PCM thickness study for a cylindrical Li-ion cell

Performed by **Sagnik Mukhopadhyay** and **Arghyo Debroy**

Transient thermal simulation of an 18650-size cell wrapped in 6, 8 and 10 mm of RT-42 paraffin. ME course project, prepared 19 Nov 2026.

1. Answer in brief

All three thicknesses work, and their differences are small. At a 3C discharge the bare cell reaches **85.9 °C** after 1200 s. With PCM it reaches **41.62 °C** (6 mm), **41.16 °C** (8 mm) and **40.80 °C** (10 mm). Going from 6 to 10 mm buys 0.82 K at 3C and 1.65 K at 2C, but almost doubles the PCM mass (24 g to 47 g).

Which is better. If the only criterion is the lowest cell temperature, 10 mm wins in every case simulated. Per gram of material added, 6 mm is clearly better: it delivers 98% of the 10 mm temperature reduction at 3C with half the PCM, and it uses its latent heat the most (10.8% melted at the end of a 3C discharge, against 2.8% for 10 mm). 8 mm, the thickness the reference paper calls optimal, sits in between on both counts.

Two findings matter more than the thickness choice. First, at 2C and 25 °C ambient none of the layers melts at all, so the latent heat that justifies using a PCM is never touched; the layer works only as a sensible heat sink. Second, the PCM layer here does not insulate the cell. Its outer radius (17 to 21 mm with the shell) is well below the critical radius k/h = 35 mm, so in continuous operation a thicker wrap lets the cell run cooler, not hotter (section 7). During a single discharge the thicker layers lose less heat to the air, because they store more of it (section 5.2).

2. Problem set-up

The geometry, materials and boundary conditions follow Alma'asfa et al., *Thermal management of cylindrical lithium-ion batteries with different fin configurations and phase change material*, J. Therm. Anal. Calorim. 150 (2025) 12643-12662 (the reference paper). The only change is the PCM thickness, which the paper fixes at 8 mm.

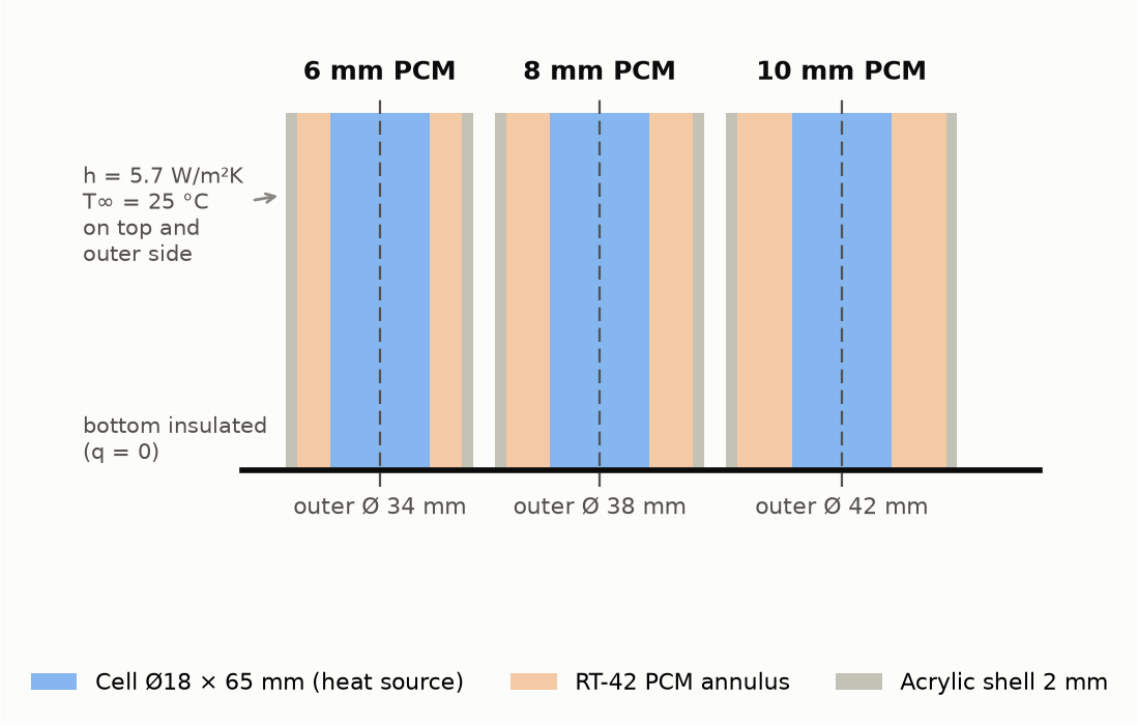


Figure 1. Half-sections of the three designs (axis dashed). Cell radius 9 mm, height 65 mm. The PCM annulus thickness is r_{outer} - r_{inner}; the 2 mm acrylic shell sits outside it. All parts are 65 mm tall.

2.1 Materials

Property	Cell (18650)	RT-42 paraffin	Acrylic shell
Density (kg/m³)	2720	820	1215
Specific heat (J/kg·K)	300	2000	1300
Thermal conductivity (W/m·K)	3.0 (isotropic)	0.2	0.17
Latent heat (J/kg)	-	165,000	-
Solidus / liquidus (°C)	-	38 / 43	-
Viscosity (kg/m·s), expansion (1/K)	-	0.02, 1e-4 (used only for the Ra check)	-

2.2 Geometry and mass of each design

Design	PCM r (mm)	Shell outer r (mm)	PCM mass (g)	Shell mass (g)	Added mass vs cell (%)	Latent capacity (J)
6 mm PCM	9 to 15	17	24.1	15.9	89	3979
8 mm PCM	9 to 17	19	34.8	17.9	117	5747
10 mm PCM	9 to 19	21	46.9	19.8	148	7736

Cell mass 45.0 g. Heat generated over a full 3C discharge is 1866 J, so even the 6 mm layer could absorb all of it as latent heat if it melted completely. It does not, because the PCM conducts heat away from the cell too slowly.

2.3 Loads and boundary conditions

Item	Value	Note
Heat generation, 2C	41,788.37 W/m³ (0.691 W)	I^2R with I = 4.8 A, R = 30 mΩ; run 1800 s
Heat generation, 3C	94,023.84 W/m³ (1.555 W)	I = 7.2 A; run 1200 s
Top surfaces (cell, PCM, shell)	convection, h = 5.7 W/m²K	h swept 5.7, 10, 15, 20
Outer side (shell, or cell if bare)	convection, h = 5.7 W/m²K	as above
Bottom	adiabatic (q = 0)	
Internal interfaces	perfect contact	continuous T and heat flux
Ambient and initial temperature	25 °C	also 30 and 35 °C (initial = ambient)
Radiation	not modelled	same as the paper

3. Numerical method

ANSYS was not available, so the model was written in Python as a 2D axisymmetric (r, z) finite-volume conduction solver. The cell is a cylinder with axisymmetric loads, so a 2D r-z model gives the same answer as a full 3D model at a small fraction of the cost. The PCM uses the enthalpy method, which is the same formulation as Fluent's Solidification & Melting model: the solver advances volumetric enthalpy $H = \rho c_p T + \rho L \beta(T)$, and the liquid fraction β rises linearly from 0 at 38 °C to 1 at 43 °C.

Governing equation (every region): $\partial H/\partial t = (1/r)\partial/\partial r(k\, r\, \partial T/\partial r) + \partial/\partial z(k\, \partial T/\partial z) + q$, with q non-zero only in the cell. Interfaces use harmonic-mean conductances, so heat flux is exactly continuous. Convective faces use the series resistance of the half cell and 1/h. Time stepping is explicit, at 90% of the stability limit rounded down to 1/n s (0.059 s on the base grid).

Why the melt is treated as conduction only. The reference paper solves buoyant flow in the liquid PCM. Here I checked whether that flow matters. Using the full gap width and the 5 K melting range, the Rayleigh number across the gap is about 356 (6 mm), 844 (8 mm) and 1649 (10 mm). Tall, narrow vertical slots stay in the conduction regime up to roughly 10^3. In these runs at most a third of the PCM melts, as a thin film next to the cell, so the real liquid layer (2 to 2.5 mm, Figure 7) is much thinner than the gap, and since Ra scales with thickness cubed its Rayleigh number is below 50. The close match with the paper in section 4, which did include convection, supports this. The assumption would fail for long runs that melt most of the layer.

3.1 Grid and time-step independence

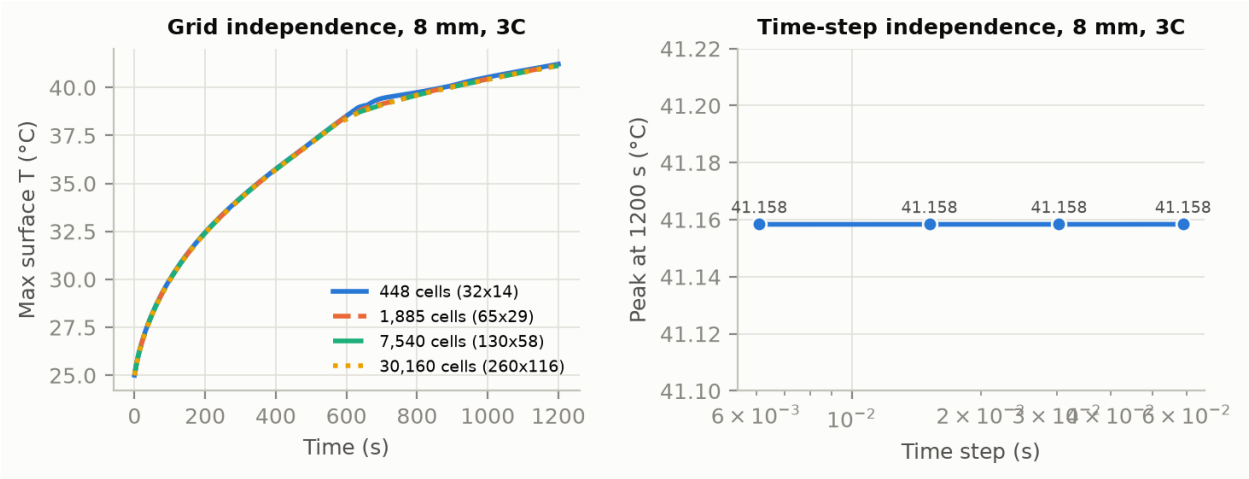


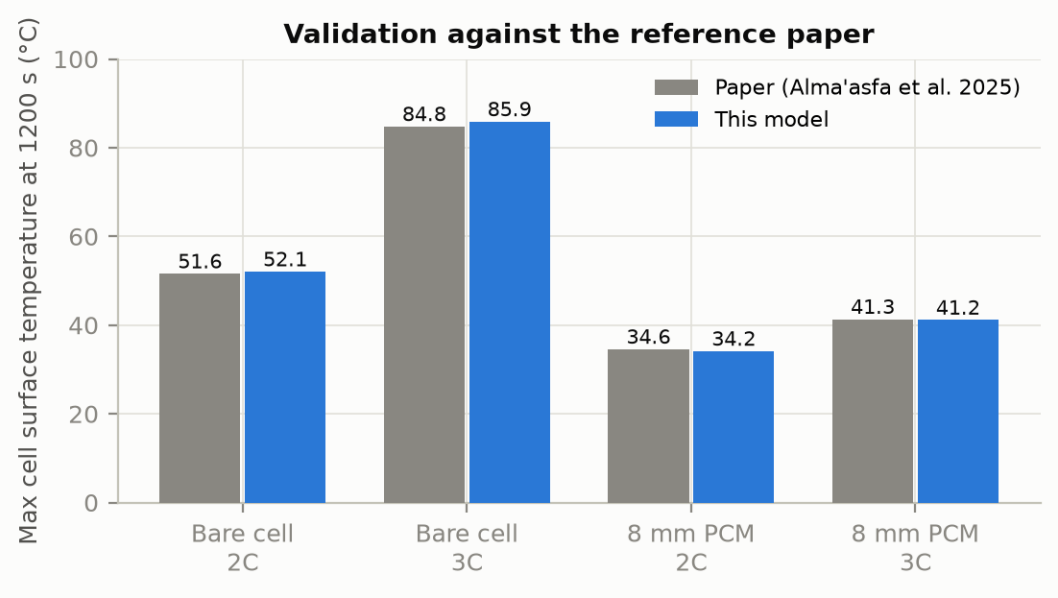
Figure 2. 8 mm design at 3C. Left: surface temperature on four grids (cell sizes scaled ×2, ×1, ×½, ×¼). Right: peak at 1200 s for four time steps on the base grid.

Grid (z × r)	Cells	Time step (s)	Peak at 1200 s (°C)	PCM melted at 1200 s (%)	Melt onset at cell surface (s)
32x14	448	0.2500	41.219	5.15	562
65x29	1,885	0.0588	41.158	5.24	564
130x58	7,540	0.0152	41.142	5.26	564
260x116	30,160	0.0038	41.137	5.26	564

The base grid (1,885 cells: 1 mm in the cell, 0.5 mm in the PCM and shell, 1 mm axially) is within 0.021 K of the finest grid. Halving the time step changes the peak by less than 0.001 K. The energy balance (heat generated = heat stored + heat lost) closes to within 5e-15 of the heat generated in every run. Melt onset is timed when the cell-PCM interface reaches 38 °C. An earlier definition based on the hottest PCM cell moved by 33 s between grids; the interface definition does not move.

4. Validation against the reference paper

The 8 mm design is the paper's "cell with pure PCM" case, and the bare cell is its baseline, so both can be compared directly with the paper's results section.



Case	Paper (°C)	This model (°C)	Difference (K)
Bare cell, 2C	51.6	52.06	+0.46
Bare cell, 3C	84.8	85.89	+1.09
8 mm PCM, 2C	34.6	34.16	-0.44
8 mm PCM, 3C	41.3	41.16	-0.19

All four agree within 1.1 K. The paper reports the PCM-only 3C value only as a 51.24% reduction, which gives 41.35 °C. The paper also gives about 580 s for the start of melting in the pure-PCM case; this model gives 564 s.

One inconsistency in the paper. Its Table 4 compares the PCM-only case with Weng et al.'s experiment at 311.13 K (38.0 °C), while its own results section gives 34.6 °C for what is described as the same case. The model here matches the results section. The experiment Weng et al. ran probably used a different heat input. Worth mentioning if you cite Table 4.

5. Results at h = 5.7 W/m²K, 25 °C

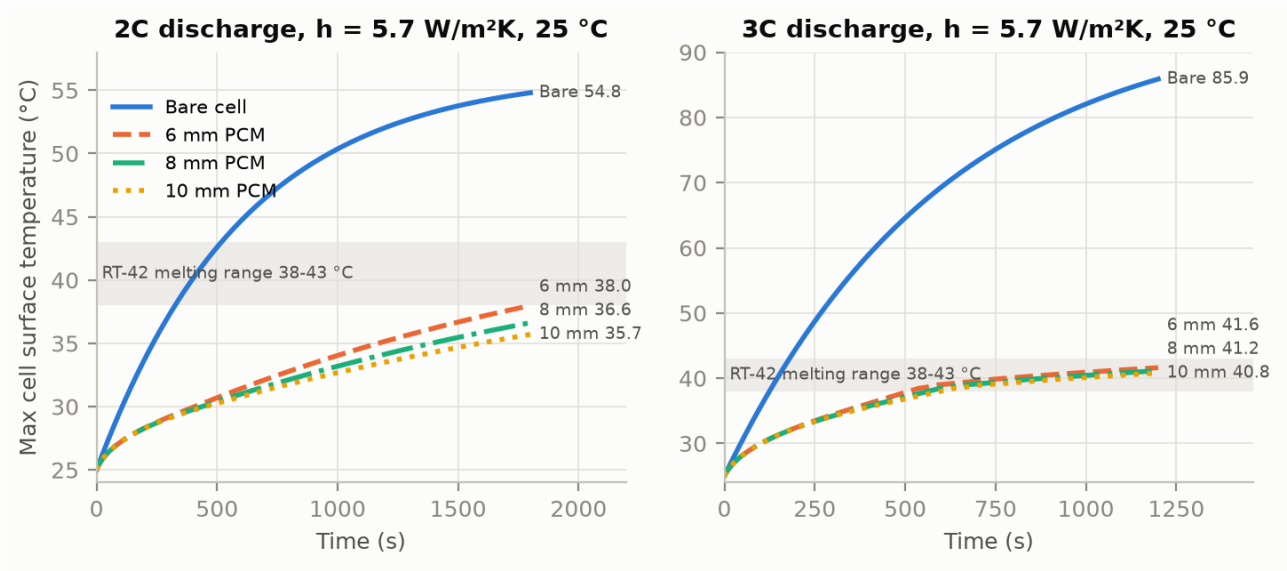


Figure 3. Maximum cell surface temperature. Grey band is the RT-42 melting range.

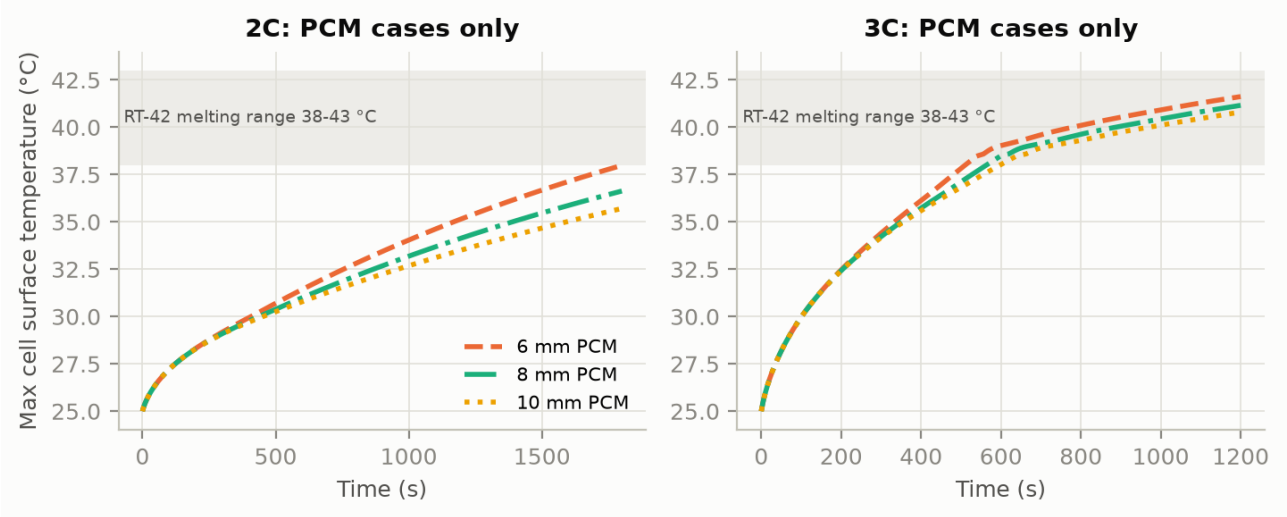


Figure 4. Same data, PCM designs only. At 3C the curves flatten once they enter the melting range; at 2C they never reach it.

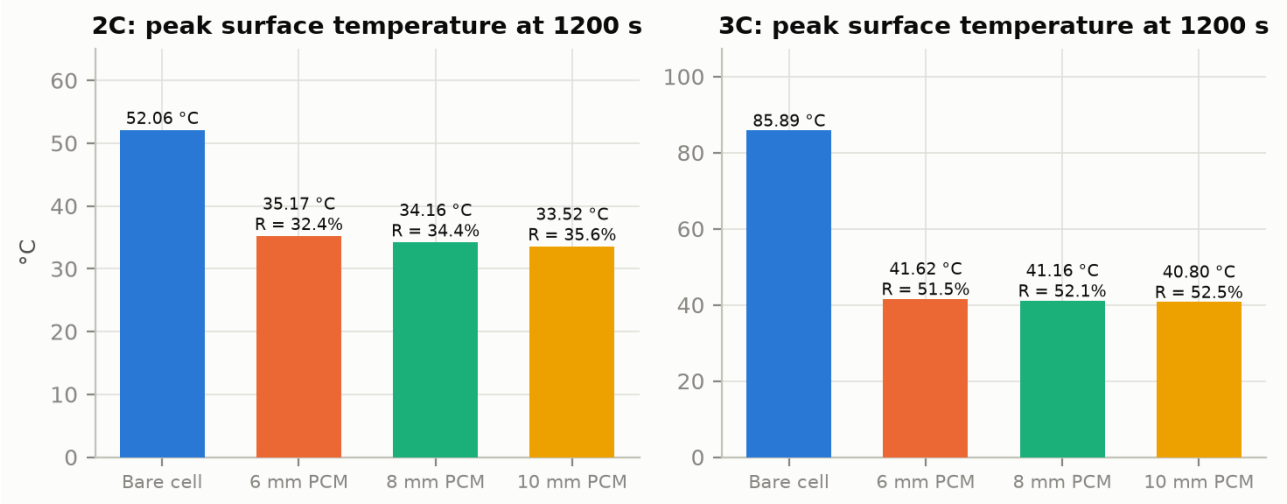


Figure 5. Peak surface temperature at 1200 s. R is the paper's reduction metric, $(T_{bare} - T)/T_{bare}$ with temperatures in °C.

Design	Rate	Peak surface T at 1200 s (°C)	Peak over whole run (°C)	R (%)	Reduction of temperature rise (%)	Cell ΔT inside (K)	Time to 40 °C surface (s)
Bare cell	2C	52.06	54.80	-	-	1.72	396
6 mm PCM	2C	35.17	37.99	32.4	62.4	1.35	never
8 mm PCM	2C	34.16	36.63	34.4	66.2	1.23	never
10 mm PCM	2C	33.52	35.71	35.6	68.5	1.14	never
Bare cell	3C	85.89	85.89	-	-	3.46	147
6 mm PCM	3C	41.62	41.62	51.5	72.7	1.23	779
8 mm PCM	3C	41.16	41.16	52.1	73.5	1.23	887
10 mm PCM	3C	40.80	40.80	52.5	74.0	1.24	972

R depends on the unit chosen: in kelvin the same results would give a far smaller percentage. The reduction of temperature *rise* above the 25 °C start, $(T_{bare} - T)/(T_{bare} - 25)$, does not depend on the unit, and is the better number to quote. "Cell ΔT inside" is the hottest minus the coolest point in the cell at the end of the run, a measure of uniformity. The whole-run peak for 2C is at 1800 s.

5.1 Melting

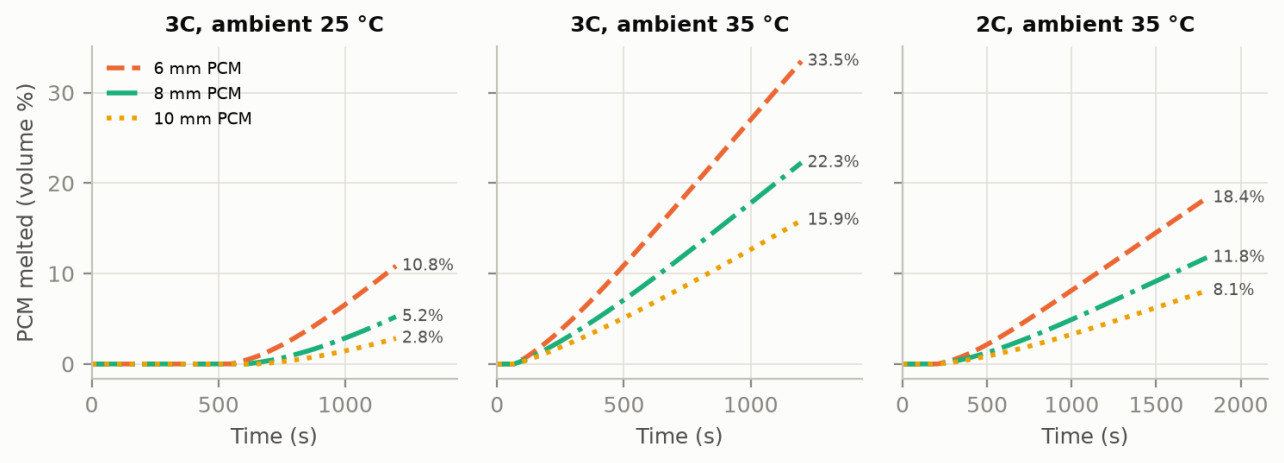


Figure 6. Volume fraction of PCM melted. At 2C and 25 °C nothing melts, so that case is not plotted.

Design	Case	Melt onset (s)	Melted at end (%)	Latent heat absorbed (J)	Time to 10% melted (s)
6 mm PCM	3C, 25 °C	511	10.8	431	1162
6 mm PCM	3C, 35 °C	46	33.5	1332	471
6 mm PCM	2C, 35 °C	168	18.4	731	1147
6 mm PCM	2C, 25 °C	no melting	0.0	0	-
8 mm PCM	3C, 25 °C	564	5.2	301	-
8 mm PCM	3C, 35 °C	46	22.3	1279	642
8 mm PCM	2C, 35 °C	169	11.8	677	1596
8 mm PCM	2C, 25 °C	no melting	0.0	0	-
10 mm PCM	3C, 25 °C	598	2.8	219	-
10 mm PCM	3C, 35 °C	46	15.9	1229	832
10 mm PCM	2C, 35 °C	169	8.1	627	-
10 mm PCM	2C, 25 °C	no melting	0.0	0	-

Thinner layers melt sooner and further because the same heat goes into less material, and the hot film next to the cell is the same thickness in all three. The layer beyond the first few millimetres stays solid and only adds sensible heat capacity.

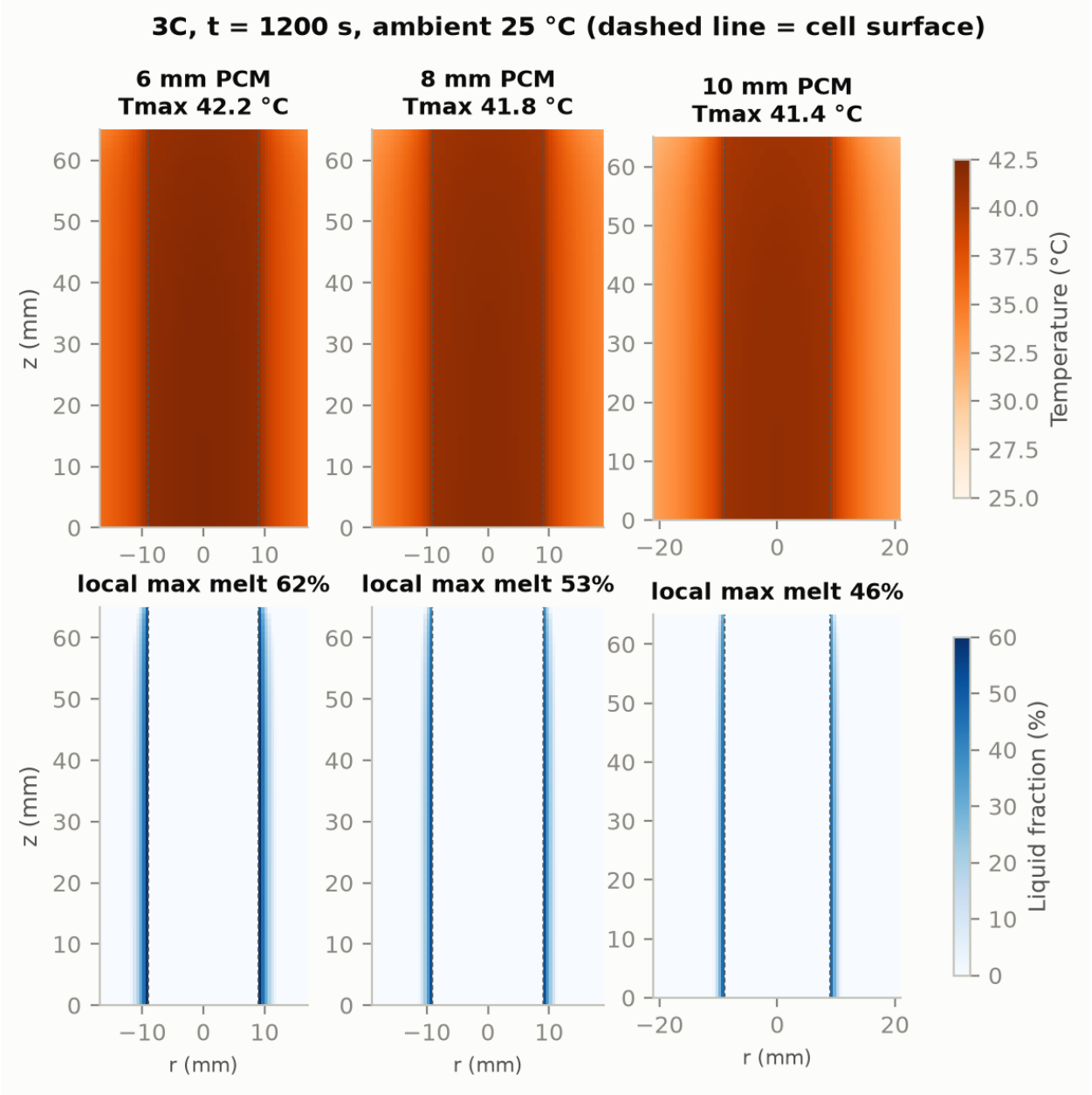


Figure 7. Temperature (top) and liquid fraction (bottom) at the end of a 3C discharge. The hottest point is at the bottom of the cell on its axis, next to the insulated base. Melting happens in a film 2 to 2.5 mm thick along the full height of the cell; the rest of the layer stays solid.

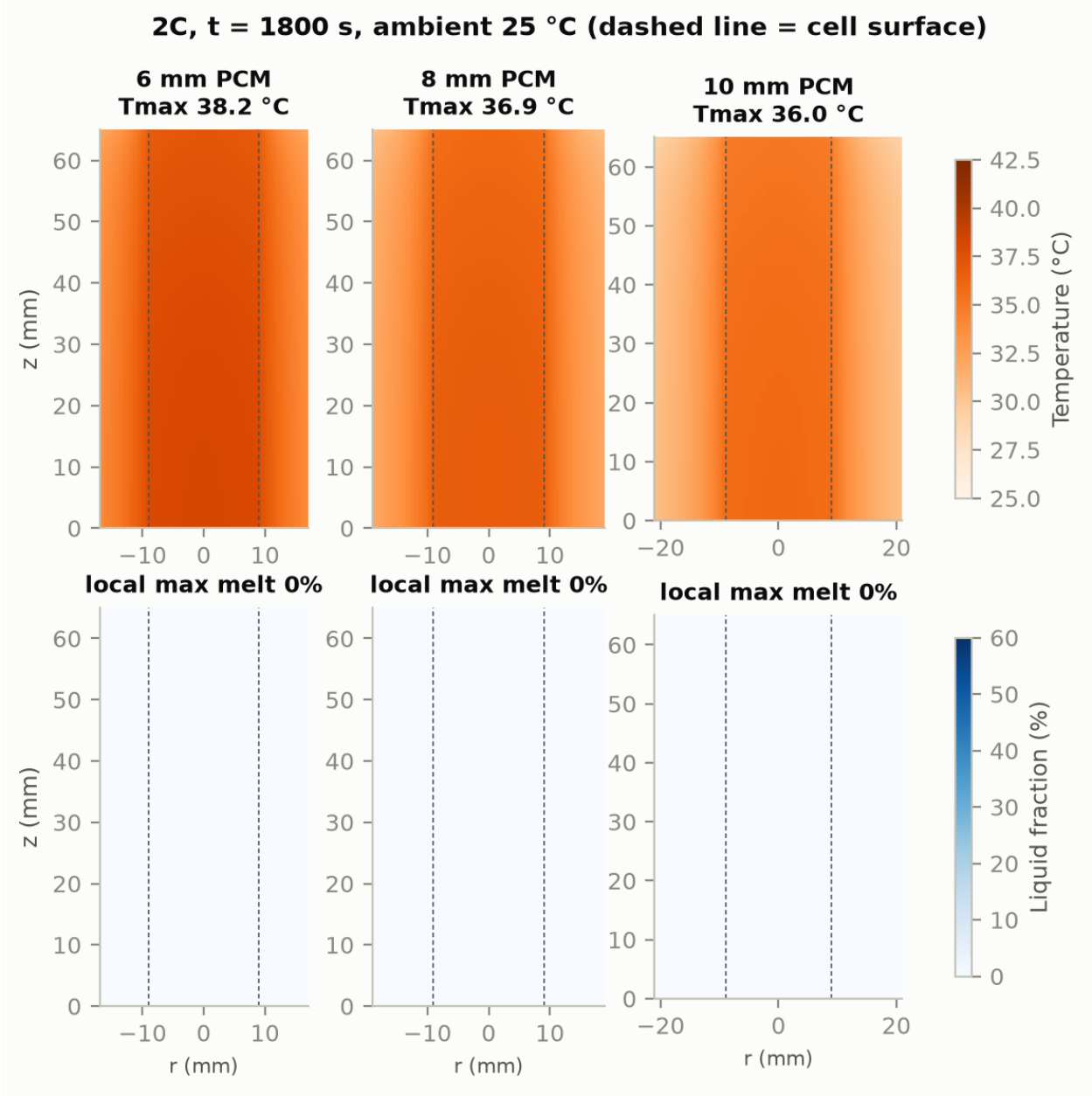


Figure 8. End of a 2C discharge (1800 s). The PCM next to the cell stays below 38 °C, so nothing melts.

5.2 Where the heat goes

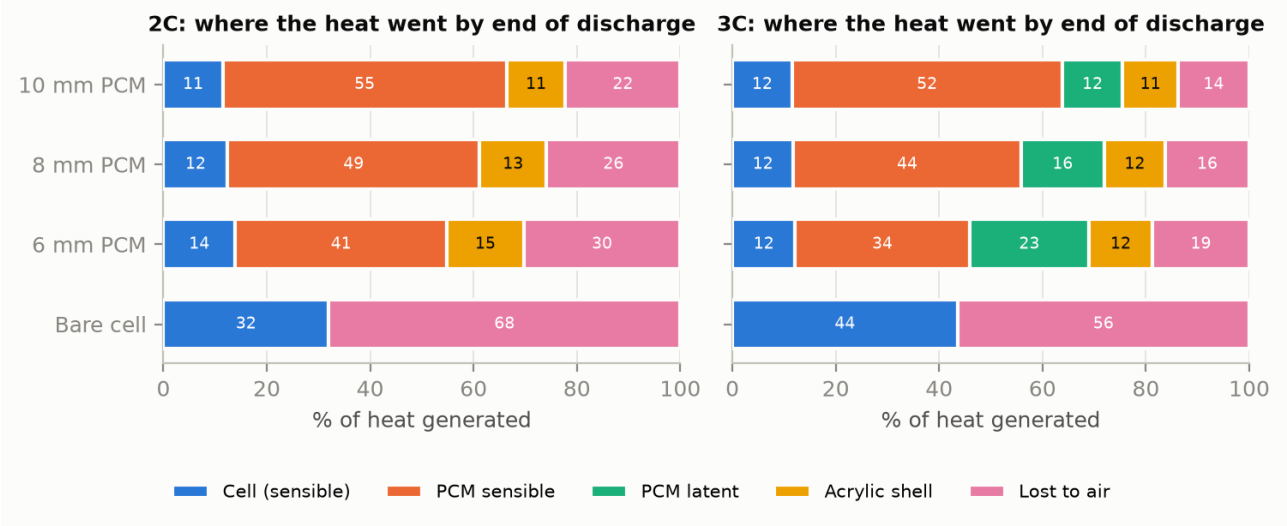


Figure 9. Energy balance at the end of discharge, as a share of the heat generated. Segments under 7% are unlabelled.

Design	Rate	Cell (%)	PCM sensible (%)	PCM latent (%)	Shell (%)	Lost to air (%)
Bare cell	2C	32.0	0.0	0.0	0.0	68.0
6 mm PCM	2C	13.9	41.0	0.0	14.8	30.3
8 mm PCM	2C	12.4	48.7	0.0	13.0	25.9
10 mm PCM	2C	11.5	54.9	0.0	11.4	22.2
Bare cell	3C	43.5	0.0	0.0	0.0	56.5
6 mm PCM	3C	12.1	33.7	23.1	12.3	18.8
8 mm PCM	3C	11.8	44.0	16.1	11.8	16.3
10 mm PCM	3C	11.5	52.2	11.8	10.7	13.8

Thicker PCM stores more heat and loses less to the air during discharge, mainly through extra sensible heat. Latent storage falls as the layer gets thicker, because less of it melts.

6. Sensitivity to cooling and ambient temperature

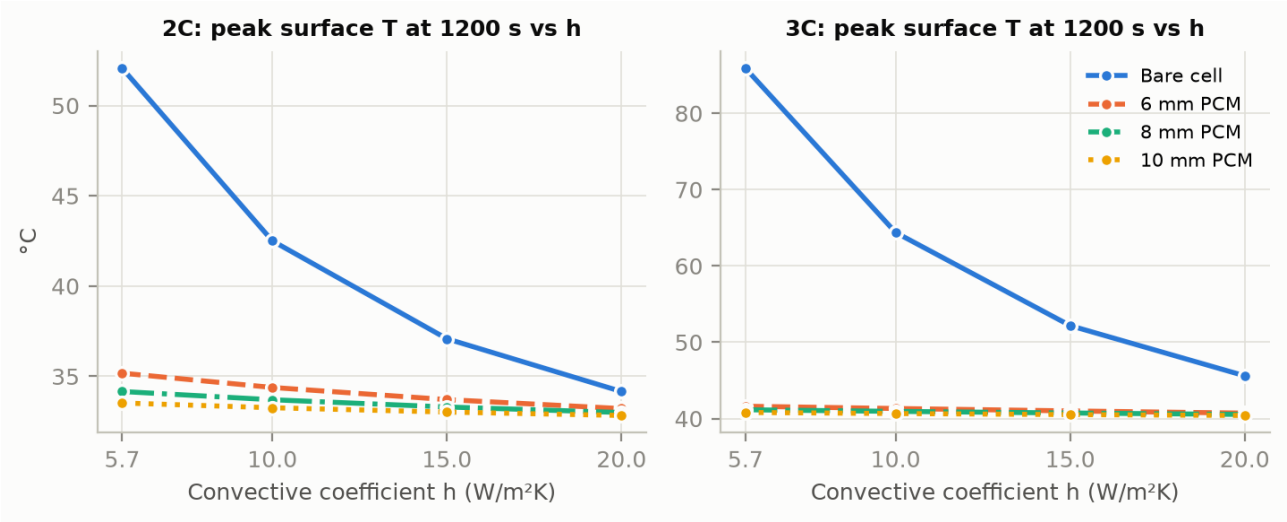


Figure 10. Peak surface temperature at 1200 s against the convective coefficient.

Design	Rate	h = 5.7	h = 10	h = 15	h = 20
Bare cell	2C	52.06	42.50	37.08	34.16
6 mm PCM	2C	35.17	34.38	33.71	33.21
8 mm PCM	2C	34.16	33.70	33.30	33.00
10 mm PCM	2C	33.52	33.26	33.02	32.83
Bare cell	3C	85.89	64.39	52.18	45.60
6 mm PCM	3C	41.62	41.32	41.01	40.72
8 mm PCM	3C	41.16	40.95	40.73	40.54
10 mm PCM	3C	40.80	40.66	40.52	40.41

Peak surface temperature at 1200 s (°C). The PCM's advantage shrinks quickly as cooling improves. At h = 20 W/m²K a bare cell at 2C peaks at 34.16 °C, about the same as the PCM designs at h = 5.7. The thickness matters even less at high h.

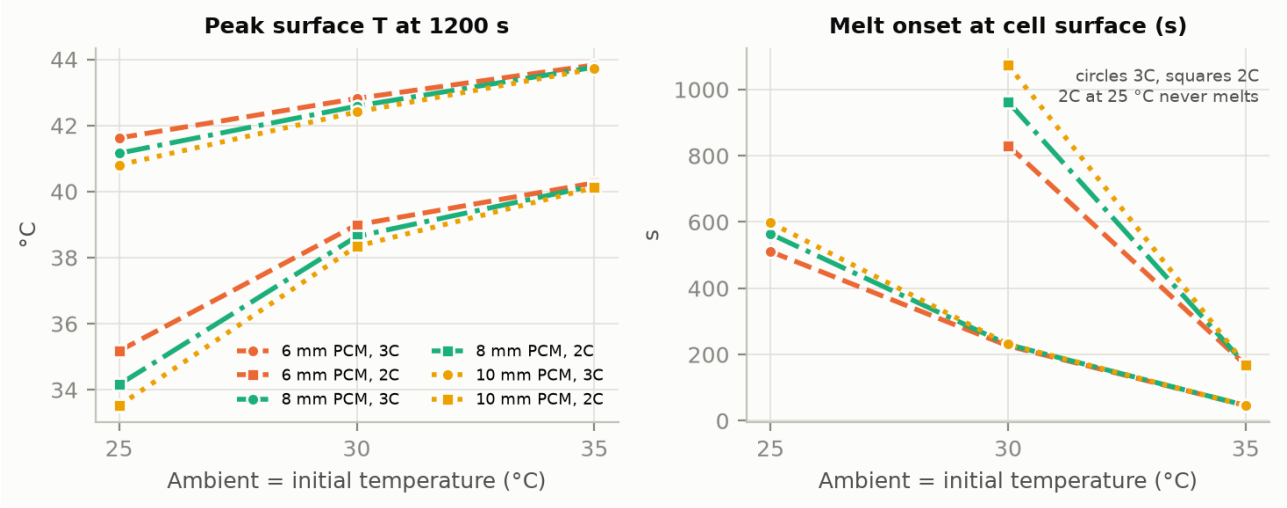


Figure 11. Ambient (and starting) temperature raised to 30 and 35 °C.

Design	Rate	25 °C	30 °C	35 °C
Bare cell	2C	52.06	57.06	62.06
6 mm PCM	2C	35.17	38.99	40.26
8 mm PCM	2C	34.16	38.64	40.18
10 mm PCM	2C	33.52	38.34	40.12
Bare cell	3C	85.89	90.89	95.89
6 mm PCM	3C	41.62	42.82	43.83

Design	Rate	25 °C	30 °C	35 °C
8 mm PCM	3C	41.16	42.58	43.76
10 mm PCM	3C	40.80	42.41	43.71

Peak surface temperature at 1200 s (°C). In a hot environment the PCM is already close to its melting point at the start. The cell temperature is then pinned near the 38-43 °C melting range, and all three thicknesses end within about 0.15 K of each other at 3C. This is the condition RT-42 is suited to. In the paper's results the initial temperature stays at 25 °C while the ambient changes. Here the initial temperature equals the ambient, because the paper's 35 °C case melts within 200 s, which only fits a warm start.

7. Insulation or heat spreader? Steady state and critical radius

For a cylinder, a layer of conductivity k increases heat loss as long as its outer radius is below r_c = k/h. For RT-42 at h = 5.7 W/m²K, r_c = 35.1 mm (acrylic: 29.8 mm). All three designs end at 17 to 21 mm, so wrapping the cell lowers its long-run temperature: the added surface area (side and top) outweighs the added conduction resistance. The steady-state run below shows the temperature the cell would settle at if it kept discharging forever, by which point the PCM is fully molten and only conduction and convection remain.

Design	Steady surface T, 2C (°C)	Steady surface T, 3C (°C)	Steady cell core, 3C (°C)
Bare cell	56.4	95.7	96.3
6 mm PCM	46.3	72.9	73.5
8 mm PCM	45.3	70.7	71.3
10 mm PCM	44.6	69.1	69.7

So the layer is not an insulator at this size. It helps in two ways: it adds thermal mass during a discharge (sensible and, above 38 °C, latent), and it adds cooled surface area. Steady-state values with molten PCM ignore convection in the melt, so they are upper bounds.

8. Simulation factors that matter, and how much

Factor	Value used	Effect seen in this study
Discharge rate (heat load)	2C, 3C	Decides whether the PCM melts at all. At 25 °C only 3C reaches 38 °C.
PCM thickness	6, 8, 10 mm	Under 1 K between 6 and 10 mm at 3C, 1.7 K at 2C; mass almost doubles.
Melting range of the PCM	38-43 °C	Must sit just above normal operating temperature. Sets the plateau in Fig. 4.
Latent heat	165 kJ/kg	23% or less of the heat goes into latent storage at 25 °C (up to 71% at 35 °C); capacity is not the limit.
PCM conductivity	0.2 W/m·K	The real limit: heat cannot reach the outer PCM, so it stays solid.
Convective coefficient h	5.7 to 20 W/m²K	Strongest external factor; PCM benefit falls from 52% to 11% (R, 3C).
Ambient / initial temperature	25, 30, 35 °C	Warm start makes the PCM melt early and pins the cell near 43 °C.
Cell properties (ρ, c_p, k)	2720, 300, 3.0	A cp of 300 is low; values reported for 18650 cells are about 900 to 1100. See section 9.
Shell	2 mm acrylic	Stores 11-15% of the heat; adds outer area.
Bottom boundary	adiabatic	Puts the hot spot at the bottom of the cell.
Mushy zone model	linear β from 38 to 43 °C	Same as Fluent; A_{mush} only matters with flow.
Grid	1885 cells (r-z)	Converged to 0.02 K (section 3.1).
Time step	0.059 s explicit	Converged; Fluent implicit with 0.5 s is fine too (paper).
Melt convection	neglected	Ra across the gap is at most 1649, so conduction dominates.

9. Assumptions and limits

1. **Cell heat capacity.** The paper's c_p of 300 J/kg·K is about a third of measured values for 18650 cells. I kept it so the results stay comparable with the paper. A realistic value would slow every temperature rise, push melt onset later, and make the PCM matter even less at 2C.

2. **Uniform, constant heat generation** (I^2R with fixed 30 mΩ). Real heat generation rises toward the end of discharge and includes entropic heat.

3. **Isotropic cell conductivity.** A jelly-roll is far more conductive along its axis than across it. Cell ΔT values here are probably underestimated.

4. **No radiation, no contact resistance**, PCM top surface open to air, constant density (no expansion on melting). All of these follow the paper.

5. **Conduction only in the melt**, justified in section 3 for these melt fractions.

6. **Single cell.** In a pack, neighbouring cells share PCM and the outer surface sees much less air.

10. Reproducing this in ANSYS Fluent

If you need Fluent output for the submission, these settings reproduce the same model. The 2D axisymmetric option keeps the mesh small enough for the Ansys Student licence.

Setting	Value
Geometry	2D axisymmetric (axis along x), or 3D as in the paper; separate bodies for cell, PCM, shell, shared topology
Mesh	Quad/hex, 0.5 mm in PCM and shell, 1 mm in cell; skewness < 0.2
General	Pressure-based, transient, gravity -9.81 m/s^2 along the cell axis
Models	Energy on; Solidification & Melting on, mushy zone constant 1e5; Viscous laminar
PCM material	Fluid; density Boussinesq 820 with expansion 1e-4; cp 2000; k 0.2; viscosity 0.02; pure solvent melting heat 165000; solidus 311.15 K; liquidus 316.15 K
Cell zone	Solid, ρ 2720, cp 300, k 3; source term energy 41788.37 (2C) or 94023.84 (3C) W/m^3
Shell zone	Solid, ρ 1215, cp 1300, k 0.17
Boundaries	Top walls and outer shell wall: Convection, h 5.7, free-stream 298.15 K. Bottom: heat flux 0. Interfaces: coupled walls
Methods	SIMPLEC, PRESTO!, second-order upwind energy and momentum
Under-relaxation	pressure 0.3, momentum 0.7, density 1, energy 1, liquid fraction 0.9
Initialization	298.15 K everywhere (or ambient for the 30 and 35 °C cases)
Time stepping	Δt 0.5 s, 20 iterations per step, 2400 steps (3C) or 3600 steps (2C)
Report definitions	Facet maximum of temperature on the cell-PCM wall; volume-average liquid fraction of the PCM zone; area-weighted heat flux on convective walls

Expect Fluent to land within about 1 K of the values in this report, as the comparison with the paper in section 4 suggests.

Appendix. Every run

Run	Peak 1200 s (°C)	Peak run (°C)	Melted end (%)	Onset (s)	Lost to air (%)	R 1200 (%)
Bare cell, 2C, h 5.7, 25 °C	52.06	54.80	0.0	-	68.0	-
Bare cell, 2C, h 10, 25 °C	42.50	42.98	0.0	-	80.8	-
Bare cell, 2C, h 15, 25 °C	37.08	37.15	0.0	-	87.1	-
Bare cell, 2C, h 20, 25 °C	34.16	34.17	0.0	-	90.3	-
Bare cell, 2C, h 5.7, 30 °C	57.06	59.80	0.0	-	68.0	-
Bare cell, 2C, h 5.7, 35 °C	62.06	64.80	0.0	-	68.0	-
6 mm PCM, 2C, h 5.7, 25 °C	35.17	37.99	0.0	-	30.3	32.4
6 mm PCM, 2C, h 10, 25 °C	34.38	36.33	0.0	-	42.9	19.1
6 mm PCM, 2C, h 15, 25 °C	33.71	35.05	0.0	-	52.3	9.1
6 mm PCM, 2C, h 20, 25 °C	33.21	34.19	0.0	-	58.5	2.8
6 mm PCM, 2C, h 5.7, 30 °C	38.99	39.84	5.9	831	27.7	31.7
6 mm PCM, 2C, h 5.7, 35 °C	40.26	40.81	18.4	168	14.7	35.1
8 mm PCM, 2C, h 5.7, 25 °C	34.16	36.63	0.0	-	25.9	34.4
8 mm PCM, 2C, h 10, 25 °C	33.70	35.57	0.0	-	37.2	20.7
8 mm PCM, 2C, h 15, 25 °C	33.30	34.71	0.0	-	45.9	10.2
8 mm PCM, 2C, h 20, 25 °C	33.00	34.12	0.0	-	51.8	3.4
8 mm PCM, 2C, h 5.7, 30 °C	38.64	39.55	2.6	963	24.9	32.3
8 mm PCM, 2C, h 5.7, 35 °C	40.18	40.74	11.8	169	14.3	35.3
10 mm PCM, 2C, h 5.7, 25 °C	33.52	35.71	0.0	-	22.2	35.6
10 mm PCM, 2C, h 10, 25 °C	33.26	35.02	0.0	-	32.3	21.8
10 mm PCM, 2C, h 15, 25 °C	33.02	34.45	0.0	-	40.2	10.9
10 mm PCM, 2C, h 20, 25 °C	32.83	34.03	0.0	-	45.8	3.9
10 mm PCM, 2C, h 5.7, 30 °C	38.34	39.29	1.2	1074	21.9	32.8
10 mm PCM, 2C, h 5.7, 35 °C	40.12	40.67	8.1	169	13.4	35.4
Bare cell, 3C, h 5.7, 25 °C	85.89	85.89	0.0	-	56.5	-
Bare cell, 3C, h 10, 25 °C	64.39	64.39	0.0	-	72.0	-
Bare cell, 3C, h 15, 25 °C	52.18	52.18	0.0	-	80.7	-
Bare cell, 3C, h 20, 25 °C	45.60	45.60	0.0	-	85.4	-
Bare cell, 3C, h 5.7, 30 °C	90.89	90.89	0.0	-	56.5	-
Bare cell, 3C, h 5.7, 35 °C	95.89	95.89	0.0	-	56.5	-
6 mm PCM, 3C, h 5.7, 25 °C	41.62	41.62	10.8	511	18.8	51.5
6 mm PCM, 3C, h 10, 25 °C	41.32	41.32	7.9	524	28.6	35.8
6 mm PCM, 3C, h 15, 25 °C	41.01	41.01	5.6	540	37.1	21.4
6 mm PCM, 3C, h 20, 25 °C	40.72	40.72	4.0	556	43.5	10.7
6 mm PCM, 3C, h 5.7, 30 °C	42.82	42.82	21.1	226	14.2	52.9
6 mm PCM, 3C, h 5.7, 35 °C	43.83	43.83	33.5	46	6.8	54.3
8 mm PCM, 3C, h 5.7, 25 °C	41.16	41.16	5.2	564	16.3	52.1
8 mm PCM, 3C, h 10, 25 °C	40.95	40.95	4.0	573	24.7	36.4
8 mm PCM, 3C, h 15, 25 °C	40.73	40.73	3.1	584	32.0	21.9
8 mm PCM, 3C, h 20, 25 °C	40.54	40.54	2.4	593	37.4	11.1
8 mm PCM, 3C, h 5.7, 30 °C	42.58	42.58	12.6	230	12.9	53.2
8 mm PCM, 3C, h 5.7, 35 °C	43.76	43.76	22.3	46	6.4	54.4
10 mm PCM, 3C, h 5.7, 25 °C	40.80	40.80	2.8	598	13.8	52.5
10 mm PCM, 3C, h 10, 25 °C	40.66	40.66	2.3	604	21.0	36.8
10 mm PCM, 3C, h 15, 25 °C	40.52	40.52	1.9	610	27.3	22.3
10 mm PCM, 3C, h 20, 25 °C	40.41	40.41	1.5	616	32.0	11.4

Run	Peak 1200 s (°C)	Peak run (°C)	Melted end (%)	Onset (s)	Lost to air (%)	R 1200 (%)
10 mm PCM, 3C, h 5.7, 30 °C	42.41	42.41	8.3	231	11.3	53.3
10 mm PCM, 3C, h 5.7, 35 °C	43.71	43.71	15.9	46	5.9	54.4

Source files: sim.py (solver), run_all.py (cases), plots.py (figures), report.py (this document). Raw results are in results/summary.json.