harvesters.

- Huge range of potential applications
- Looking for partners to develop these devices

Conclusions

- Comparison of a mean field and an empirical fit for nano-enhanced PCMs
  - Mean field Maxwell&Brinkman model mostly overestimates heat transfer rate
  - Empirical fit shows the need to choose appropriate parameters to optimize PCM in thermoregulation and energy recovery
- Marangoni driving very efficient mechanism to enhance heat transfer rate of PCMs in microgravity (three-to-five times faster in cases presented)
  - Confirmed in experiments in parabolic flights by the E-USOC (ESA center)
- Collaboration with experimental group
  - Good modeling of experimental results on melting of tetracosane
  - New plume coarsening state induced by the moving interface
  - Thermal, kinematic boundary layers, number of plumes follow power laws
  - Exponents of the turbulent regime agree with a body of theoretical and experimental results of classic Rayleigh-Bénard convection
  - Turbulent state is the main dynamic regime of PCMs in large domains with vertical heating

- *Melting dynamics of a phase change material (PCM) with dispersed metallic nanoparticles using transport coefficients from empirical and mean field models.* S. Madruga and G.S. Mischlich. Applied Thermal Engineering. **124**, 1123-1133 (2017).
- *Enhancement of heat transfer rate on phase change materials with thermocapillary flows*. S. Madruga and C. Mendoza. European Physical Journal Special Topics. **226**, 1169-1176 (2017).
- *Heat transfer performance and melting dynamic of a phase change material subjected to thermocapillary effects*. S. Madruga and C. Mendoza. International Journal of Heat and Mass Transfer. **109**, 501-510 (2017).
- *Dynamic of plumes and scaling during the melting of a Phase Change Material heated from below*. S. Madruga and J. Curbelo. Submitted to International Journal of Heat and Mass Transfer.
- *Experimental and numerical study of melting of the phase change material tetracosane*. S. Madruga, A. Haruki, A. Horibe. In preparation.

More information:
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