Numerical simulation of Phase Change Material (PCM) – water heat storage

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Objective and method

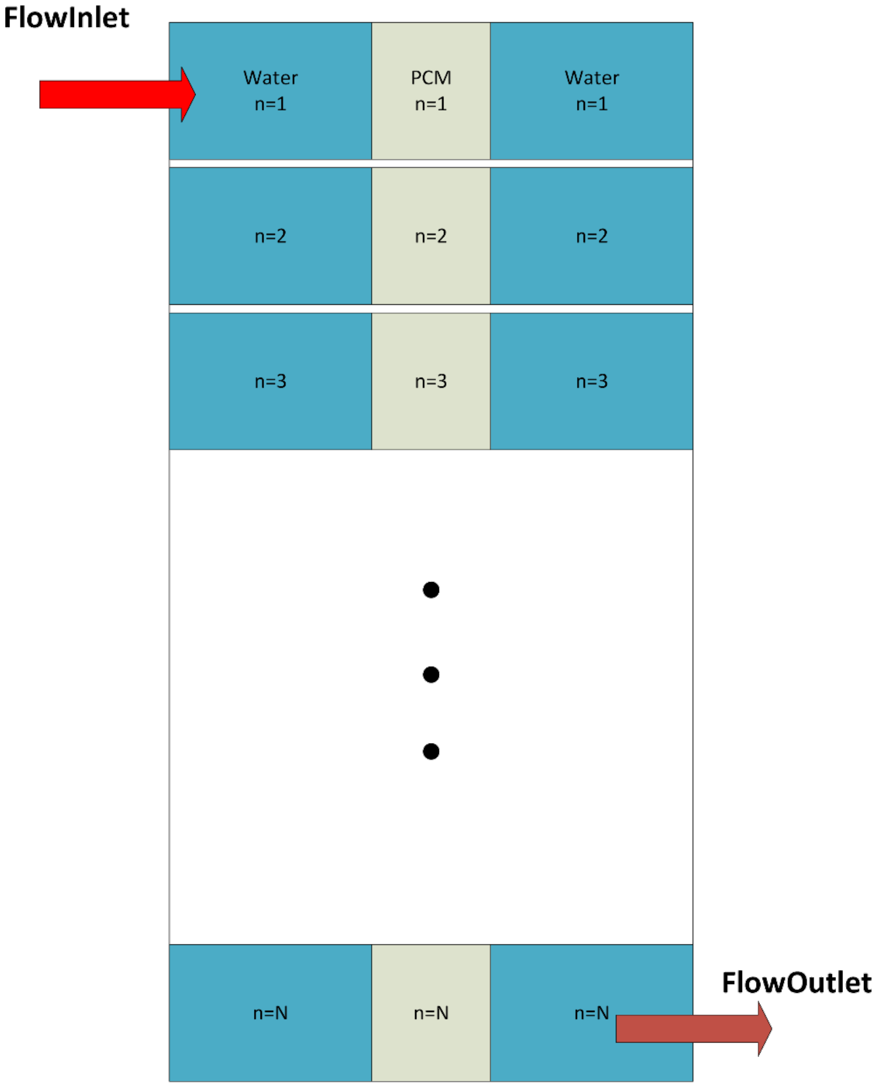
Objectives:

- Simulate a PCM - water tank heat storage
- Not to optimize the tank design
- Used as a component for **all year system** simulation

Method:

- Rough mesh numerical heat transfer method
- All implicit CFD method
- Assume an uniform velocity field.
- Only solve the energy equations.

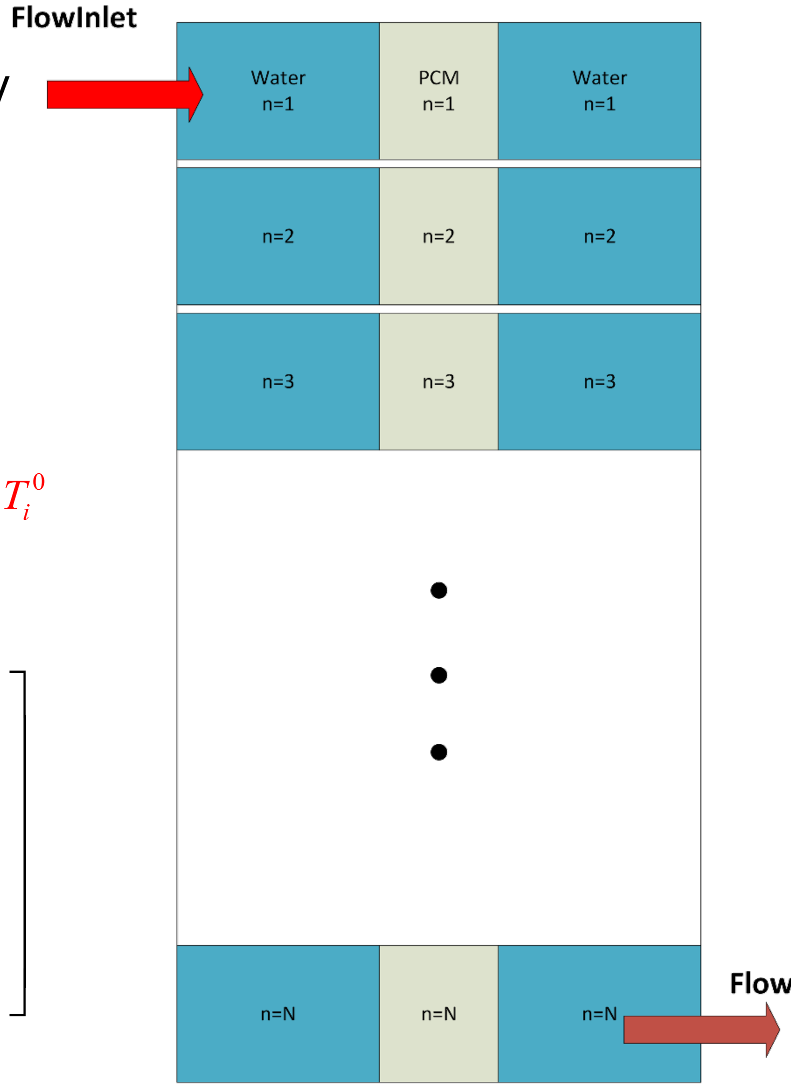
- Independent water model
- Independent PCM model
- Coupling calculation method for water – PCM model



Content

- Water tank development
- PCM tank development
- Coupling calculation of PCM – water tank
- Functionality extension
- Discussion

A little bit review of Numerical method by a 1D water tank simulation example



- The governing equation for 1D multi-layer vertical tank unsteady state energy

$$\frac{\partial \rho c T_w}{\partial t} + \frac{\partial \rho c u T_w}{\partial x} = \frac{\partial}{\partial x}\left(k \frac{\partial T_w}{\partial x}\right) + h_{hl} A_s (T_a - T_w) / V + \Gamma A_{pw} (T_p - T_w) / V$$

- All implicit discrete equation

$$\left(-\frac{kA_c}{\Delta x} - \dot{m}c\right) T_{i-1} + \left(\frac{mc}{\Delta t} + \frac{2kA_c}{\Delta x} + h_{hl} A_s + \dot{m}c + \Gamma A_{pw}\right) T_i + \left(-\frac{kA_c}{\Delta x}\right) T_{i+1} = h_{hl} A_s T_a + \Gamma A_{pw} T_{pi} + \frac{mc}{\Delta t} T_i^0$$

$$aT_{i-1} + bT_i + cT_{i+1} = d$$

- For example N = 5, in one time step:

$$\begin{bmatrix} b,c,0,0,0 \\ a,b,c,0,0 \\ 0,a,b,c,0 \\ 0,0,a,b,c \\ 0,0,0,a,b \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \\ d_5 \end{bmatrix}$$

- The Gauss Elimination method or TDMA for 1D meshing

- The same simulation accuracy as TRNSYS type 534

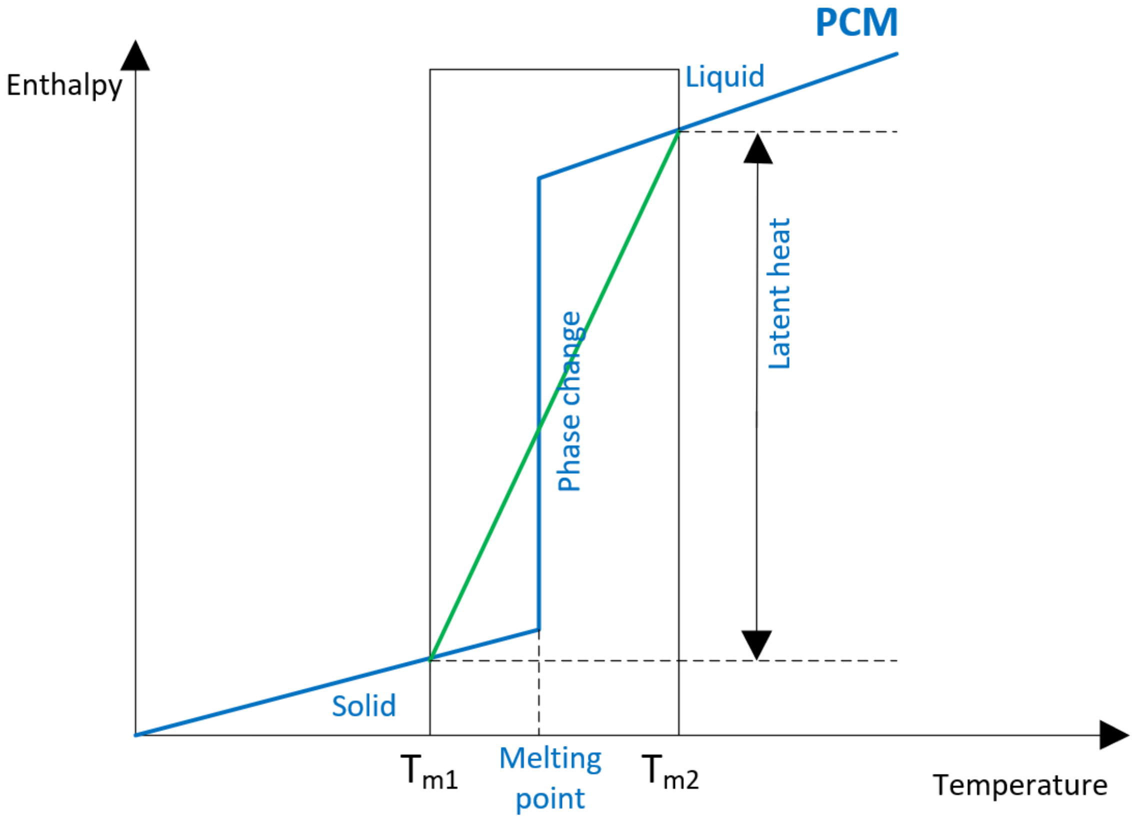
1D PCM tank model

- Suppose a 1D vertical PCM surrounded by water. The governing equation for PCM tank in unsteady state

$$\frac{\partial \rho H_p}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T_P}{\partial x}\right) + \Gamma A_{pw}(T_w - T_p)/V$$

- The discontinuity of PCM energy is described by the piecewise enthalpy equations

$$H_p = \begin{cases} c_s T & T < T_{m1} \\ c_s T_{m1} + \dfrac{E_L (T - T_{m1})}{T_{m2} - T_{m1}} & T_{m1} \le T \le T_{m2} \\ c_s T_{m1} + E_L + c_l (T - T_{m2}) & T > T_{m2} \end{cases}$$



Linearization of the enthalpy equation

The enthalpy can be rewritten into a temperature linear equation with a fixed format with S1 and S2

$$H_p = S_1 T + S_2$$

$$\begin{cases} S_1 = c_s,\, S_2 = 0 & T \le T_{m1} \\ S_1 = \dfrac{E_L}{T_{m2} - T_{m1}},\, S_2 = c_s T_{m1} - \dfrac{E_L T_{m1}}{T_{m2} - T_{m1}} & T_{m1} < T \le T_{m2} \\ S_1 = c_l,\, S_2 = E_L + c_s T_{m1} - c_l T_{m2} & T > T_{m2} \end{cases}$$

Then the governing equation can be discrete as follows

$$m\frac{S_1 T + S_2}{\Delta t} - m\frac{S_1^0 T^0 + S_2^0}{\Delta t} = kA_c \frac{T_{i-1} - T_i}{\Delta x} + kA_c \frac{T_{i+1} - T_i}{\Delta x} + \Gamma A_s (T_w - T)$$

$$m\frac{S_1 T}{\Delta t} = kA_c \frac{T_{i-1} - T_i}{\Delta x} + kA_c \frac{T_{i+1} - T_i}{\Delta x} + \Gamma A_s (T_w - T) + m\frac{S_1^0 T^0 + S_2^0 - S_2}{\Delta t}$$

The all implicit discrete equation of PCM

The all implicit discrete equation

$$-\frac{kA_c}{\Delta x}T_{i-1}+\left(\frac{mS_1}{\Delta t}+\frac{2kA_c}{\Delta x}+\Gamma A_s\right)T_i-\frac{kA_c}{\Delta x}T_{i+1}=\Gamma A_s T_w+m\frac{S_1^0 T^0+S_2^0-S_2}{\Delta t}$$

The coefficient of the algebraic Equations

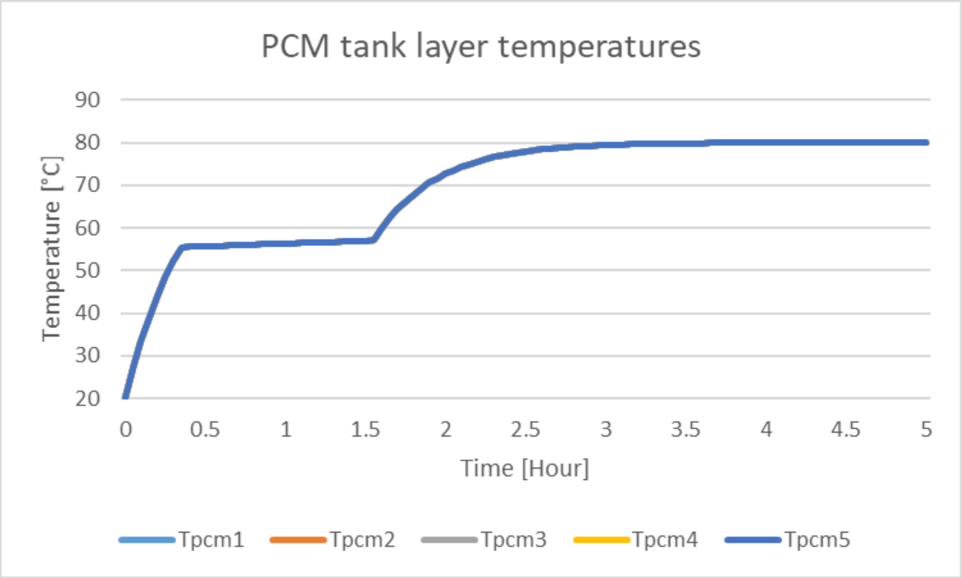
$$a=c=-\frac{kA_c}{\Delta x}$$

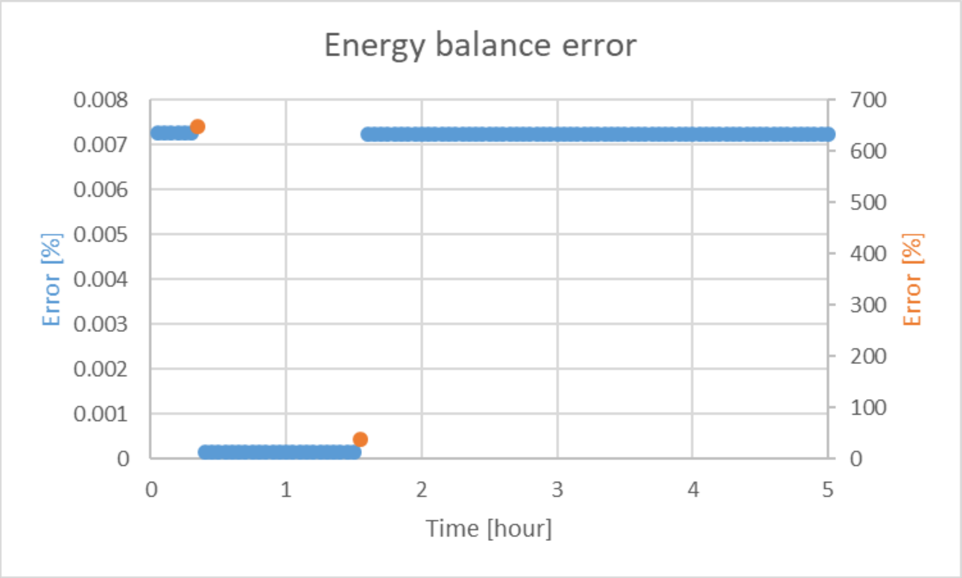
$$b=\frac{mS_1}{\Delta t}+\frac{2kA_c}{\Delta x}+\Gamma A_s$$

$$d=\Gamma A_s T_w+m\frac{S_1^0 T^0+S_2^0-S_2}{\Delta t}$$

The same procedure used for solving as the water tank section. The only extra requirement is to change the S1 and S2 according to the current PCM temperatures.

Simulation results of a simple case for PCM tank


PCM tank layer temperatures


Energy balance error

Volume of tank = 1 m^3; Height of tank = 1.5 m;
Tank layer = 5; Initial tank temp. = 20 °C
Water temp. = 80 °C;
Heat transfer coefficient PCM Water = 500 W/K

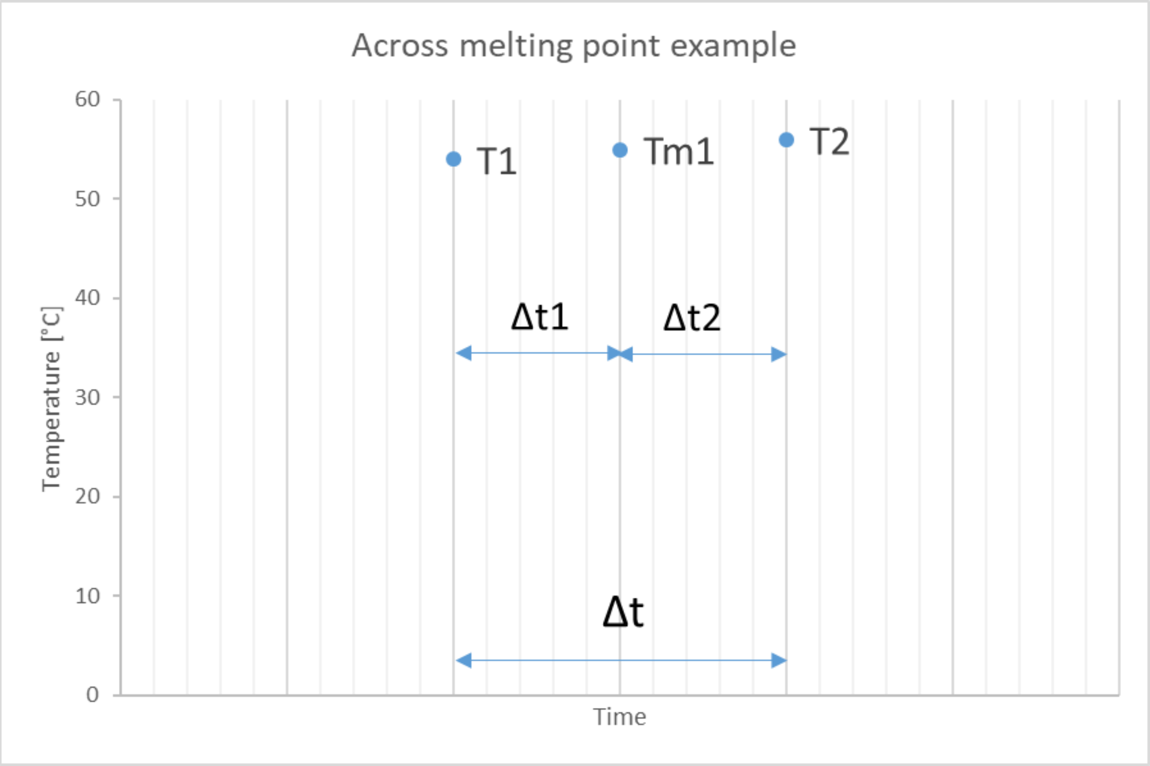
PCM properties:
melting temperature start = 55 °C
melting temperature end = 57 °C
Latent heat of fusion = 250000 J/kg
Solid heat capacity = 2540 J/kg/K
Liquid heat capacity = 2551 J/kg/K
Density = 1301 kg/m^3
Thermal conductivity = 0.3 W/m/k

Simulation time duration = 5 hour;
Time step = 0.05 hour

The big error happens at the two melting points of T_{m1} and T_{m2}.

Reason and solution

- The big energy balance error happens at the time steps that cross the melting point.
- The S1 and S2 differ before and after the melting points.



Reason and solution

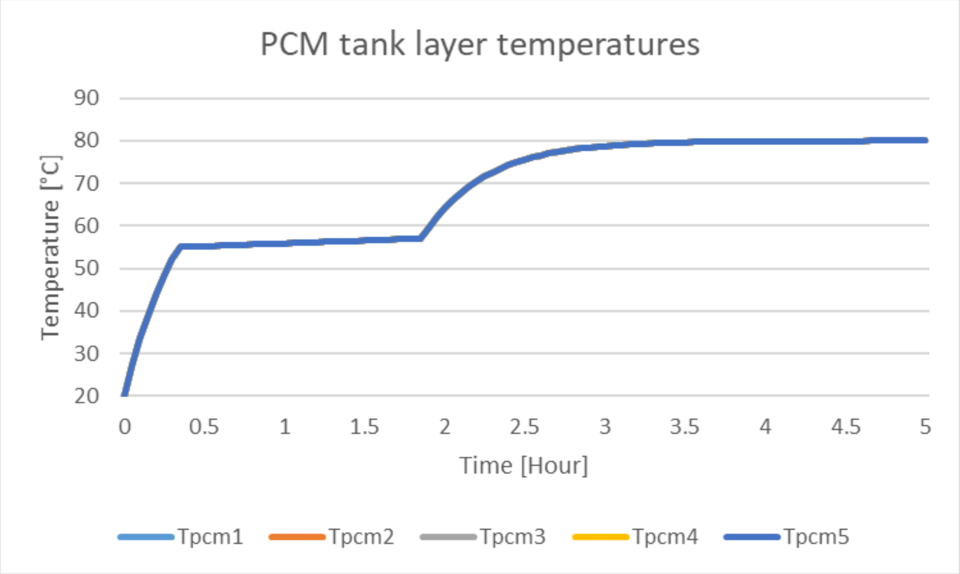
- Assign different S1 S2 and calculate Δt_1 and Δt_2

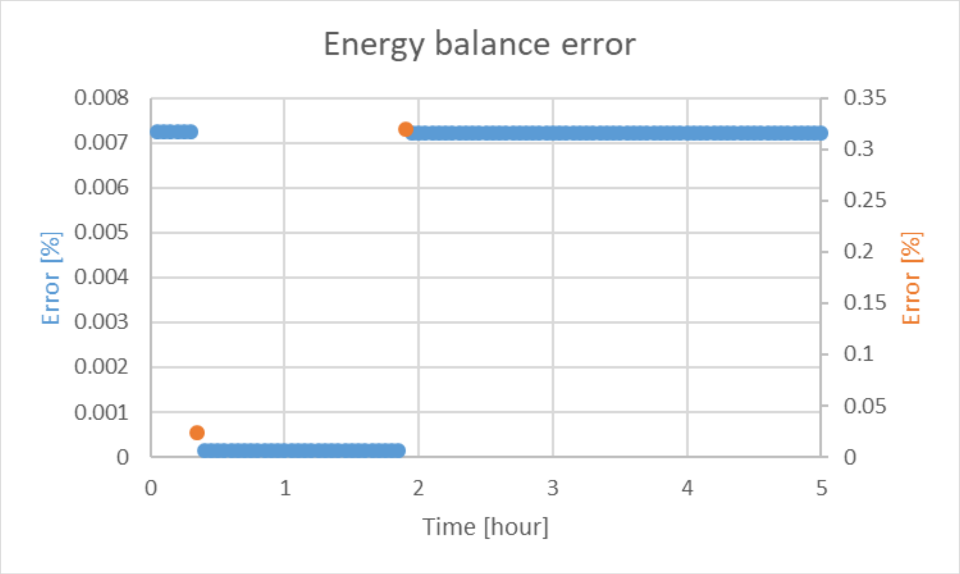
$$m\frac{S_1 T + S_2}{\Delta t} - m\frac{S_1^0 T^0 + S_2^0}{\Delta t} = \frac{d}{dx}(kA_c \frac{dT}{dx}) + \Gamma A_s (T_w - T)$$

$$m\frac{S_{1a} T_{m1} + S_{2a}}{\Delta t_1} = kA_c \frac{T_{i-1} - T_{m1}}{\Delta x} + kA_c \frac{T_{i+1} - T_{m1}}{\Delta x} + \Gamma A_s (T_w - T_{m1}) + m\frac{S_{1a} T^0 - S_{2a}}{\Delta t_1}$$

$$m\frac{S_{1b} T_i}{\Delta t_2} = kA_c \frac{T_{i-1} - T_i}{\Delta x} + kA_c \frac{T_{i+1} - T_i}{\Delta x} + \Gamma A_s (T_w - T_i) + m\frac{S_{1a} T_{m1} + S_{2a} - S_{2b}}{\Delta t_2}$$

Simulation results of the new method





Old method

Time	Tpcm1	Tpcm2	Tpcm3	Tpcm4	Tpcm5	Melting1	Melting2	Melting3	Melting4	Melting5	MeltingAll	QL	Qp	dE	Error
0.3	52.10454	52.10817	52.10818	52.10817	52.10454	0	0	0	0	0	0	12551.98	12551.06	-0.91152	0.007262
0.35	55.44741	55.45115	55.45115	55.45115	55.44741	0.223705	0.225573	0.225574	0.225573	0.223705	0.224826	11047.66	82685.61	71637.95	648.4448
1.5	56.9593	56.96281	56.96282	56.96281	56.9593	0.979652	0.981406	0.981408	0.981406	0.979652	0.980705	10367.37	10367.35	-0.0153	0.000148
1.55	57.02288	57.02638	57.02639	57.02638	57.02288	1	1	1	1	1	1	10338.76	6358.724	-3980.03	38.49624

New method

Time	Tpcm1	Tpcm2	Tpcm3	Tpcm4	Tpcm5	Melting1	Melting2	Melting3	Melting4	Melting5	MeltingAll	QL	Qp	dE	Error
0.3	52.10454	52.10817	52.10818	52.10817	52.10454	0	0	0	0	0	0	12551.98	12551.06	-0.91152	0.007262
0.35	55.01033	55.0104	55.0104	55.0104	55.01033	0.005164	0.005202	0.005202	0.005202	0.005164	0.005187	11245.33	11247.95	2.622438	0.02332
1.85	56.99838	56.99846	56.99846	56.99846	56.99838	0.999192	0.99923	0.99923	0.99923	0.999192	0.999215	10350.71	10350.69	-0.01528	0.000148
1.9	59.6842	59.6875	59.6875	59.6875	59.6842	1	1	1	1	1	1	9141.219	9170.427	29.20752	0.319515

PCM water heat storage

- Governing equations:

$$\rho c \frac{\partial T_w}{\partial t} = \frac{d}{dx}\left(k_w \frac{dT_{ww}}{dx}\right) + \rho u c \frac{dT_{ww}}{dx} + h_{loss} \frac{dT_{wa}}{d\delta_{wa}} + h_{wp} \frac{dT_{wp}}{d\delta_{wp}} + \frac{d}{d\delta_{wp}}\left(k_{wp} \frac{dT_{wp}}{d\delta_{wp}}\right)$$

→ Tw()

$$\rho \frac{\partial H_p}{\partial t} = \frac{d}{dx}\left(k_p \frac{dT_{pp}}{dx}\right) + h_{wp} \frac{dT_{pw}}{d\delta_{wp}} + \frac{d}{d\delta_{wp}}\left(k_{wp} \frac{dT_{pw}}{d\delta_{wp}}\right)$$

→ Tp()

- Two equations model

  Tw() represents the water tank model

  Tp() represents the inside PCM model

- Iteration method to derive the correct water and PCM temperature

Step 1: $T_{w1} = Tw(T_{wo}, T_{po})$ $T_{p1} = Tp(T_{w1}, T_{po})$

Step 2: $T_{w2} = Tw(T_{wo}, T_{p1})$ $T_{p2} = Tp(T_{w2}, T_{po})$

… …

Until

Step n: $T_{wn} – T_{wn-1}$ and $T_{pn} – T_{pn-1}$ are extremely small

Functionality extension

- All the new functionalities are development based on the same governing equation, discrete method and the all-implicit solver of the algebraic equation set.
- No new assumptions or special techniques were used.

Auxiliary heater

$$-\frac{kA_c}{\Delta x}T_{i-1}+\left(\frac{mc}{\Delta t}+\frac{2kA_c}{\Delta x}+hA_s+\dot{m}c\right)T_i+\left(-\frac{kA_c}{\Delta x}-\dot{m}c\right)T_{i+1}=hA_sT_a+\frac{mc}{\Delta t}T_i^0+Q_i$$

$$aT_{i-1}+bT_i+cT_{i+1}=d$$

- The auxiliary heater can be added into any tank layers.

Separate heat losses on top and at bottom

- Three heat losses coefficients: h_side, h_top, h_bot

$$-\frac{kA_c}{\Delta x}T_{i-1}+\left(\frac{mc}{\Delta t}+\frac{2kA_c}{\Delta x}+hA_s+\dot{m}c\right)T_i+\left(-\frac{kA_c}{\Delta x}-\dot{m}c\right)T_{i+1}=hA_sT_a+\frac{mc}{\Delta t}T_i^0$$

$$aT_{i-1}+bT_i+cT_{i+1}=d$$

- The only effected nodes are the first (top) and last (bottom) node.

$$b_1=b_1+h_{top}A_{cross} \qquad b_N=b_N+h_{bot}A_{cross}$$

$$d_1=d_1+h_{top}A_{cross}T_a \qquad d_N=d_N+h_{bot}A_{cross}T_a$$

- If uneven h_side are defined by users, the same method can be used.

- The same method can be used for the PCM tank if needed.

Flexible inlet/outlet for the enter/exit flow

User can assign the pair ports of the flow enters and exits at any tank layers.

Only one pair port was modelled for this model.

Method:

$$mc\frac{T_i - T_i^0}{\Delta t} = kA_c\frac{T_{i-1} - T_i}{\Delta x} + kA_c\frac{T_{i+1} - T_i}{\Delta x} + F_1\dot{m}c(T_{i-1} - T_i) + F_2\dot{m}c(T_{i+1} - T_i) + hA_s(T_a - T_i)$$

$$(-\frac{kA_c}{\Delta x} - F_1\dot{m}c)T_{i-1} + (\frac{mc}{\Delta t} + \frac{2kA_c}{\Delta x} + hA_s + F\dot{m}c)T_i + (-\frac{kA_c}{\Delta x} - F_2\dot{m}c)T_{i+1} = hA_sT_a + \frac{mc}{\Delta t}T_i^0$$

The methodology is to create three flow coefficient lists a, b, c, which contains series number of 0 or 1, to determine whether there is flow or not in the specific layer.

Fx, a 5 layer water tank, the inlet layer is 2 and outlet layer is 4. Then

F_1 = [0,0,1,1,0] F = [0,1,1,1,0] F_2 = [0,0,0,0,0]

Do not forget to model the boundary condition for the enter flow layer.

It is allowed to assign the inlet and outlet in the same layer.

Mixing effect for water tank

- Mixing effect is caused by the thermally unstable of layers temperature – a layer temperature is higher than the layer above.

- Reference the methods of TRNSYS type 534, we provide three options for users for the mixing effect.

1. No mixing effect
2. Complete mixing (Infinite reverse flow rate)
3. User-defined inverse flow rate

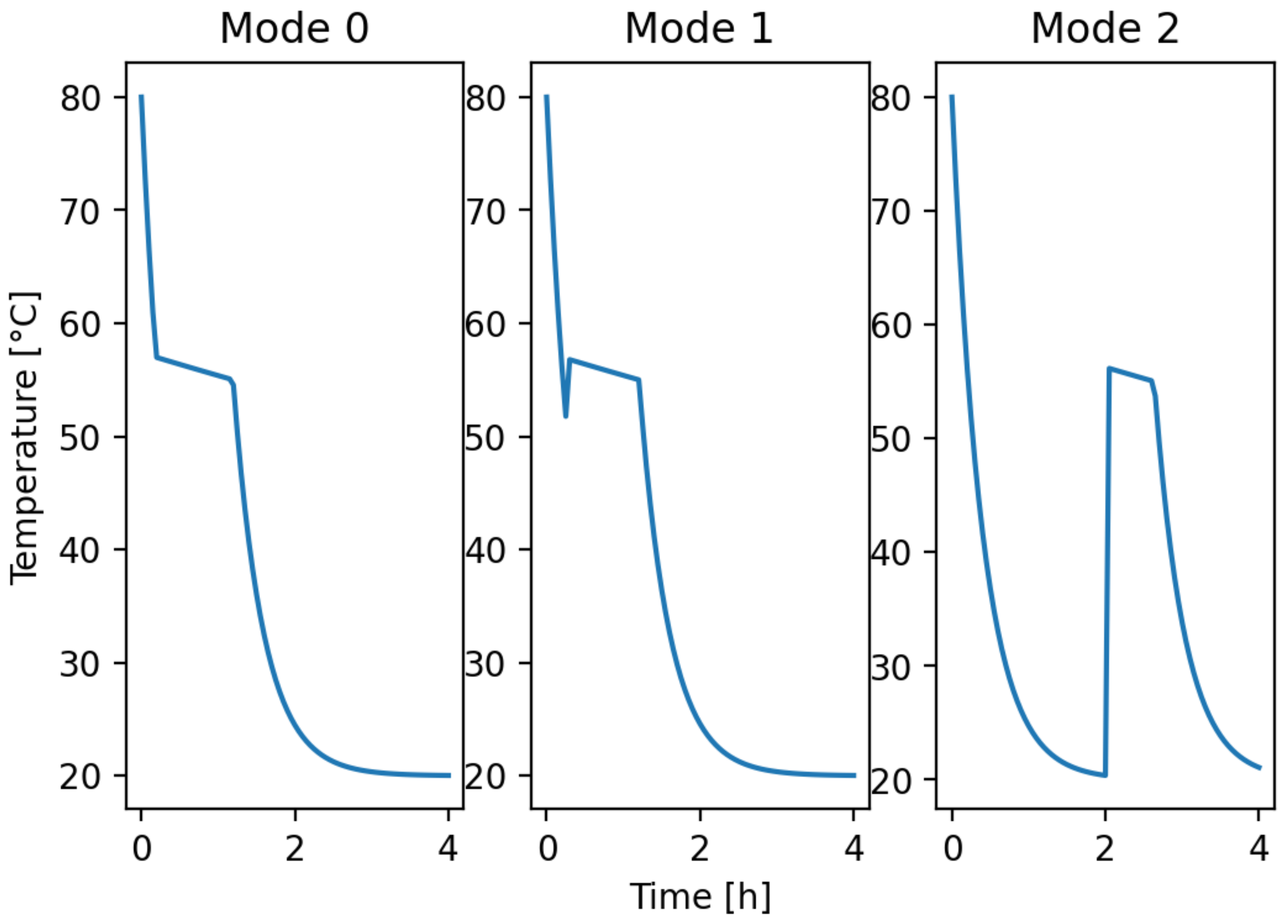
- Complete mixing method:

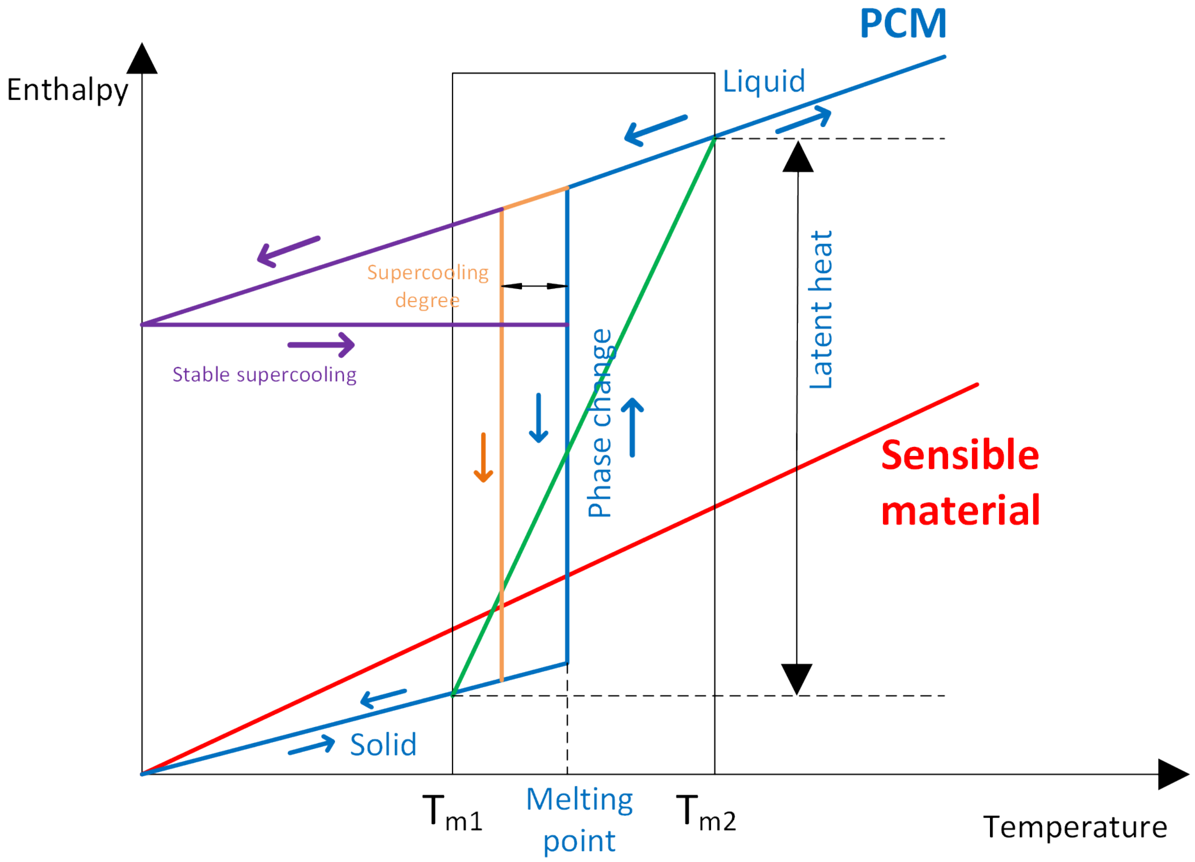
The unstable layers temperature is assigned as the average temperature of the two unstable layers.

PCM supercooling modes

Mode = 0 : No supercooling. Mode = 1 : Supercolling degree provided by user.

Mode = 2 : Stable supercooling. The PCM will start solidification by activation signals provided by user/control unit.





Discussion

Physical model:

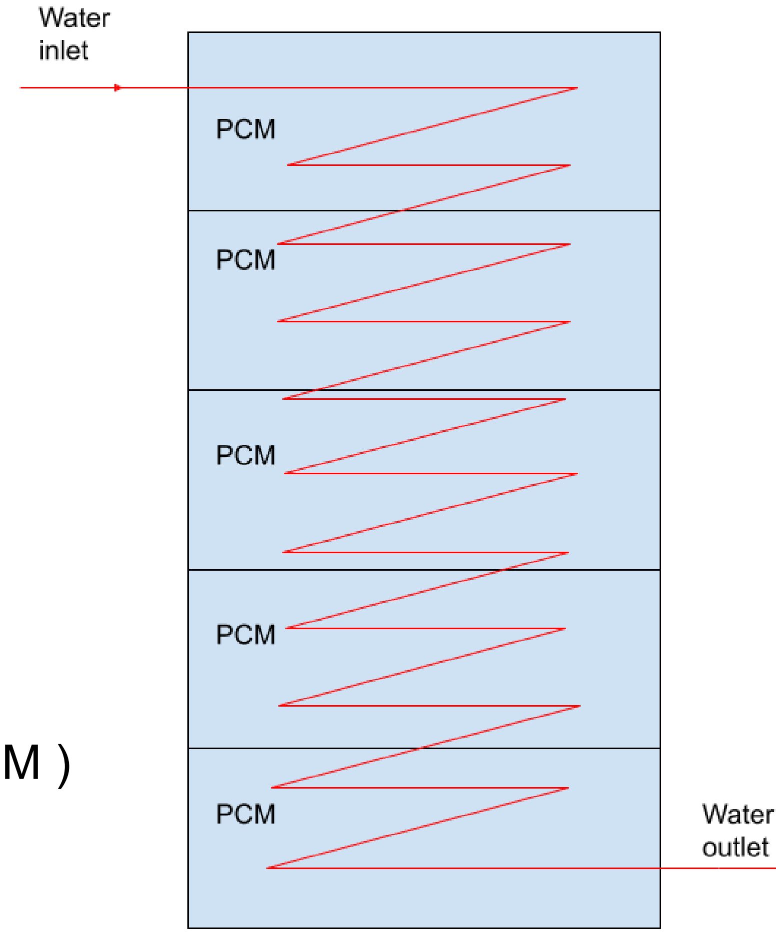
- Application: Single water tank, single PCM tank and PCM water tank.
- Potential: Fx, a PCM tank with water heat exchanger inside.

Limitation:

- No simulation on flow details. It is difficult for users to estimate the Mixing flow.
- 2D PCM tank is needed for rectangular PCM shape.

Further development:

- Heat exchanger for water tank
- PCM in the middle of the water tank (Layers of water tank > layers of PCM)
- 2D PCM tank
- Automatic mixing flow/momentum equation?… …



Publication and Acknowledgment

- Weiqiang Kong, Gang Wang, Gerald Englmair, Elsabet Nomonde Noma Nielsen, Janne Dragsted, Simon Furbo, Jianhua Fan, A simplified numerical model of PCM water energy storage, Journal of Energy Storage,Volume 55, Part A, 2022, https://doi.org/10.1016/j.est.2022.105425.

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