# Phase Change Materials

## Modeling Approach to Facilitate Thermal Energy Management in Buildings

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# Introduction

What are PCMs and what are their application areas?

- Materials with a characteristically large enthalpy of fusion
- Latent heat energy storage systems
- Decouple energy supply and demand → increase efficiency
- Wide range of applications from -40 to 500°C, *i.e.* space to photovoltaics

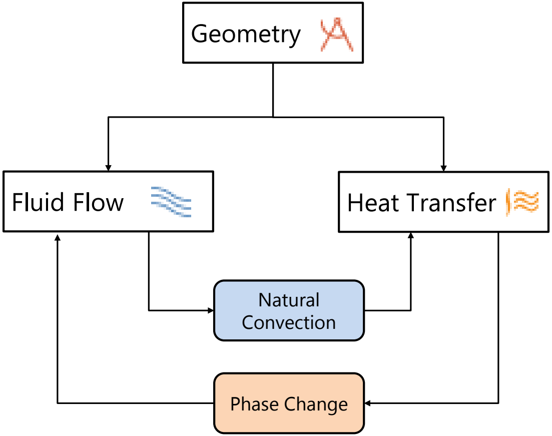
# Introduction

## The need for modeling PCM

- Obtain fundamental understanding for freezing and melting cycle
- Predict the complex behavior well enough
- Efficiently choose among the vast selection of suitable PCM
- Design improvements
- Reduce development costs

# Physical Model

## Multiphysical couplings

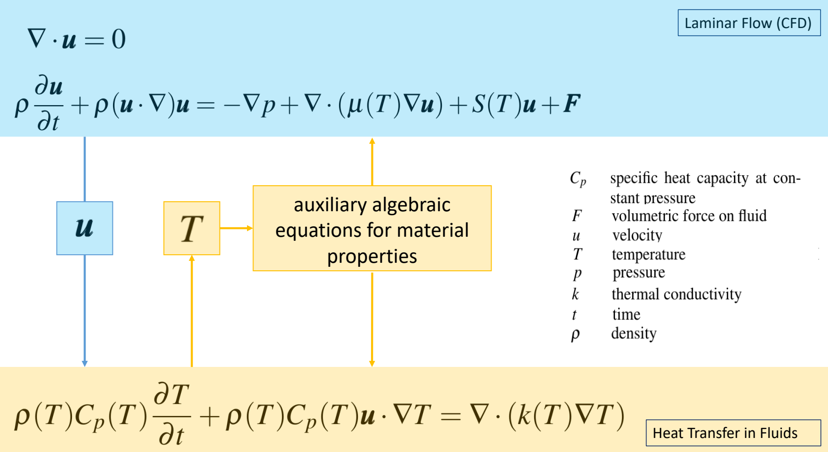


# Numerical Model

## Implementation into COMSOL Multiphysics

$$\nabla \cdot \boldsymbol{u} = 0$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\nabla p + \nabla \cdot (\mu(T)\nabla \boldsymbol{u}) + S(T)\boldsymbol{u} + \boldsymbol{F}$$



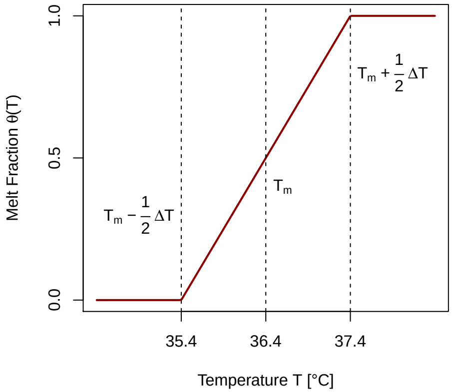

$$\rho(T)C_p(T)\frac{\partial T}{\partial t} + \rho(T)C_p(T)\boldsymbol{u} \cdot \nabla T = \nabla \cdot (k(T)\nabla T)$$

| | |
|---|---|
| $C_p$ | specific heat capacity at constant pressure |
| $F$ | volumetric force on fluid |
| $u$ | velocity |
| $T$ | temperature |
| $p$ | pressure |
| $k$ | thermal conductivity |
| $t$ | time |
| $\rho$ | density |

# Numerical Model

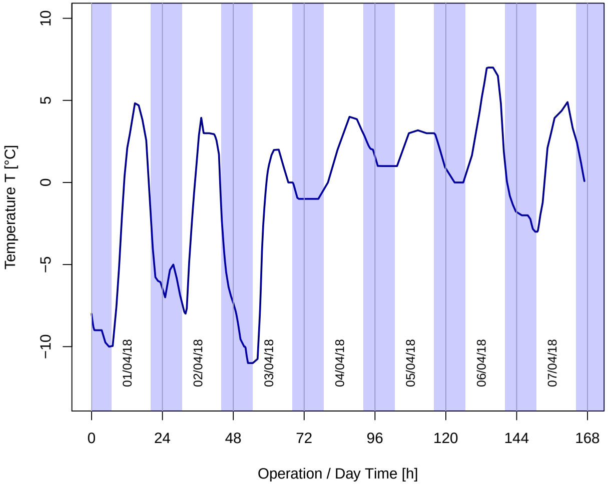
## Melted fraction $\theta(T)$

$$\theta(T) = \begin{cases} 0, & \text{solid} \\ \frac{T-(T_m-\Delta T/2)}{\Delta T}, & \text{mushy} \\ 1, & \text{liquid} \end{cases} \quad (1)$$



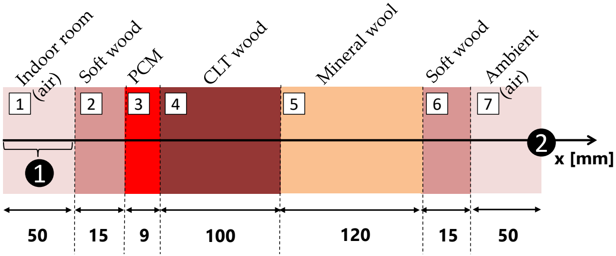
# Application Example

## Observed week in Oslo, temperature profile



# Application Example

## Wall crossection of a typical Norwegian building



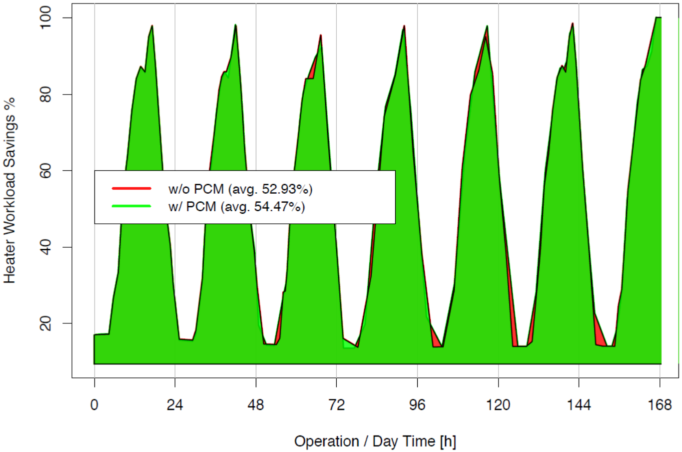

1 Thermostat: Keep $19 < T < 26$ °C + internal heat gains

2 Weather data for T

| Layer | Width [mm] | $\rho$ [kg m$^{-3}$] | $C_p$ [J kg$^{-1}$ K$^{-1}$] | $k$ [W m$^{-1}$ K$^{-1}$] |
|---|---|---|---|---|
| 1 7 | 50 | 1.3 | 1000 | 0.13 |
| 2 6 | 15 | 390 | 1600 | 0.13 |
| 3 (s) | 9 | 1400 | 2200 | 2.5 |
| 3 (l) | 9 | 850 | 4500 | 0.15 |
| 4 | 100 | 410 | 1300 | 0.098 |
| 5 | 120 | 60 | 850 | 0.04 |

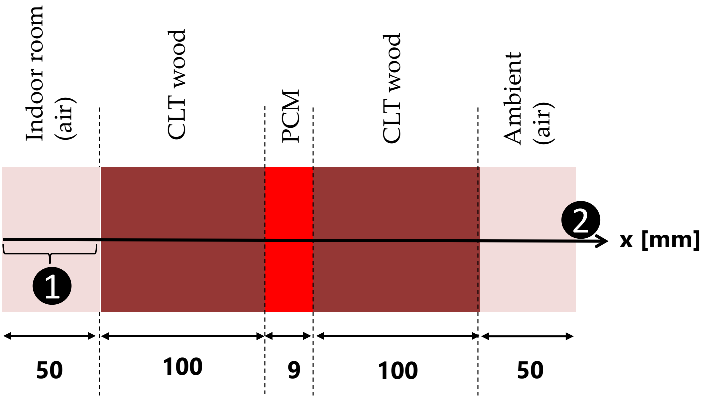
# Application Example

## Results - energy savings?



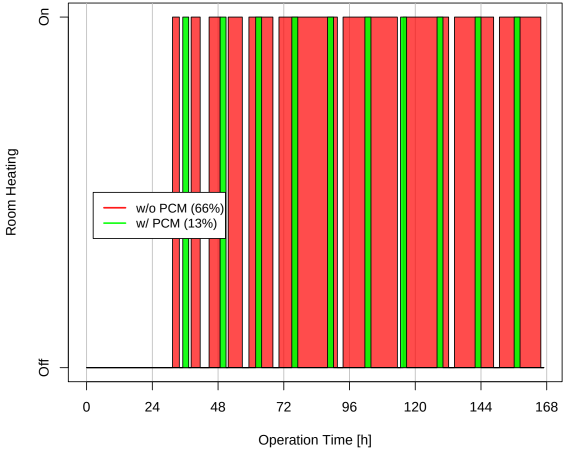
# Application Example

## A less instulated wall crosssection



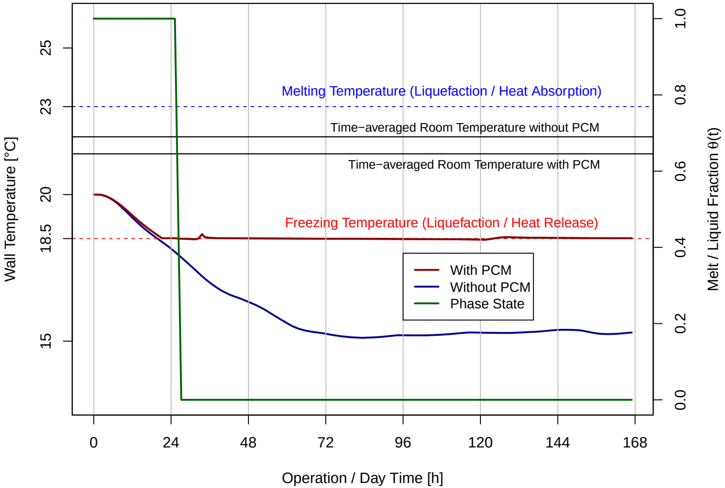
# Application Example

## Results - substantial energy savings!



# Application Example

## Wall core temperature



# Final Remarks

## Discussion

- Release heat to reduce heating demand
- For well insulated walls $\rightarrow$ marginal savings!
- But: PCM reduces peak temperatures on both extremes
- Cold climates $\rightarrow$ main benefit in summer

## Conclusion

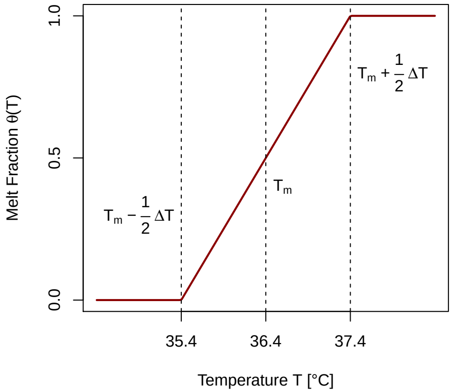
- Comprehensive and suitable modeling approach for phase change phenomena developed
- Rapid orientation whether a PCM meets thermal, technical and economic requirements
- Model shows the importance of including indoor dynamics to assess the PCM potential
- Numerically stable model, extendable to enhanced PCM

Thank you for your attention!

# A - Modeling Functions

## Melt Fraction $\theta(T)$

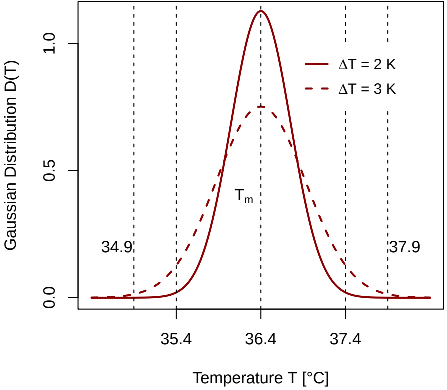
$$\theta(T) = \begin{cases} 0, & \text{solid} \\ \frac{T-(T_m-\Delta T/2)}{\Delta T}, & \text{mushy} \\ 1, & \text{liquid} \end{cases} \quad (2)$$



# A - Modeling Functions

## Gaussian Distribution Function $D(T)$

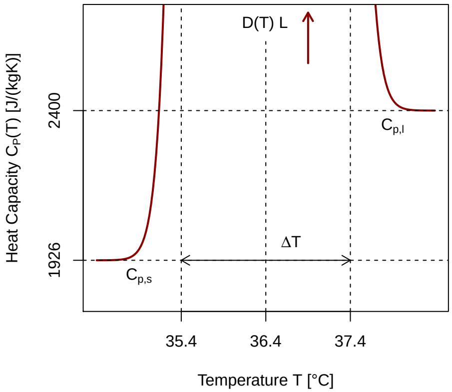
$$D(T) = \frac{e^{-\frac{(T-T_m)^2}{(\Delta T/4)^2}}}{\sqrt{\pi(\Delta T/4)^2}} \quad (3)$$



# A - Modeling Functions

## Modified Heat Capacity $C_p(T)$

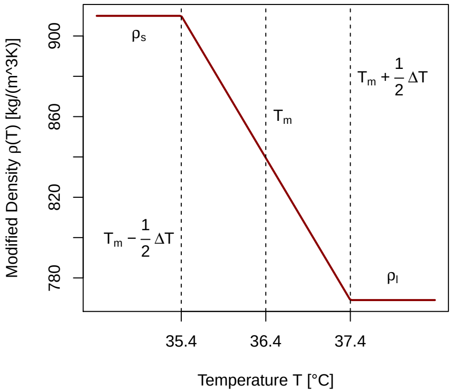
$$C_p(T) = C_{p,s} + \theta(T)(C_{p,l} - C_{p,s}) + D(T)L \quad (4)$$



# A - Modeling Functions

## Modified Material Density $\rho(T)$

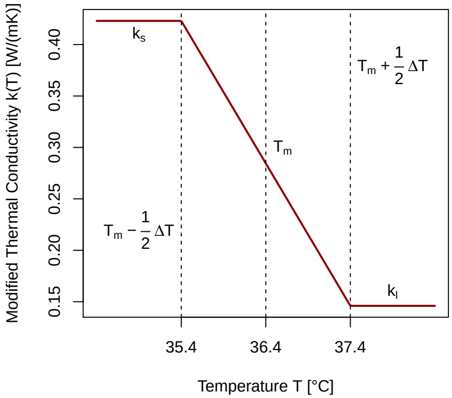
$$\rho(T) = \rho_s + \theta(T)(\rho_l - \rho_s) \tag{5}$$



# A - Modeling Functions

## Modified Thermal Conductivity $k(T)$

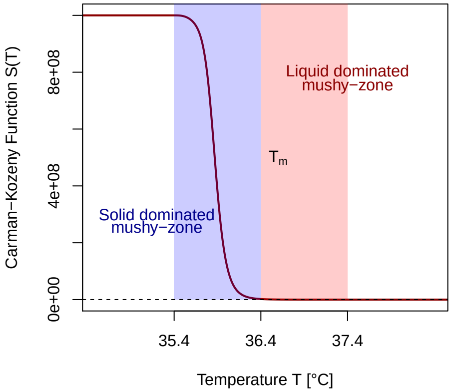
$$k(T) = k_s + k(T)(k_l - k_s) \quad (6)$$



# A - Modeling Functions

## Carman-Kozeny Porosity Function $S(T)$

$$S(T) = A_m \frac{(1-\theta(T))^2}{\theta(T)^3 + \varepsilon} \quad (7)$$

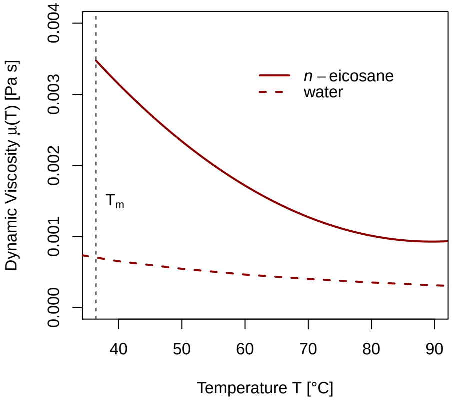



Ali C. Kheirabadi and Dominic Groulx. "Simulating Phase Change Heat Transfer using COMSOL and FLUENT: Effect of the Mushy-Zone Constant". In: *Computational Thermal Sciences: An International Journal* 7.5-6 (2015). DOI: 10.1615/ComputThermalScien.2016014279

# A - Modeling Functions

## Viscosity of *n*-eicosane $\mu(T)$

$$\mu(T) = (9\times10^{-4}\ T^2 - 0.6529\ T + 119.94)\times10^{-3} \tag{8}$$



# A - Modeling Functions

## Basic numerical requirements to govern the physics of PCM

| conservation equation | solid fraction | liquid fraction |
|---|---|---|
| continuity | | ✓ |
| momentum | | ✓ |
| energy | ✓ | ✓ |

→ direct approach: two subdomains for liquid and solid fraction with front tracking algorithm

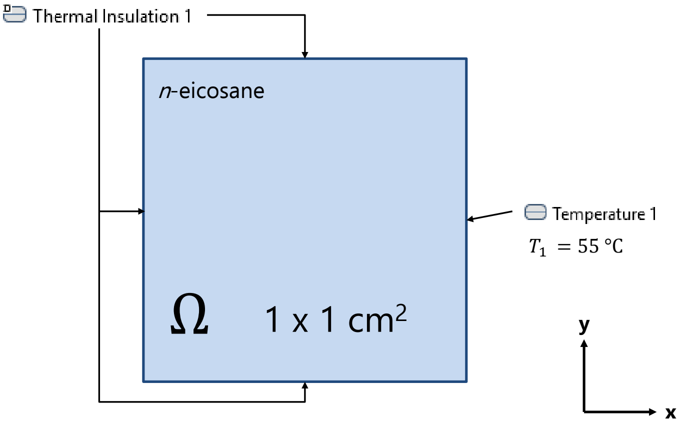
# A - Modeling Functions

## Alternative approach: introduction of a mushy zone

- Idea: material properties are smeared out over an user-defined melting temperature range
- Method: use of porosity formulation, liquid and solid co-exist in the mushy zone
- Benefits:
  - avoid numerical singularities
  - use one single mesh
  - easy to implement
- Setback: highly mesh-dependent solution in terms of physical accuracy

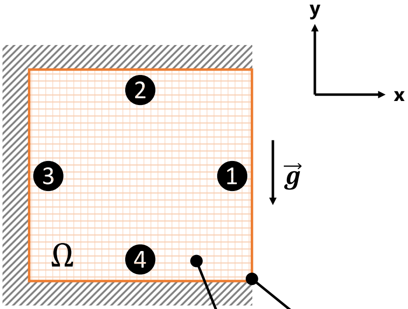
# A - Modeling Functions

## 2D Test-case



# A - Modeling Functions

## Boundary conditions and setup




| Boundary | CFD | Heat Transfer |
|---|---|---|
| 1 | No slip wall | $T_R = 40, 55, 70\ °C$ |
| 2 | No slip wall | Thermal insulation |
| 3 | No slip wall | Thermal insulation |
| 4 | No slip wall | Thermal insulation |

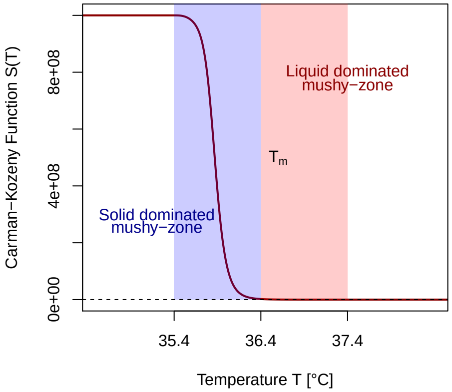
Pressure constraint point, $p = 0$ Pa

Transient study, $0 < t < 1000$ s

# A - Modeling Functions

## Carman-Kozeny porosity function $S(T)$

$$S(T) = A_m \frac{(1-\theta(T))^2}{\theta(T)^3 + \varepsilon} \tag{9}$$

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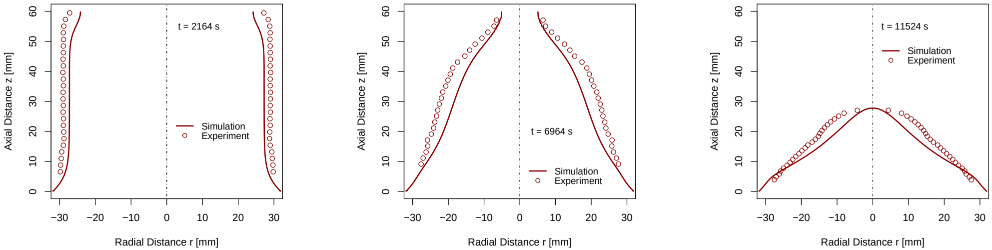
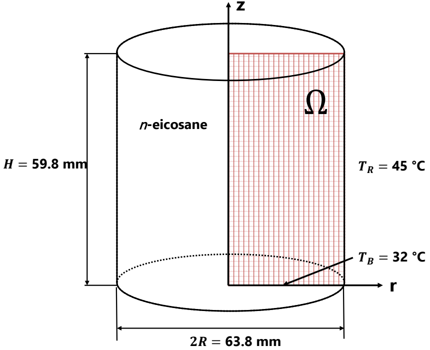
# B - Comparison to Experimental Data

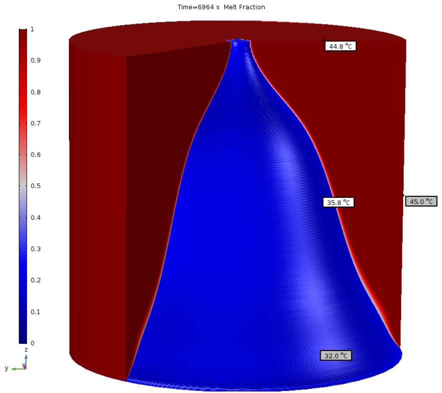
## Results



# B - Comparison to Experimental Data

## Model Setup



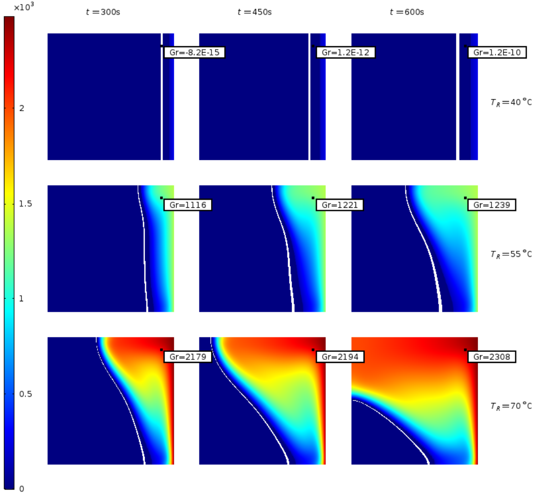
# B - Comparison to Experimental Data

## Material properties of *n*-eicosane, comparison with water

| | *n*-eicosane | | water | |
|---|---|---|---|---|
| | *solid* | *liquid* | *solid* | *liquid* |
| density $\rho$ [$kg\,m^{-3}$] | 910 | 769 | 916 | 997 |
| thermal conductivity $k$ [$W\,m^{-1}\,K^{-1}$] | 0.423 | 0.146 | 1.6 | 0.6 |
| heat capacity $C_p$ [$kJ\,kg^{-1}\,K^{-1}$] | 1.9 | 2.4 | 2.1 | 4.2 |
| melting temperature $T_m$ [$^\circ C$] | 36.4 | - | 0 | - |
| latent heat of fusion $L$ [$kJ\,kg^{-1}$] | 248 | - | 334 | - |

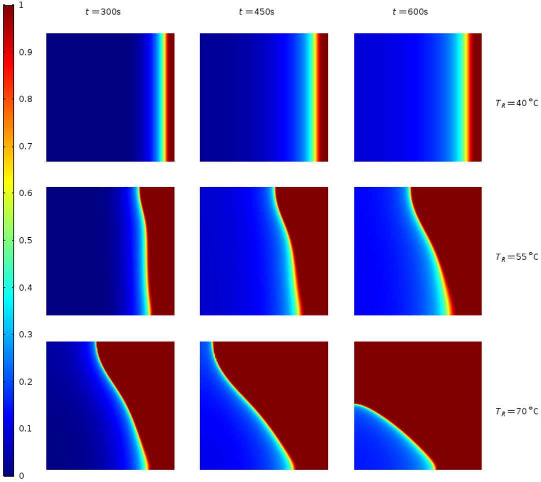
# C - Results

## Grashof Number



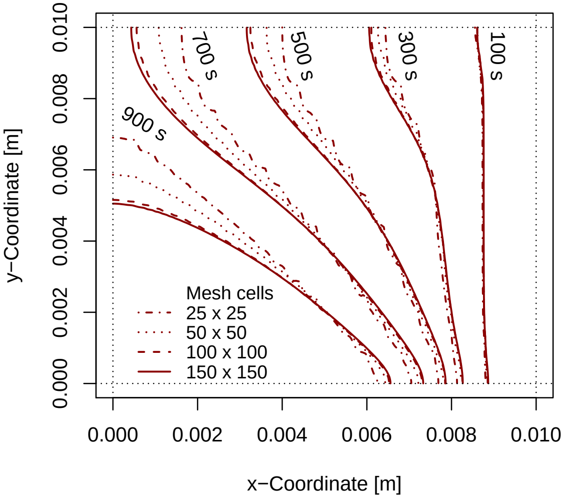
# C - Results

## Melt Fraction



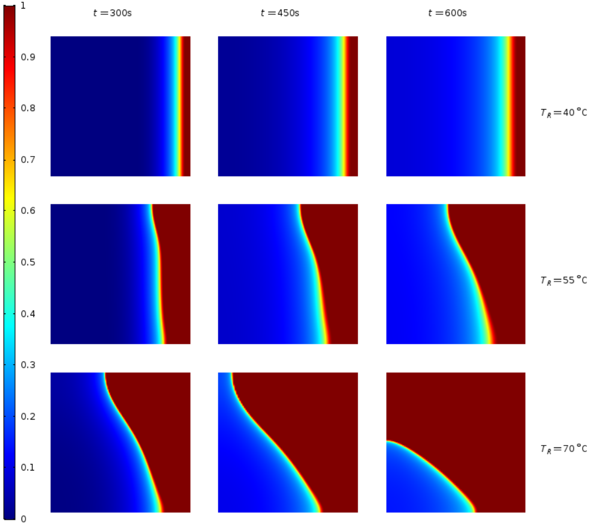
# C - Results

## Mesh sensitivity - melting front prediction



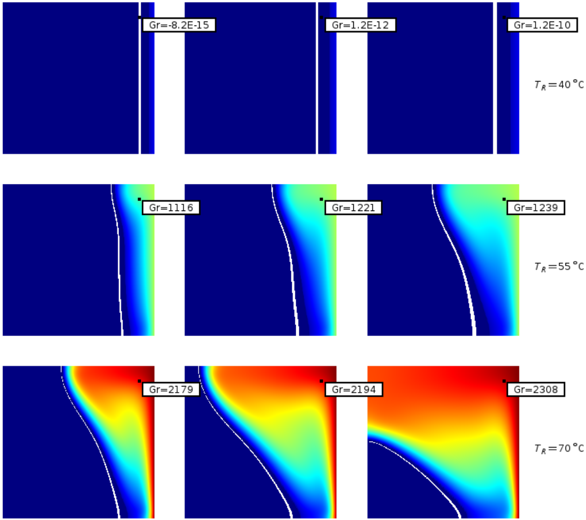
# C - Results

## Melt fraction - curvature of melting front



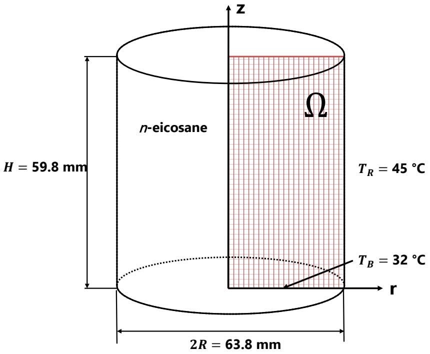
# C - Results

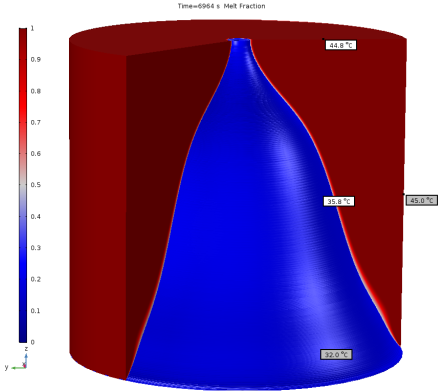
## Local Grashof number - influence of natural convection



# C - Results

## Validation case - setup

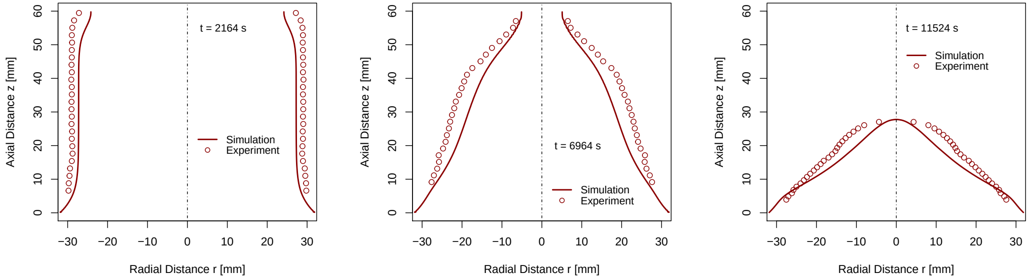



Benjamin J. Jones et al. "Experimental and numerical study of melting in a cylinder". In: *International Journal of Heat and Mass Transfer* 49.15-16 (2006), pp. 2724–2738

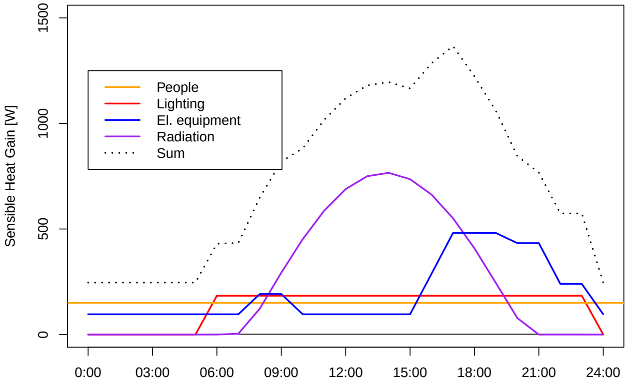
# C - Results

## Validation case - comparison to experimental data



# D - Application Example

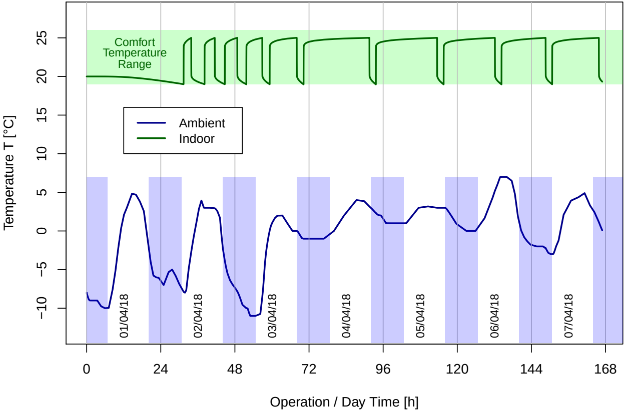
## Internal Heat Gains, Hourly




Komité-SN/K-034. *Bygningers energiytelse, Beregning av energibehov of energiforsyning (engl.: Energy performance of buildings, calculation of energy needs and energy supply)*. URL: https://www.standard.no/no/Nettbutikk/produktkatalogen/Produktpresentasjon/?ProductID=859500. 2016

# D - Application Example

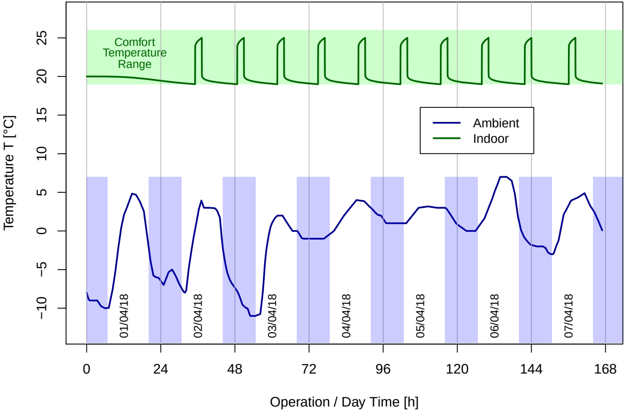
## Indoor Temperature w/o PCM




*Weather Forecast Oslo*. 2018. URL: https://www.wunderground.com/weather/no/oslo

# D - Application Example

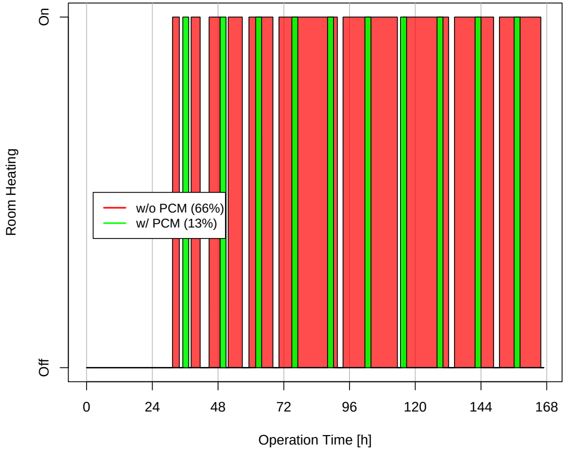
## Indoor Temperature w/ PCM




*Weather Forecast Oslo*. 2018. URL: https://www.wunderground.com/weather/no/oslo

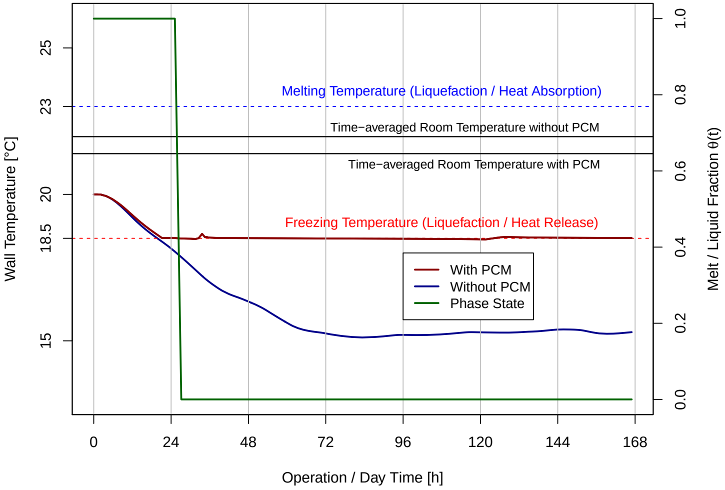
# D - Application Example

## Thermostat



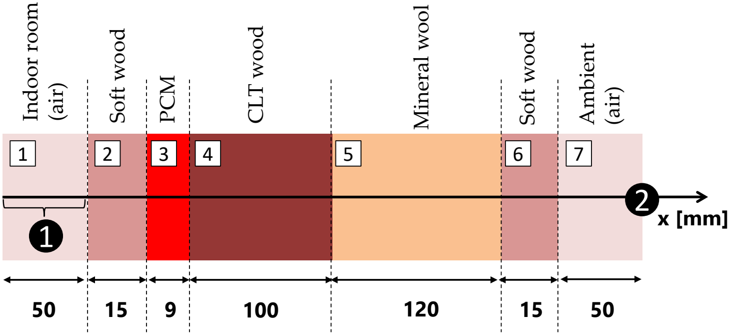
# D - Application Example

## Wall Core Temperature



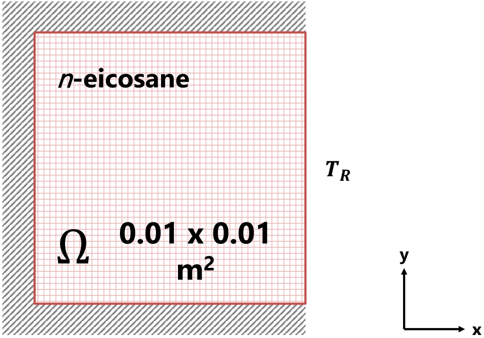
# D - Application Example

## Wall Cross-Section



# E - 2D Test-Case

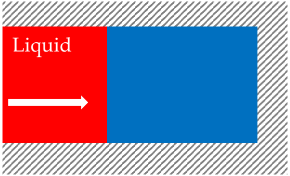
## 2D Test-Case

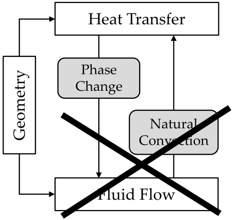


# E - 2D Test-Case

## Multiphysical couplings

$T_R > T_m$




$T_R$: Boundary Temperature

$T_m$: Melting Temperature

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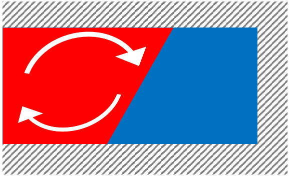
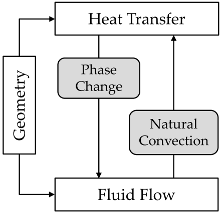
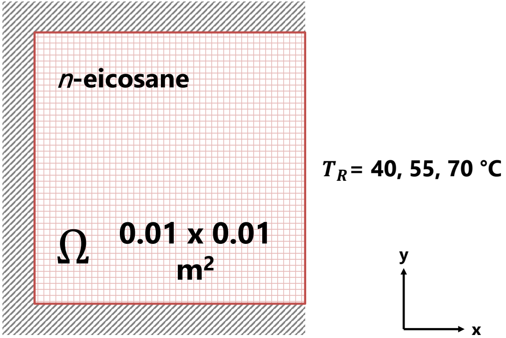
$T_R \gg T_m$





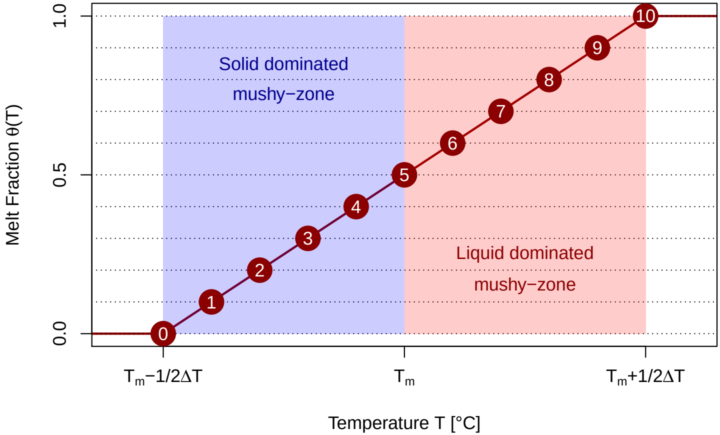
# E - 2D Test-Case

## 2D Test-case



# F - Dimensionless Estimation

## Mushy Zone Investigation



# F - Dimensionless Estimation

## Scaling Variables

$$\tilde{x} = \frac{x}{H} \qquad \tilde{y} = \frac{y}{H} \qquad \tilde{p} = \frac{p - p_{ref}}{\rho {u_0}^2}$$

$$\tilde{t} = \frac{u_0 t}{H} \qquad \tilde{\boldsymbol{u}} = \frac{\boldsymbol{u}}{u_0} \qquad \tilde{T} = \frac{T - T_{ref}}{T_R - T_{ref}}$$

$$\tilde{\Phi}_v = \left(\frac{H}{u_0}\right)^2 \Phi_v \qquad \tilde{\nabla} = H\nabla \qquad \frac{D}{D\tilde{t}} = \left(\frac{H}{u_0}\right)\frac{D}{Dt}$$

# F - Dimensionless Estimation

## Dimensionless Equations

$$\tilde{\nabla} \cdot \tilde{\boldsymbol{u}} = 0 \tag{10}$$

$$\frac{D\tilde{\boldsymbol{u}}}{D\tilde{t}} = -\tilde{\nabla}\tilde{p} + \left[\frac{\mu}{u_0 \rho H}\right]\tilde{\nabla}^2\tilde{\boldsymbol{u}} - \left[\frac{g\beta(T_R - T_m)H}{{u_0}^2}\right]\left(\frac{\boldsymbol{g}}{g}\right)(\tilde{T} - \tilde{T}_m) \tag{11}$$

$$\frac{D\tilde{T}}{D\tilde{t}} = \left[\frac{k}{u_0 \rho H C_p}\right]\tilde{\nabla}^2\tilde{T} + \left[\frac{\mu u_0}{\rho H C_p (T_R - T_m)}\right]\tilde{\Phi}_v \tag{12}$$

# F - Dimensionless Estimation

## Dimensionless Numbers

| | | |
|---|---|---|
| Brinkman | $\mathrm{Br} = \frac{\mu {u_0}^2}{k \Delta T}$ | heat production visc. dissipation vs heat transport by cond. |
| Grashof | $\mathrm{Gr} = \frac{g \beta \Delta T H^3}{\nu^2}$ | buoyant forces vs viscous forces |
| Prandtl | $\mathrm{Pr} = \frac{\nu}{\alpha}$ | momentum diffusivity vs thermal diffusivity |
| Rayleigh | $\mathrm{Ra} = \frac{g \beta \Delta T H^3}{\alpha \nu} = \mathrm{GrPr}$ | heat transport conv. vs cond. |
| Reynolds | $\mathrm{Re} = \frac{\rho u_0 H}{\mu}$ | inertial vs viscous forces |

# F - Dimensionless Estimation

## Values For Liquid Fraction

| Dimensionless group | $T_R$ | | |
|---|---|---|---|
| | 40 °C | 55 °C | 70 °C |
| $\left[\frac{\mu}{u_0 \rho H}\right] = \frac{1}{\text{Re}}$ | 1 | 1 | 1 |
| $\left[\frac{g\beta(T_R - T_m)H}{{u_0}^2}\right] = \frac{\text{Gr}}{\text{Re}^2} = \frac{\text{Ra}}{\text{PrRe}^2}$ | 266 | 1376 | 2486 |
| $\left[\frac{k}{u_0 \rho H C_p}\right] = \frac{1}{\text{RePr}}$ | 0.008 | 0.008 | 0.008 |
| $\left[\frac{\mu u_0}{\rho H C_p (T_R - T_m)}\right] = \frac{\text{Br}}{\text{RePr}}$ | $1.25 \times 10^{-10}$ | $2.42 \times 10^{-11}$ | $1.34 \times 10^{-11}$ |