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Introduction

Physical Model

Numerical Model

Application Example

Final Remarks

Phase Change Materials

Modeling Approach to Facilitate Thermal Energy Management in Buildings

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COMSOL CONFERENCE 2018 LAUSANNE

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 \rightarrow increase efficiency
- Wide range of applications from -40 to 500°C, *i.e.* space to photovoltaics

PCM

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Introduction

The need for modeling PCM

PCM

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- 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



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Numerical Model

Implementation into COMSOL Multiphysics



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Numerical Model Implementation Melted fraction

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$$heta(au) = egin{cases} 0, & ext{solid} \ rac{ au-(au_m-\Delta au/2)}{\Delta au}, & ext{mushy} \ 1, & ext{liquid} \ (1) \end{cases}$$





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Wall core

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Operation / Day Time [h]

Application Example

Observed week in Oslo, temperature profile

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Application Example

Wall crossection of a typical Norwegian building



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Crossection 1

Results

Crosssection

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Application Example

Results - energy savings?



Operation / Day Time [h]



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Room Heating

₽

0

24

48

72

Operation Time [h]

96

120

144

168

Application Example

Results - substantial energy savings!

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Application Example

Wall core temperature



Operation / Day Time [h]

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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

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Thank you for your attention!

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A - Modeling Functions

Melt Fraction

Gaussian Heat Capacity Density Th. Conductivity Carman-Kozeny Viscosity Viscosity Requirements Mushy zone 2D Test-case BC Carman-Kozeny

 $heta(au) = egin{cases} 0, & ext{solid} \ rac{ au-(au_m-\Delta au/2)}{\Delta au}, & ext{mushy} \ 1, & ext{liquid} \end{cases}$

(2)

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A - Modeling Functions Melt Fraction $\theta(T)$



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A - Modeling Functions

Melt Fraction

Gaussian

Density Th. Condu Carman-Ko Viscosity Requirement

Mushy zoi

2D Test

BC

Carman-Kozer

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

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A - Modeling Functions Gaussian Distribution Function D(T)



Temperature T [°C]

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A - Modeling Functions Modified Heat Capacity $C_p(T)$



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

A - Modeling Functions Modified Material Density $\rho(T)$



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

Modified Thermal Conductivity k(T) [W/(mK)]





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A - Modeling Functions Melt Fraction Gaussian Heat Capacity Density Th. Conductivity

Carman-Kozeny

Viscosity Requirements Mushy zone 2D Test-case BC Carman-Kozei $S(T) = A_m rac{(1- heta(T))^2}{ heta(T)^3 + arepsilon}$

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A - Modeling Functions Carman-Kozeny Porosity Function S(T)



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

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Viscosity

Requirement: Mushy zone 2D Test-case BC Carman-Koze

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$$\mu(T) = (9 \times 10^{-4} T^2 - 0.6529 T + 119.94) \times 10^{-3}$$
(8)

A - Modeling Functions

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



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A - Modeling Functions

Basic numerical requirements to govern the physics of PCM

conservation equation	solid fraction	liquid fraction
continuity		\checkmark
momentum		\checkmark
energy	\checkmark	\checkmark

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

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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



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A - Modeling Functions

Boundary conditions and setup



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 $S(T) = A_m rac{(1- heta(T))^2}{ heta(T)^3 + arepsilon}$

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Carman-Kozeny

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A - Modeling Functions Carman-Kozeny porosity function S(T)



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

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Model Setup Material properties

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8

8

10

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-30

Vxial Distance z [mm]

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F -Dimensionles Estimation

B - Comparison to Experimental Data Results



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B - Comparison to Experimental Data Model Setup





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A - Modeling Functions

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Material properties

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B - Comparison to Experimental Data

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

.

	<i>n-</i> eicosane		water	
	solid	liquid	solid	liquid
density $ ho$ [kg m ⁻³]	910	769	916	997
thermal conductivity $k [\text{W} \text{m}^{-1} \text{K}^{-1}]$	0.423	0.146	1.6	0.6
heat capacity $\mathit{C_p} \; [extsf{kJ} extsf{kg}^{-1} extsf{K}^{-1}]$	1.9	2.4	2.1	4.2
melting temperature T_m [°C]	36.4	-	0	-
latent heat of fusion L [kJ kg ⁻¹]	248	-	334	-

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C - Results Grashof Number



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Grashof Number

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Mesh sensitivity - melting front prediction



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Melt fraction - curvature of melting front



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Local Grashof number - influence of natural convection



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C - Results Grashof Number Melt Fraction Mesh sensisitvity Melt fraction

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Validation I Validation II

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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

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Validation case - comparison to experimental data



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Internal Heat Gains, Hourly

Indoor Temperatur w/o PCM

Indoor Temperatur w/ PCM

Thermostat

Wall Core Temperature

Wall Cross-Section

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F -Dimensionless Estimation





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

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Indoor Temperature w/o PCM



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

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D - Application Example

Wall Core Temperature



Operation / Day Time [h]





Wall Core Temperature

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Couplings

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Heat Transfer Liquid Phase Geometry Change $T_R > T_m$ Natura Com T_R: Boundary Temperature luid Flow T_m: Melting Temperature Heat Transfer Phase Geometry Change $T_R \gg T_m$ Natural Convection Fluid Flow

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E - 2D Test-Case

Multiphysical couplings

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Mushy Zone Investigation

Scaling Variable

Dimensionless Equations

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Values For Liquid Fraction

F - Dimensionless Estimation

Mushy Zone Investigation



Temperature T [°C]

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Mushy Zone Investigation

Scaling Variables

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Values For Liquid Fraction

F - Dimensionless Estimation Scaling Variables

$$\begin{split} \tilde{x} &= \frac{x}{H} & \tilde{y} &= \frac{y}{H} & \tilde{p} &= \frac{p - p_{ref}}{\rho u_0^2} \\ \tilde{t} &= \frac{u_0 t}{H} & \tilde{u} &= \frac{u}{u_0} & \tilde{T} &= \frac{T - T_{ref}}{T_R - T_{ref}} \\ \tilde{\Phi}_v &= \left(\frac{H}{u_0}\right)^2 \Phi_v & \tilde{\nabla} &= H\nabla & \frac{D}{D\tilde{t}} &= \left(\frac{H}{u_0}\right) \frac{D}{Dt} \end{split}$$

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Dimensionless Equations

$$\begin{split} \tilde{\nabla} \cdot \tilde{\boldsymbol{u}} &= 0 \quad (10) \\ \frac{D\tilde{\boldsymbol{u}}}{D\tilde{t}} &= -\tilde{\nabla}\tilde{\rho} + \left[\frac{\mu}{u_0\rho H}\right]\tilde{\nabla}^2\tilde{\boldsymbol{u}} - \left[\frac{g\beta(T_R - T_m)H}{u_0^2}\right]\left(\frac{\boldsymbol{g}}{g}\right)(\tilde{T} - \tilde{T}_m) \quad (11) \\ \frac{D\tilde{T}}{D\tilde{t}} &= \left[\frac{k}{u_0\rho HC_p}\right]\tilde{\nabla}^2\tilde{T} + \left[\frac{\mu u_0}{\rho HC_p(T_R - T_m)}\right]\tilde{\Phi}_v \quad (12) \end{split}$$

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Mushy Zone Investigation Scaling Variabl Dimensionless

Dimensionless Numbers

Values For Liquid Fraction

F - Dimensionless Estimation Dimensionless Numbers

heat production visc. dissipation vs heat transport by cond.

buoyant forces vs viscous forces

momentum diffusivity vs thermal diffusivity

RayleighRa = $\frac{g\beta\Delta TH^3}{\alpha\nu}$ = GrPrheat transport conv. vs cond.ReynoldsRe = $\frac{\rho u_0 H}{\mu}$ inertial vs viscous forces

 $\mathsf{Br} = \frac{\mu u_0^2}{k \Lambda T}$

 $\mathsf{Pr} = \frac{\nu}{-}$

 $Gr = \frac{g\beta\Delta TH^3}{v^2}$

Brinkman

Grashof

Prandtl

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Equations

Dimensionles Numbers

Values For Liquid Fraction

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
$\left[\frac{g\beta(T_R-T_m)H}{{u_0}^2}\right] = \frac{\mathrm{Gr}}{\mathrm{Re}^2} = \frac{\mathrm{Ra}}{\mathrm{Pr}\mathrm{Re}^2}$	266	1376	2486
$\left[\frac{k}{u_0\rho HC_p}\right] = \frac{1}{\text{RePr}}$	0.008	0.008	0.008
$\left[\frac{\mu u_0}{\rho H C_{\rho}(T_R - T_m)}\right] = \frac{Br}{RePr}$	$1.25 imes 10^{-10}$	2.42×10^{-11}	$1.34 imes10^{-11}$