



Simplified Model Taking into Account the Natural Convection during Melting of PCM

Farah SOUAYFANE, Pascal-Henry BIWOLE, Farouk FARDOUN

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fsouayfane@unice.fr

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I. Introduction

- In thermal engineering applications, phase change problem is simplified
- Building models with integrated PCM ignore the convection effect in the liquid region
- Only conduction in the energy equation is considered
- Complexity of CFD models and high computational time

Why should we take the convection effect into consideration ?

Hasan, 1994

- Model considering only conduction heat transfer does not describe the melting process correctly
- The convection has a significant role

Lacroix et al, 1998

- During melting, natural convection is the principal heat transfer mechanism

Velraj ,1999

- Natural convection in liquid PCM increases heat transfer rate during melting

Groulx, 2011

- Neglecting the role of natural convection in liquid PCM result an under prediction of heat transfer rate



Model is needed in which convective heat transfer is accounted for in liquid PCM

Models based on CFD

(solution of N-S equations)

FVM (FLUENT)

FEM (COMSOL)

- Enthalpy porosity approach (**Brent & Voller** 1988)
- TTM (Cao and Faghri,1990)
- Equivalent thermal capacity method (**Morgan**,1981)
- Modified heat capacity method (**Groulx**,2014)
- Lattice Boltzmann method (**Chatterjee**,2005)

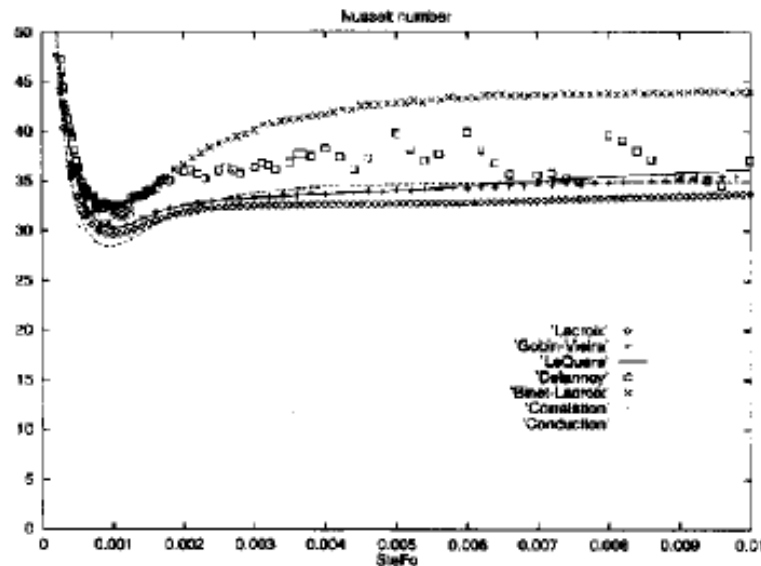
Simplified methods

- Enhanced conductivity approach (**Farid**,1990, **Vidalain**,2009) + scaling theory (**Bejan**,1988)

Literature review:

- Melting process consists mainly of three regimes: conduction-dominated regime, mixed conduction-convection regime and convection-dominated regime
- These regimes are reflected by the average Nusselt number curve function of time

- Average Nusselt number: key parameter in convection dominated problem
- The choice of a suitable correlation for the average Nu and appropriate characteristic length in Nu formula is very important

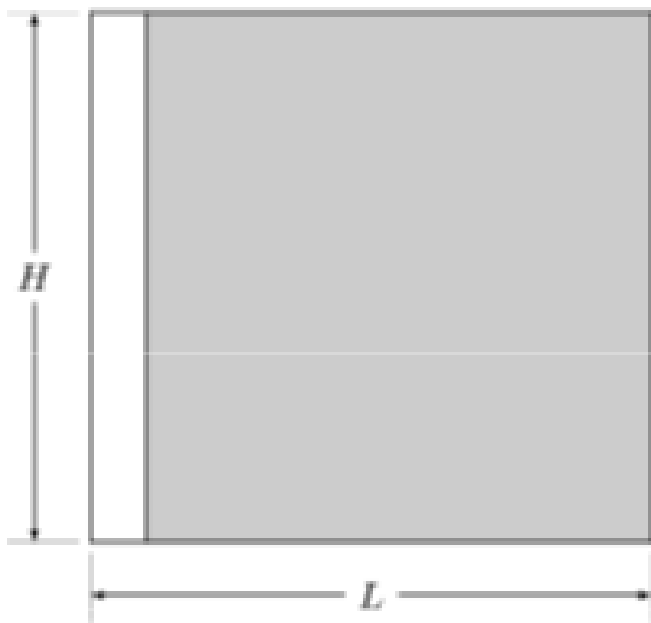


II. objectives

- Investigate the process of PCM melting in a square enclosure heated from its left vertical wall
- Get a clear understanding of the role of natural convection in the melt region
- Develop a simplified model based on the scaling theory and the enhanced thermal conductivity approach to be implemented in MATLAB
- Validate the obtained results with those of CFD model (COMSOL), in addition to numerical Benchmark results

III. Physical phenomena

During melting, convection occurs in the liquid PCM under the action of **buoyancy forces**, due to the variations of temperature gradients

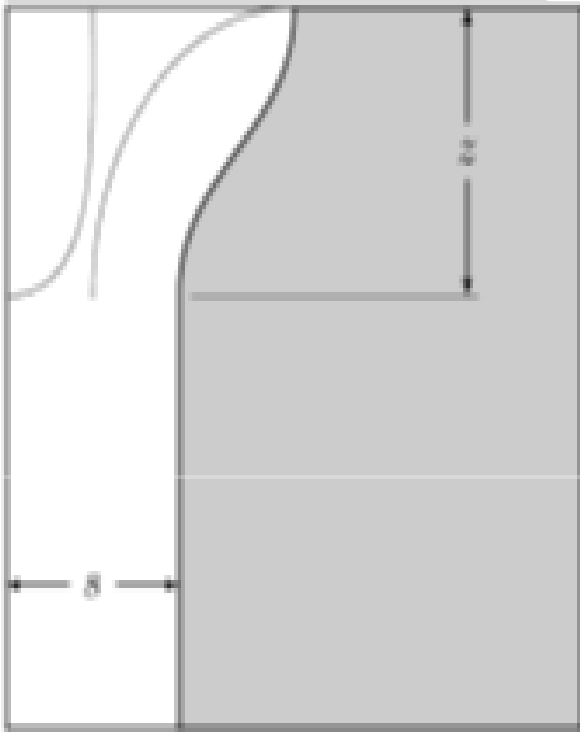


(a) pure conduction regime

heat transfer dominated
by conduction

Melting front moves
parallel to the left heated
wall

(b) mixed regime

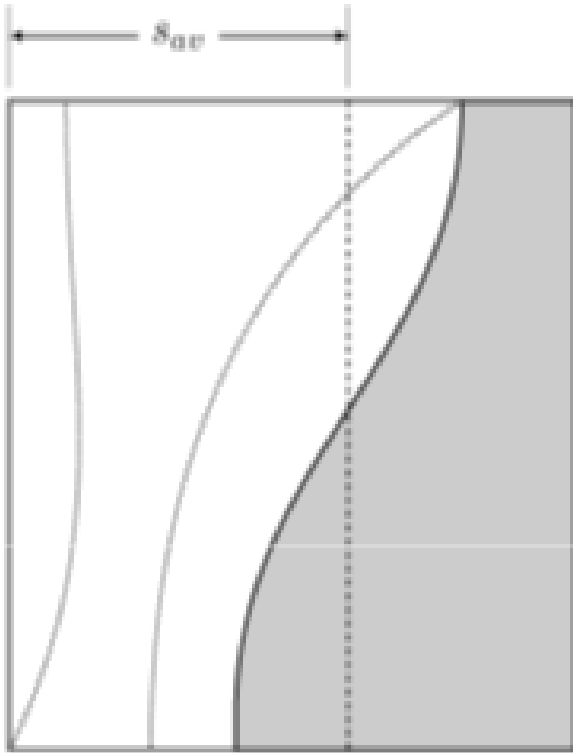


variation in density \rightarrow hot fluid rises and brings heat to the solid via the interface

Non-uniform distribution of heat and slight deformation of the melting front

Heat transfer is mixed: convection in the superior part and conduction in the lower part

(c) convective regime



temperature rises \rightarrow the fluid motion is more important

heat transfer larger at the top than the bottom.

The deformation of the melting front is more important and dominated by the convective heat transfer

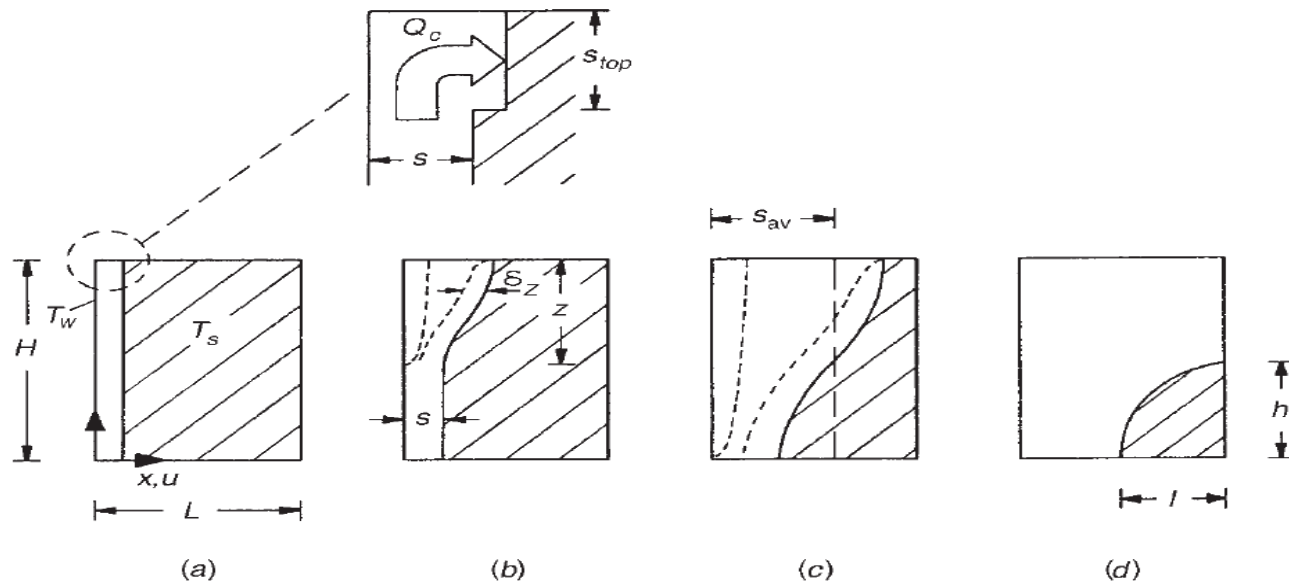
Scaling theory proposed by **Bejan, 1987**

- Convection in the upper left corner appears when

$$\delta z \sim s$$

δz : boundary layer thickness

s : thickness of the molten layer



- z : height of convective zone in the upper region of melt layer

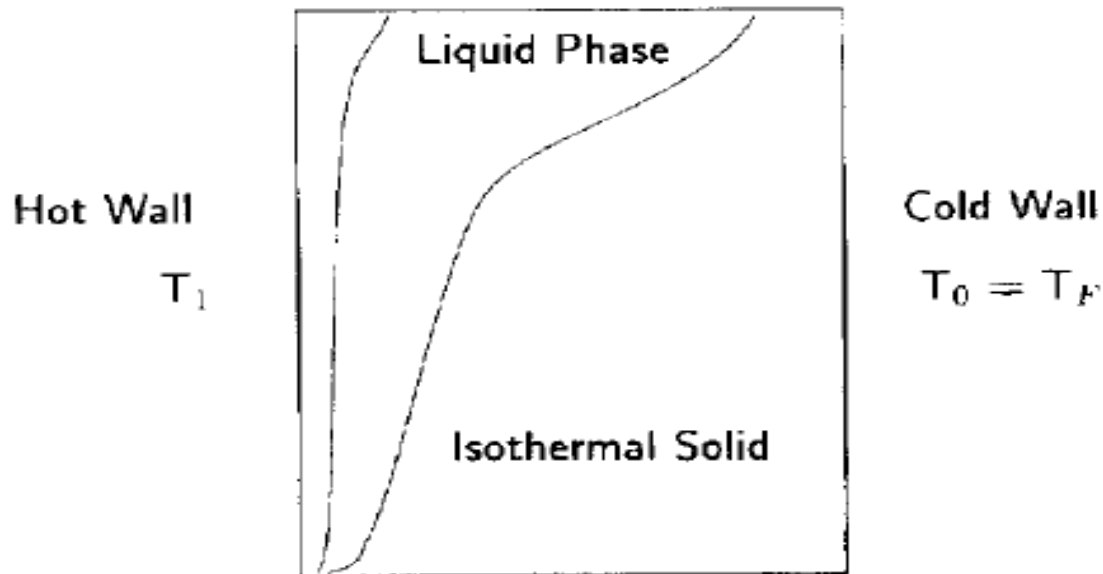
- Criterion to determine the start of convective effects

$$\frac{z}{H} \sim \left(\frac{s}{H}\right)^{-1/4} Ra_H$$

- Enhancement of k performed in “convective zone” $z \times z$ squared-shaped domain located in the upper left corner of the domain
- Assume $z = s(y = H)$

IV. Case study

Melting of Octadecane with natural convection in a 2D square cavity of $H = 0.1\text{m}$



Property	value
k (W.m/K)	0.2
Cp _s = Cp _l (J.kg/K)	1250
ρ _s = ρ _l (kg/m ³)	800
α (m ² /s)	2.10 ⁻⁷
ν (m ² /s)	10 ⁻⁵
L _H (J/kg)	1.25.10 ⁵
T _m (K)	303.15
ΔT (K)	10
T _h (K)	313.15
T _c (K)	303.15
T ₀ (K)	303.15
Ste	0.1
β (1/K)	2.10 ⁻³
g (m/s ²)	10
Pr	50
Gr	2.10 ⁶
Ra	10 ⁸

V. Numerical procedure

1. Simplified model (enhanced conduction model)

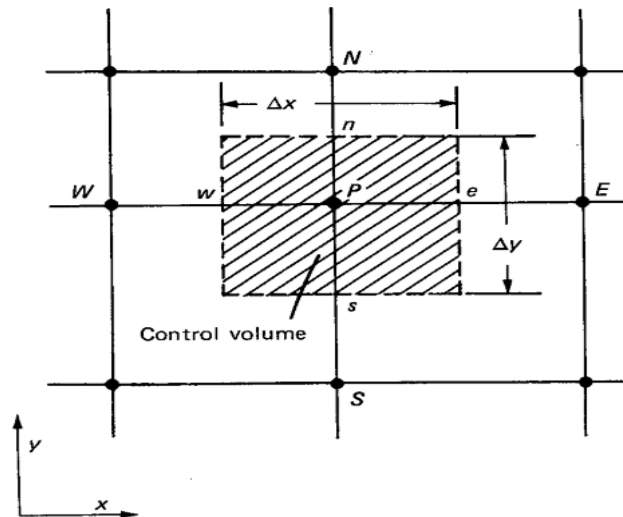
- Model phase change problem: modified “enthalpy” method (**Zivkovic**,2001)
- Calculate the temperature and the liquid fraction separately
- Two-dimensional equation for phase change is:

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k}{\rho} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k}{\rho} \frac{\partial T}{\partial y} \right) - L_H \frac{\partial f_l}{\partial t}$$

$$f_l = \begin{cases} 0 & \text{if } T < T_m \text{ (solid)} \\]0,1[& \text{if } T = T_m \text{ (mushy)} \\ 1 & \text{if } T > T_m \text{ (liquid)} \end{cases}$$

Firstly totally solid or liquid $\frac{\partial f_l}{\partial t} = 0$:

- To solve 2D phase change problem: implicit finite volume method (**Patankar**, 1980)
- Domain divided into rectangular control volumes CV
- Integrate the equation over a typical control volume and with respect to time t over a small interval Δt



After integration, we obtain the discretization equation as following:

$$a_P T_P^{t+\Delta t} = a_W T_W^{t+\Delta t} + a_E T_E^{t+\Delta t} + a_S T_S^{t+\Delta t} + a_N T_N^{t+\Delta t} + b$$

$$a_W = k_w \frac{\Delta y}{(\Delta x)_w}$$

$$a_E = k_e \frac{\Delta y}{(\Delta x)_e}$$

$$a_S = k_s \frac{\Delta x}{(\Delta y)_s}$$

$$a_N = k_n \frac{\Delta x}{(\Delta y)_n}$$

$$a_P = a_W + a_E + a_S + a_N + a_P^0$$

$$a_P^0 = \frac{\rho C p \Delta x \Delta y}{\Delta t}$$

$$b = a_P^0 T_P^0$$

$$A * T = b$$

Secondly phase change occurs:

$$T_{i,j} \equiv T_m$$

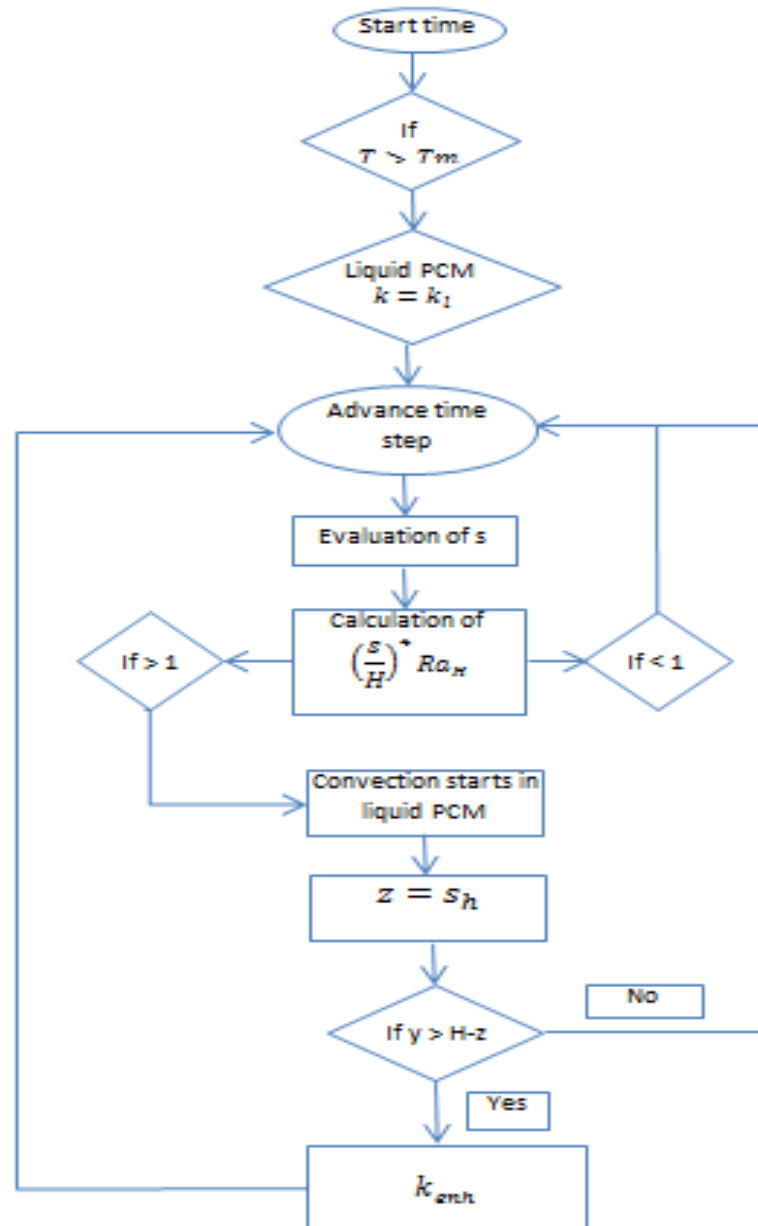
$$\frac{\partial h}{\partial t} \equiv 0$$

$$L_H \frac{\partial f_l}{\partial t} = \frac{\partial}{\partial x} \left(\frac{k}{\rho} \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k}{\rho} \frac{\partial T}{\partial y} \right)$$

$$f_{l,i,j} = f_{l,i,j}^0 + \frac{k_e \Delta t}{\rho L \Delta x^2} (T_E - T_m) - \frac{k_w \Delta t}{\rho L \Delta x^2} (T_m - T_W) + \frac{k_n \Delta t}{\rho L \Delta y^2} (T_N - T_m) - \frac{k_s \Delta t}{\rho L \Delta y^2} (T_m - T_S)$$

At each time step:

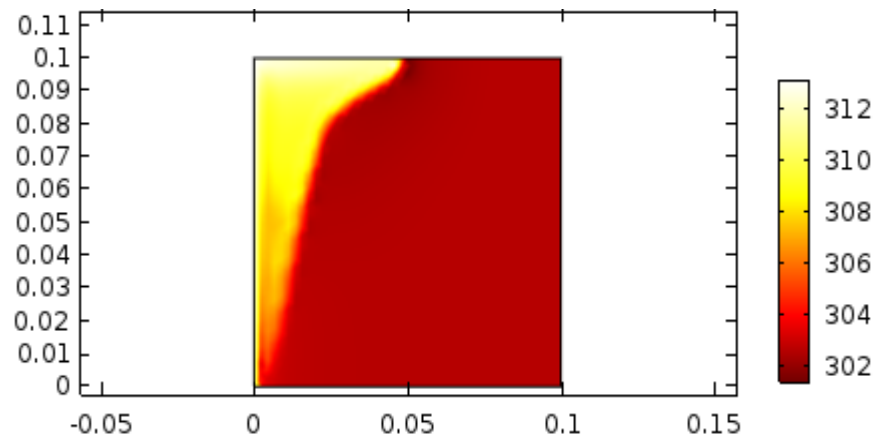
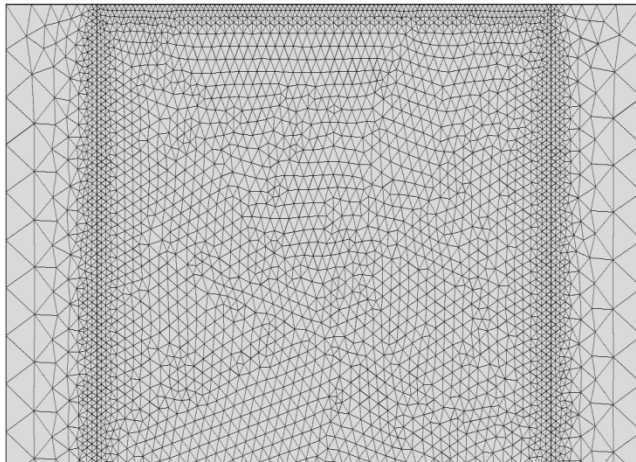
- Test the start of natural convection effect
- Evaluate z
- Calculate Ra_z and $\overline{Nu_z}$ numbers
- Enhance the thermal conductivity of liquid PCM



- Code written in MATLAB®
- Simulations performed with a grid size comprising 225 control volumes after a grid sensitivity analysis
- The dimensionless time step is $\Delta\theta = 2 \times 10^{-5}$ for a total simulation dimensionless time of $\theta = \text{SteFo} = 0.01$ (5000s).

2. CFD model

- CFD model created and implemented in COMSOL
- Modified heat capacity method is used
- Simulations finally performed with 15268 triangular elements of maximum size $1.3\text{e-}3\text{m}$ and minimum size $1.5\text{e-}5\text{m}$



3. comparison between MATLAB and CFD simulations

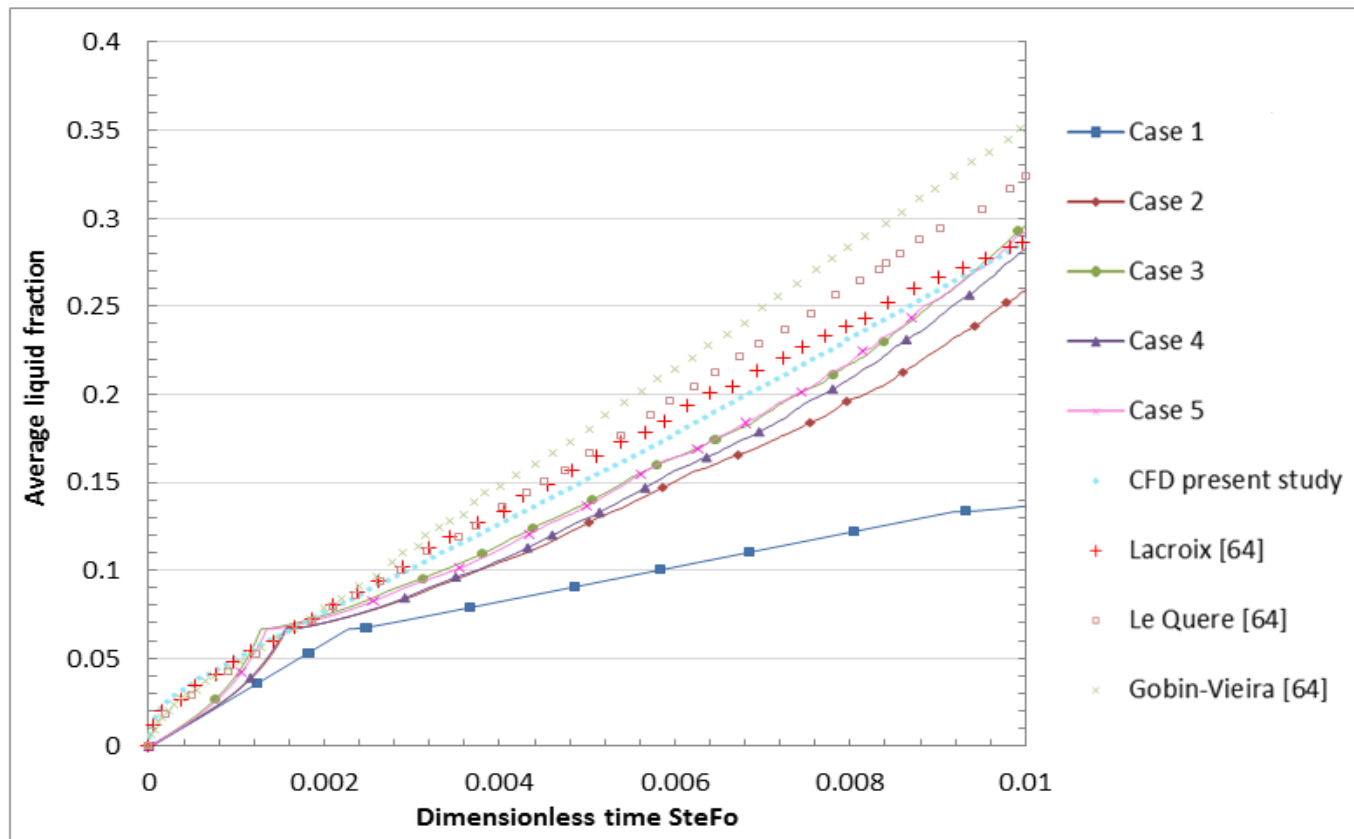
- Simulations conducted with enhanced conduction model run at least 45 times faster than those of CFD simulations
- The average Nusselt number was correlated from CFD model as a function of $\theta = Ste \cdot Fo$
- The correlation was found for a very specific case ($Ra=10^8$, $Ste=0.1$ and $Pr=50$)
- Least square fitting used to correlate Nuz function of θ ($R^2=0.998$)

Cases conducted in the simplified model

cases	Nusselt number correlation	Enhanced conductivity
1	$Nu_z = 1$ (conduction only)	$k_{enh} = \overline{Nu_z} \cdot k_l = k_l$
2	$Nu_z = 0.18 \left(\frac{Pr}{0.2 + Pr} Ra_z \right)^{0.29}$	$k_{enh} = \overline{Nu_z} \cdot k_l$
3	$Nu_z = 0.18 \left(\frac{Pr}{0.2 + Pr} Ra_z \right)^{0.29}$	$k_{enh} \sim k_l (1 + \overline{Nu_z})$
4	Correlation from CFD $Nu_z(\theta) = 2150 \cdot (SteFo) - 0.17$	$k_{enh} = \overline{Nu_z} \cdot k_l$
5	Correlation from CFD $Nu_z(\theta) = 2150 \cdot (SteFo) - 0.17$	$k_{enh} \sim k_l (1 + \overline{Nu_z})$

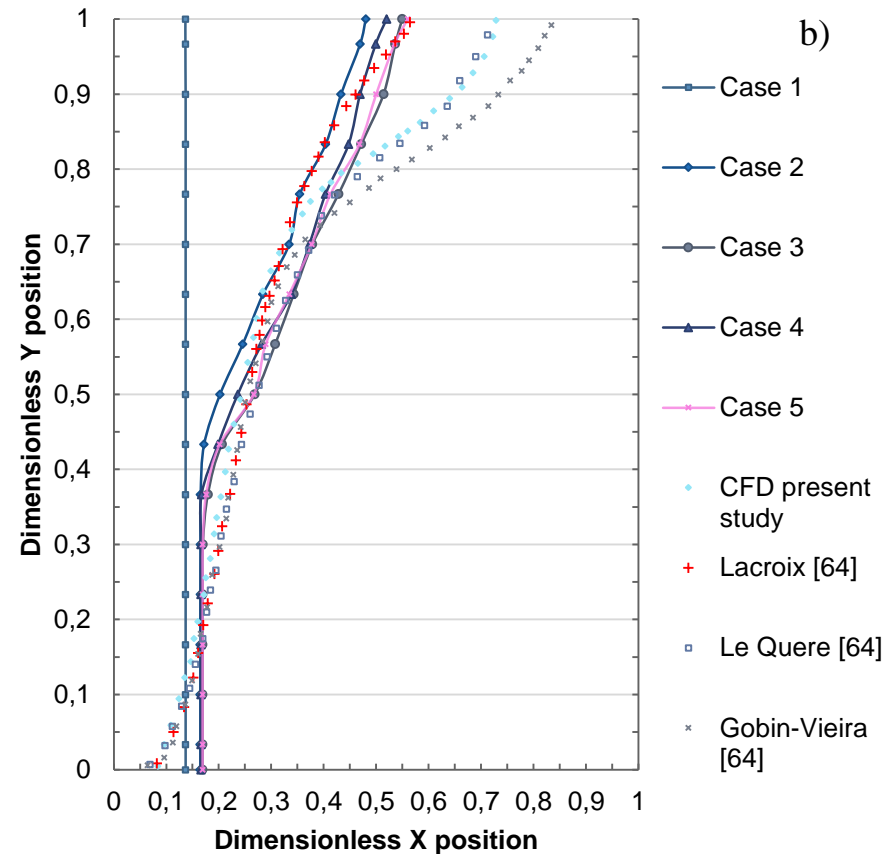
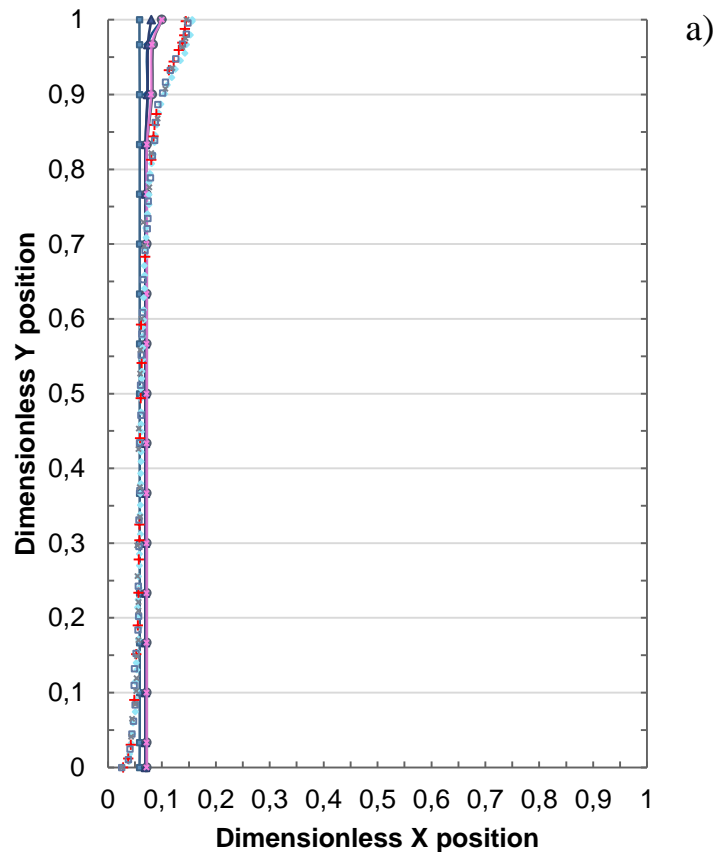
VI. Results

1. **Average liquid fraction** in function of dimensionless time from the model and the numerical benchmark



- Very good agreement between CFD model and the simplified model especially in cases 3 & 5 (The average difference less than 6%)
- The results of these both cases are very close → compatibility between the Nu correlated from CFD and the general correlation proposed by Berkovsky and Polevikov
- Average difference about 5% Comparing the results with those of Lacroix
- Average dispersion around 10% comparing with the results of Le Quere and about 12% with those of Gobin-Vieira
- Comparing with case 1, the average fraction of liquid is enhanced by about 40%

2. Comparison of **melting front positions** from the model and the numerical benchmark at a) $SteFo = 0.002$. b) $SteFo = 0.01$



- Results of simplified model close to those of CFD model, and in good agreement for the overall shape of the solid-liquid interface especially for cases 3 and 5
- Results of simplified model also compared to numerical Benchmark results of Lacroix, Le Quere and Gobin-vieira (**Bertrand** et al,1988)
- The average melting front position enhanced by about at about 55% at $SteFo = 0.01$ for cases 3 and 5 compared to case 1

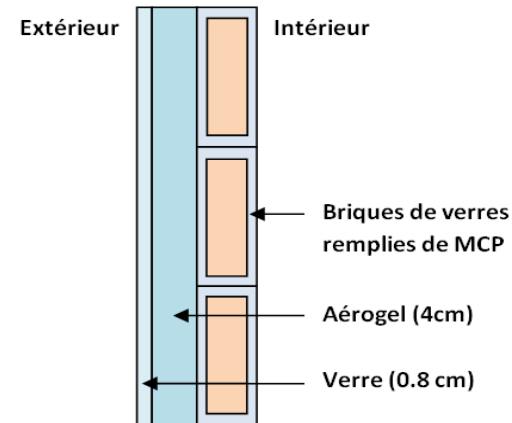
VII. conclusion

- The simplified model showed very good agreement compared to CFD and benchmark solutions
- Results were enhanced by about 40% to 55% taking the convection effect into consideration
- Simple to implement & Its computer simulations run much faster than those of the CFD model
- Developed specifically for practical thermal engineering applications (yearly energy performance evaluation)

Perspective

- To model the solar radiation (short-wave radiation) through transparent PCM filled in a cavity
- To integrate the obtained validated simplified model in an energy simulation tool of a building for yearly basis (for example TRNSYS or Energy Plus)

- To use the model to study the thermal behavior of a solar wall made of transparent PCM and super-insulating silica aerogel



A 2D heatmap plot is shown in the background. The plot has a color gradient ranging from dark blue to red. A bright yellow and orange diagonal band runs from the bottom-left towards the top-right. The rest of the plot is predominantly dark blue. The text "Thank you for your attention!" is overlaid in a large, blue, sans-serif font with a black outline.

Thank you for your
attention!