THERMAL ANALYSIS PROJECTIONS FOR SCALE UP FROM 18650 TO 21700

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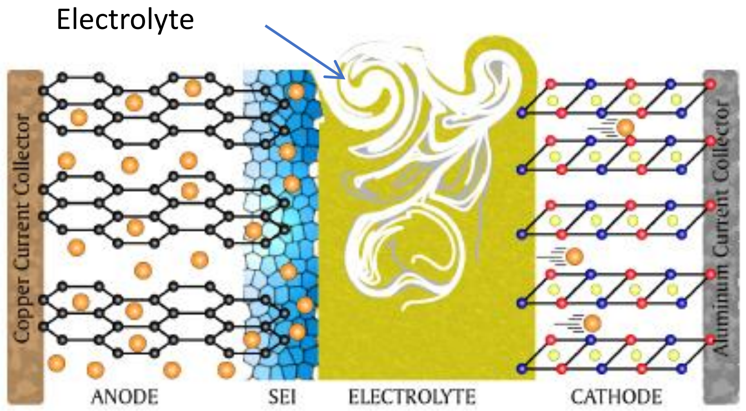
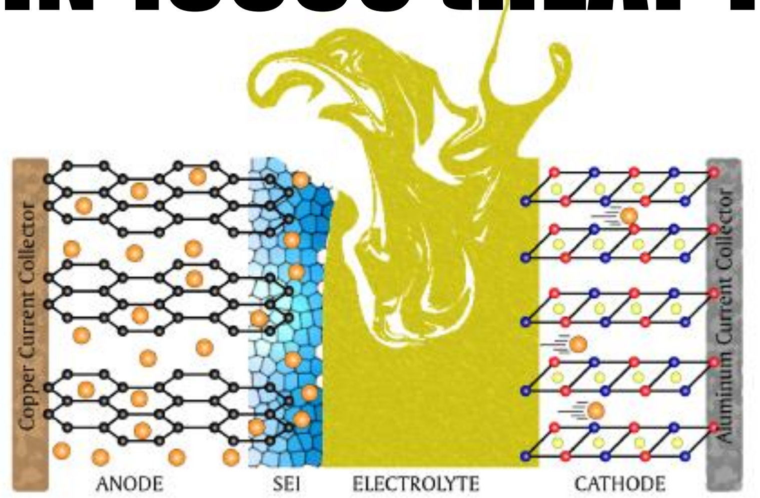
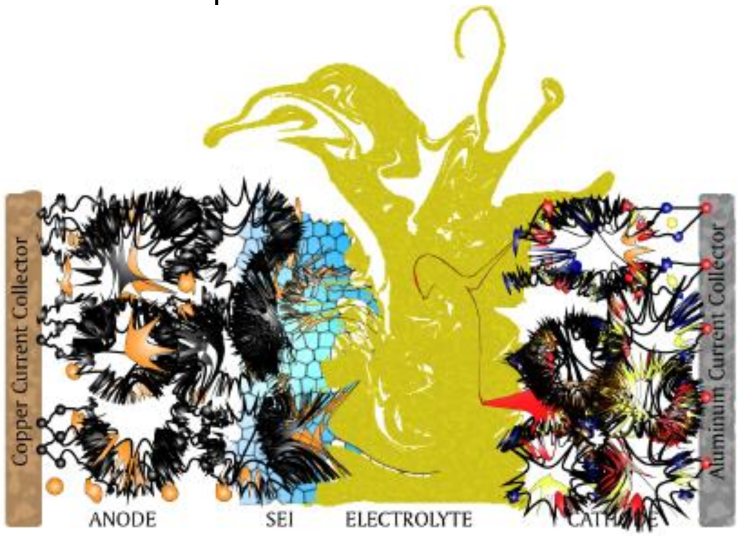
THERMAL RUNAWAY IN 18650 (HEAT TRIGGER)



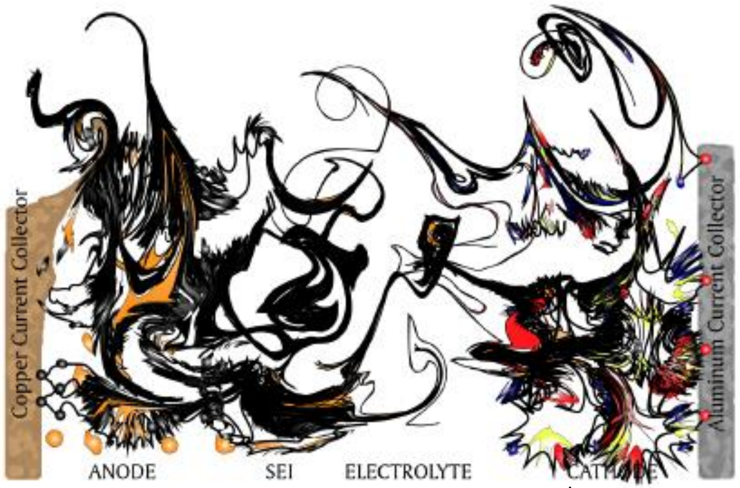
a) The pressure inside increases



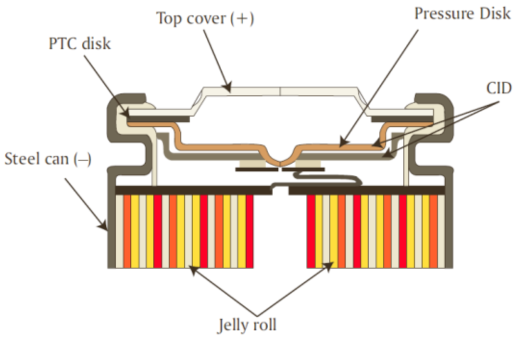
b) The CID membrane opens (1st venting)

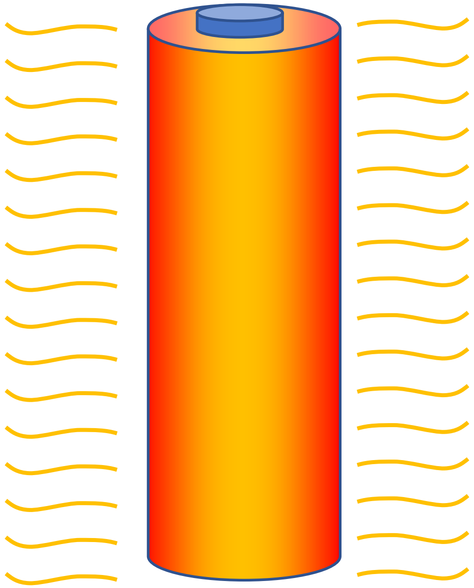


c) The Decomposition are activated



d) Parts of the solids are ejected out (2nd venting)





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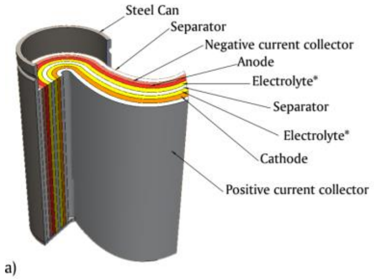
TRANSITION FROM FUNDAMENTALS TO REAL-LIFE



$$V_{cell}\rho_{jr}(y)Cp_{jr}\frac{dT}{dt} = \sum \dot{Q}_{net}$$

$$\dot{Q}_{vap} = -m_e h_{vap}\frac{dy}{dt} - V_h\frac{dP}{dt}$$

$$\dot{Q}_c = m_c h_c \frac{d\alpha}{dt}$$

$$\rho_{jr}(y) = \rho_{jr} - \frac{(m_e+m_{ej})y}{V_{cell}}$$

$$\dot{Q}_{vent} = -m_e h_{vap}\frac{dy}{dt} - m_e Cp_e T\frac{dy}{dt}$$

$$\dot{Q}_{sei} = m_a h_{sei}\frac{dx_{sei}}{dt}$$

$$\frac{dy}{dt} = \frac{P_{vent}v_{vent}A_{vent}M_e}{RT_{vent}m_e}$$

$$\frac{dx_a}{dt} = -A_a x_a \exp\left(-\frac{z}{z_0} - \frac{E_a}{k_b T}\right)$$

$$\frac{d\alpha}{dt} = A_c\,\alpha(1-\alpha)\exp\left(-\frac{E_c}{k_b T}\right)$$

$$\frac{dx_s}{dt} = -A_s x_s \exp\left(-\frac{E_s}{k_b T}\right)$$

$$\frac{dz}{dt} = A_a x_a \exp\left(-\frac{z}{z_0} - \frac{E_a}{k_b T}\right)$$

$$\frac{dSoC}{dt} = -A_{ec}(1-\alpha)x_a \exp\left(-\frac{E_{ec}}{k_b T}\right) + \left(\frac{d\alpha}{dt} - \frac{dx_a}{dt}\right)SoC$$

$$\dot{Q}_{ejecta} = -m_{ej}C_{p_{jr}}T\frac{dy}{dt}$$

$$\dot{Q}_{ec} = -(m_c + m_a)h_{ec}\frac{dSoC}{dt}$$

$$\frac{d\theta}{dt} = -A_e\theta_e \exp\left(-\frac{E_e}{k_b T}\right)$$

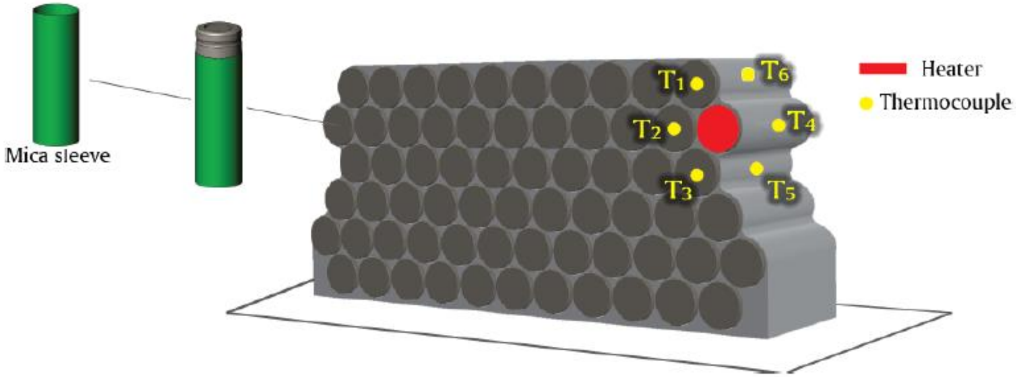
$$\dot{Q}_a = -m_a h_a \frac{dx_a}{dt}$$

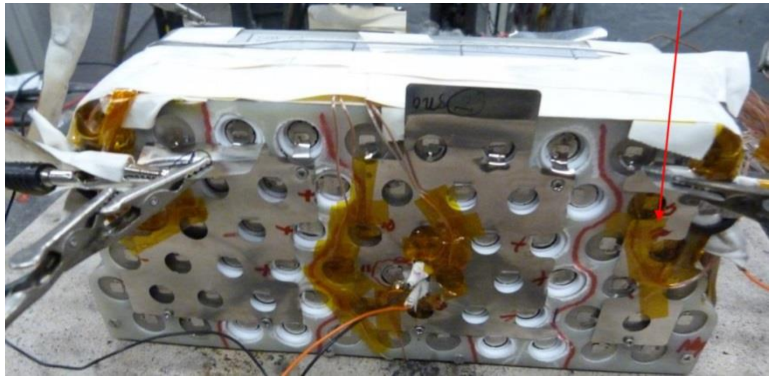
$$\dot{Q}_{conv} = -h_{conv}A_{surf}(T - T_{amb})$$

$$P = \frac{m_e RT(1-\theta_e-y)}{V_h M_e} + P_0$$

$$\dot{Q}_{rad} = -\epsilon\sigma A_{surf}(T^4 - T_{amb}^4)$$

$$\dot{Q}_{in} = 1.05\ [W]$$





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SIMPLIFICATION OF PACK TR

- Energy Balance (using effective properties):

$$m_{cell}Cp_{eff}\frac{dT}{dt} = \dot{Q}_a + \dot{Q}_c + \dot{Q}_{sei} + \dot{Q}_{ec,ISC} + \dot{Q}_{conv} + \dot{Q}_{rad} + \dot{Q}_{heater}$$

- Heat Sources and fluxes:
  - Decomposition of anode:

    $$\dot{Q}_a = m_a h_a \frac{dx_a}{dt}$$
  - Decomposition of cathode:

    $$\dot{Q}_c = m_c h_c \frac{d\alpha}{dt}$$
  - Decomposition of SEI:

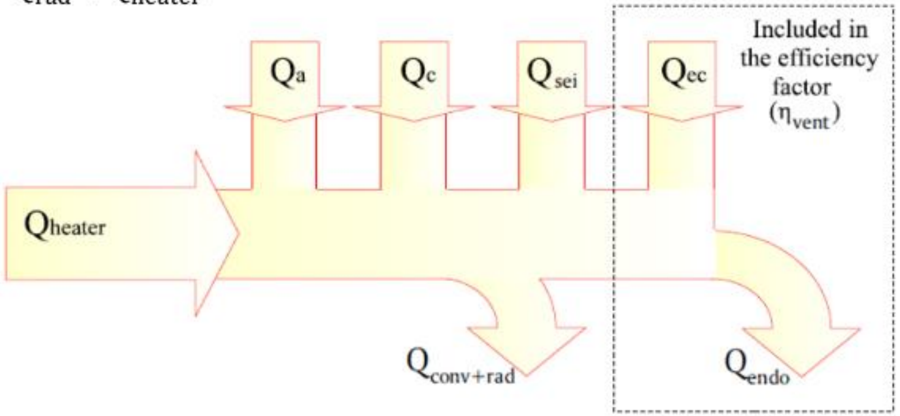
    $$\dot{Q}_{sei} = m_a h_{sei} \frac{dx_{sei}}{dt}$$
  - Electrochemical reactions:

    $$\dot{Q}_{ec} = \eta H_{ec} \frac{dSoC}{dt}$$
  - Heat rate due to radiation:

    $$\dot{Q}_{rad} = -\epsilon\sigma A_{surf}(T^4 - T_{amb}^4)$$
  - Heat rate due to convection:

    $$\dot{Q}_{conv} = -h_{conv}A_{surf}(T - T_{amb})$$

$\eta = 0.28$



– State of Charge Equation

$$\frac{dSoC}{dt} = ISC_{cond}SoC \cdot A_{ISC}\exp\left(-\frac{E_{isc}}{k_bT}\right)$$

Simplified SoC

– Triggering condition:

$$ISC_{cond} = \begin{cases} 0 \text{ if } T \leq 57°C \\ 1 \text{ if } T > 57°C \end{cases}$$

P.T.Coman, E.C.Darcy, C.T.Veje and R.E.White,"Modelling Li-ion cell thermal runaway triggered by an internal short circuit by using an efficiency factor and Arrhenius formulations," J.Electrochem.Soc.,vol.164,no.4,pp.A1–A7,2017

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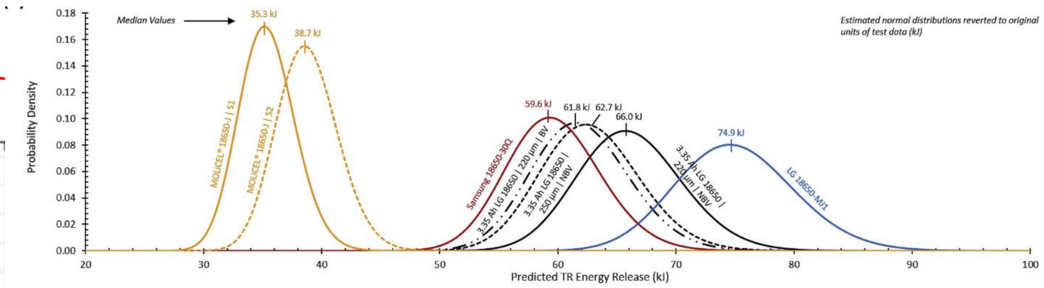
SIMPLIFICATION



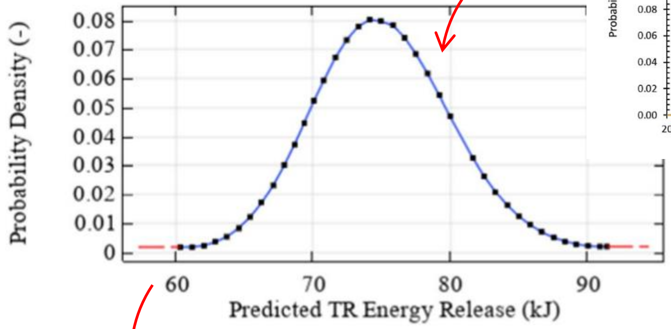


Figure 2. Predicted TR Energy for an LG 18650 MJ1 cell.[26]

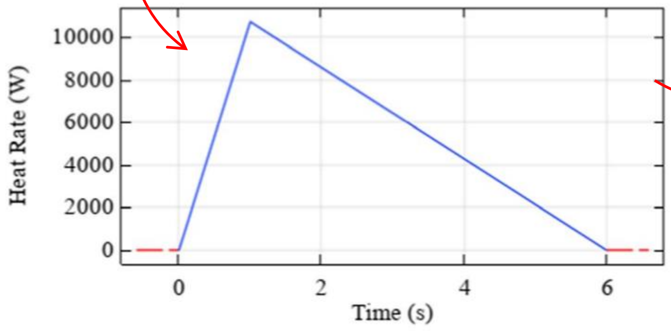
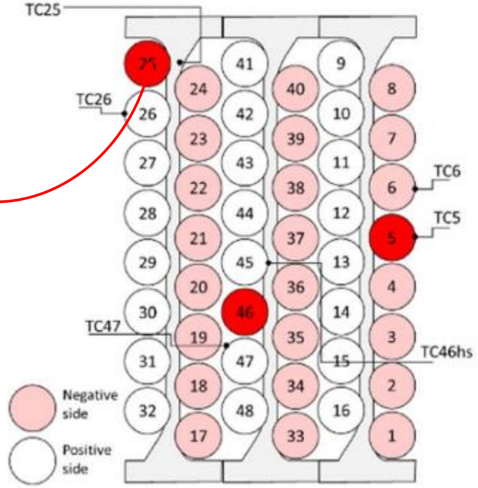
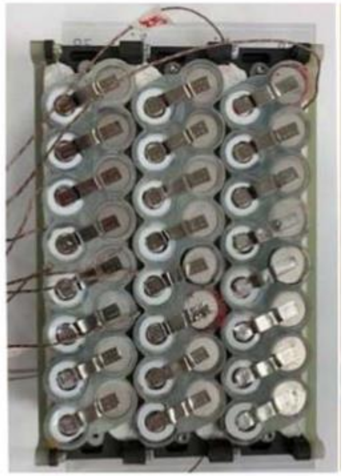
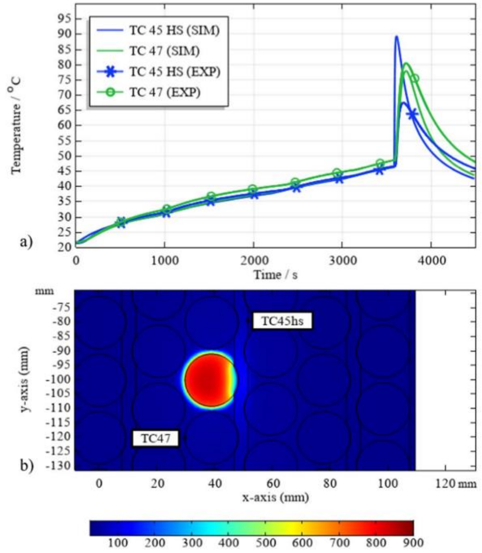
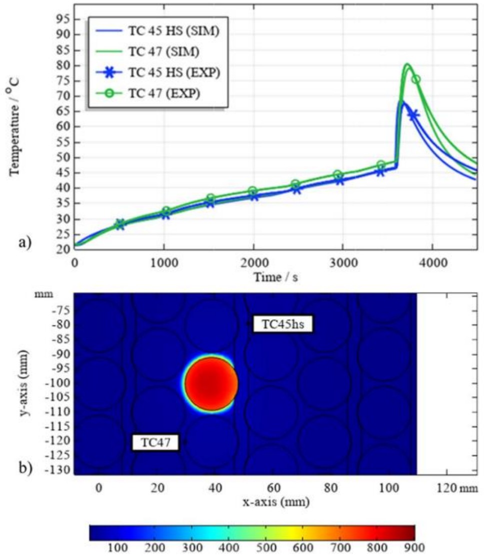


Figure 3. Approximated heat generation rate for MJ1 cells. Integrated over time, the heat rate yields a total energy of 32.2 kJ.









Paul T. Coman, Eric C. Darcy and Ralph E. White, Simplified Thermal Runaway Model for Assisting the Design of a Novel Safe Li-Ion Battery Pack, 2022 *J. Electrochem. Soc.* **169** 040516

William Q. Walker, John J. Darst, Donal P. Finegan, Gary A. Bayles, Kenneth L. Johnson, Eric C. Darcy, Steven L. Rickman, Decoupling of heat generated from ejected and non-ejected contents of18650-format lithium-ion cells using statistical methods, Journal of Power Sources, 415 (2019) 207-218

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SAMPLE FOR LG18650-MJ1

LG 18650-MJ1

Item	Unit	Orion-Run4	Orion-Run5	Orion-Run7	Orion-Run8	Orion-Run10	Orion-Run11	Orion-Run13	DLS-Run55	DLS-Run56	DLS-Run59	DLS-Run60	DLS-Run62	Orion-Run1	Orion-Run2	Orion-Run12	NBR Avg.	NBR St. Dev.	BR Avg.	BR St. Dev.	GLOBAL Avg.	GLOBAL St. Dev.
Total Energy	kJ	78.3	76.9	82.4	79.7	77.7	73.7	82.9	75.2	66.6	70.2	59.4	77.3	81.8	67.6	78.0	75.0	6.8	75.8	7.4	75.2	6.6
Electrochemical Ratio	$kJ\ kJ^{-1}$	1.73	1.70	1.82	1.76	1.71	1.63	1.83	1.66	1.47	1.55	1.31	1.71	1.81	1.49	1.72	1.66	0.15	1.67	0.16	1.66	0.15
Distribution $E_{Cell\ Body}$	kJ	17.6	14.3	13.2	10.2	10.3	15.6	18.8	17.2	11.7	19.7	8.6	20.6	17.4	19.2	30.3	14.8	4.0	22.3	7.0	16.3	5.4
Distribution $E_{Ejecta\ and\ Gas}$ (+)	kJ	60.4	62.2	68.7	69.1	67.0	57.4	63.1	56.5	54.2	49.7	50.0	55.7	57.4	35.2	36.2	59.5	6.7	42.9	12.5	56.2	10.2
Distribution $E_{Ejecta\ and\ Gas}$ (-)	kJ	0.4	0.5	0.5	0.5	0.4	0.7	1.0	1.5	0.7	0.8	0.7	1.0	7.0	13.1	11.5	0.7	0.3	10.5	3.2	2.7	4.2
Percent $E_{Cell\ Body}$	%	22.5	18.6	16.0	12.8	13.3	21.2	22.7	22.9	17.6	28.1	14.5	26.6	21.3	28.4	38.8	19.7	5.1	29.5	8.8	21.7	6.9
Percent $E_{Ejecta\ and\ Gas}$ (+)	%	77.1	80.9	83.4	86.7	86.2	77.9	76.1	75.1	81.4	70.8	84.2	72.1	70.2	52.1	46.4	79.3	5.3	56.2	12.4	74.7	11.6
Percent $E_{Ejecta\ and\ Gas}$ (-)	%	0.5	0.7	0.6	0.6	0.5	0.9	1.2	2.0	1.1	1.1	1.2	1.3	8.6	19.4	14.7	1.0	0.4	14.2	5.4	3.6	5.9
Avg. Heater Power	W	905.0	899.0	893.0	923.0	944.0	942.0	940.0						990.0	772.0	941.0	920.9	21.8	901.0	114.4	914.9	57.6
Time to Trigger	s	92.3	93.5	91.7	96.2	91.8	94.2	95.4	107.0	116.7	94.9	97.0	92.5	83.9	105.9	90.6	96.9	7.5	93.5	11.3	96.2	8.0
Avg. Cell Casing Temperature at Trigger	°C	242.5	252.1	256.9	250.3	280.8	291.4	298.8	247.4	239.4	271.7	263.4	269.1	253.2	250.3	275.9	263.7	19.2	259.8	14.0	262.9	17.9
Cell Mass (Pre-TR)	g	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0	47.0						
Cell Mass (Post-Tr)	g	11.3	10.5	12.0	7.6	9.4	9.8	13.9	13.4	10.0	17.3	8.3	16.1	11.3	15.2	20.2	11.6	3.0	15.6	4.5	12.4	3.6
Pos. Ejecta Mating Soot Mass (Post-TR)	g	4.0	8.5	0.2	5.4	7.5	8.2	0.6	0.5	6.6	1.2	8.2	2.1	3.6	2.1	0.4	4.4	3.4	2.0	1.6	3.9	3.2
Pos. Ejecta Bore Soot Mass (Post-TR)	g	14.3	15.2	20.0	21.1	17.4	14.3	17.8	17.6	15.9	17.1	17.1	18.3	13.0	14.1	8.2	17.2	2.1	11.8	3.1	16.1	3.1
Neg. Ejecta Mating Soot Mass (Post-TR)	g	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.4	0.9	1.3	0.0	0.0	0.9	0.5	0.2	0.4
Neg. Ejecta Bore Soot Mass (Post-TR)	g	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	1.9	3.5	2.4	0.0	0.1	2.6	0.8	0.5	1.1
Estimated Mass Ejected from System	g	17.4	12.8	14.8	12.9	12.7	14.7	14.7	15.1	14.5	11.4	13.4	10.5	16.8	11.2	14.5	13.7	1.8	14.2	2.8	13.8	2.0
Casing Thickness	µm	150	150	150	150	150	150	150	150	150	150	150	150	150	150	150						

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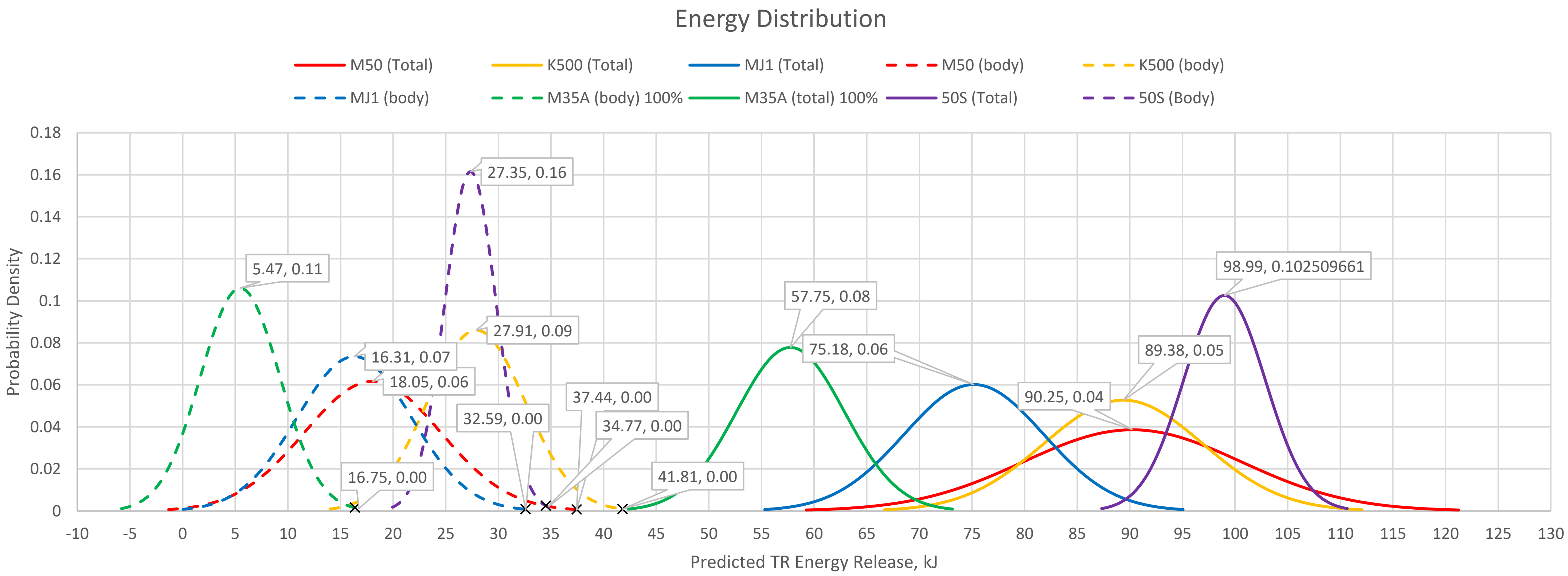
KULR 21700 – K500 (FROM NREL DATA BANK)

Item	Units	Experiment													
Experiment ID	-	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_Fe	ESRF18_O	ESRF18_O	ESRF18_O
Date of Experiment		12/12/19	12/12/19	12/12/19	12/12/19	12/12/19	12/13/19	12/14/19	12/14/19	12/14/19	12/14/19	02/16/19	10/27/18	10/27/18	10/27/18
Trigger		Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (IS	Heater (N	Heater (N	Heater (N	Heater (N
Cell failure Mechanism		Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top and B
Capacity	Ah	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00
OCV	V	4.156	4.168	4.153	4.153	4.189	4.190	4.168	4.179	4.180	4.170	4.153	4.153	4.152	4.150
Initial Cell Mass	g	73.0000	72.6000	73.2000	72.5000	72.0480	71.9930	72.9900	72.7940	72.7000	72.7000	72.9381	70.4393	70.4892	70.5057
DPA Cell Mass	g	39.5000	31.2000	32.9000	39.3000	33.3000	30.5000	43.0000	33.8000	40.7000	38.9000	33.4000	41.9560	38.0560	41.9577
Post-Test-Mass-Positive-Ejecta-Mating-g	g	2.4000	3.1000	0.6000	4.1000	3.8000	2.8000	2.5000	2.0000	1.2000	3.9000	1.4400	0.5500	4.4750	2.3000
Post-Test-Mass-Positive-Ejecta-Bore-Baffles-g	g	4.8000	3.0000	5.2000	4.7000	5.9000	6.1000	6.3000	10.8000	4.0000	4.3000	2.9400	2.6500	6.8150	7.6400
Post-Test-Mass-Positive-Copper-Mesh-g	g	0.1000	1.1100	0.0000	1.5000	0.0000	2.1000	0.4000	0.2000	0.3000	0.3000	2.5400	0.6000	2.2200	2.2400
Post-Test-Mass-Negative-Ejecta-Mating-g	g	1.7000	7.0000	4.4000	1.9000	2.5000	4.8000	1.6000	0.8000	0.7000	4.5000	2.3400	1.2100	0.4000	0.4492
Post-Test-Mass-Negative-Ejecta-Bore-Baffles-g	g	3.0000	5.9000	0.9000	3.7000	9.1000	10.5000	3.3000	7.2000	7.4000	3.0000	7.6400	6.8900	3.8600	1.2327
Post-Test-Mass-Negative-Copper-Mesh-g	g	0.0000	1.3000	0.0000	0.8100	2.5000	0.0000	0.9000	0.7000	0.6000	0.2100	3.1400	1.1400	0.4470	0.4167
Post-Test-Mass-Unrecovered-g	g	21.5000	19.9900	29.2000	16.4900	14.9480	15.1930	14.9900	17.2940	17.8000	17.5900	19.4981	15.4433	14.2162	14.2694
Energy Trigger	kJ	88.7775	104.9524	67.2907	69.4641	63.9560	105.8905	90.3078	38.9490	40.0783	92.6363	96.3477	101.9220	88.3005	99.3759
Heater Power	W	956.7142	929.3360	951.7815	924.5232	929.1241	933.9485	941.3726	930.0860	935.2720	937.0686	971.1702	956.0369	505.1184	955.8221
Heater Time	s	93.0137	113.0937	70.9578	75.4576	69.0667	113.6693	96.2170	42.1005	43.1056	99.1231	99.0601	106.4695	413.1214	103.9203
Ejected (Unrecovered) Mass Heat Loss Negative		3.0895	1.4858	4.5957	0.6763	1.0803	1.3085	0.8130	1.5768	1.1394	0.8667	1.6777	0.3528	0.6107	0.2962
Ejected (Unrecovered) Mass Heat Loss Positive	kJ	1.1575	1.1789	2.9339	0.9944	0.8345	0.5713	0.8681	1.0476	0.8492	1.0750	1.3171	0.9414	0.9555	1.0669
Heat Loss Corrected Total Energy Yield	**kJ**	**81.3607**	**96.4229**	**94.1028**	**84.6141**	**89.6461**	**81.1001**	**82.4824**	**90.2981**	**81.3227**	**76.7936**	**84.0068**	**77.5769**	**85.5504**	**79.7885**
Energy Fractio Cell Body	kJ	28.4039	26.1796	24.5978	27.4956	25.0668	18.6278	37.2740	30.4983	31.8785	23.2074	23.7593	34.1611	29.7259	29.8003
Energy Fraction Positive Ejecta	kJ	25.6764	25.4684	40.1435	34.6917	27.7434	20.2383	26.6144	31.0601	20.6944	28.9373	20.7641	33.4344	38.0215	41.7230
Energy Fraction Negative Ejecta	kJ	27.2804	44.7748	29.3615	22.4267	36.8360	42.2340	18.5940	28.7396	28.7498	24.6489	39.4834	9.9813	17.8030	8.2653
Percent Cell Body	%	34.91%	27.15%	26.14%	32.50%	27.96%	22.97%	45.19%	33.78%	39.20%	30.22%	28.28%	44.04%	34.75%	37.35%
Percent Positive Ejecta	%	31.56%	26.41%	42.66%	41.00%	30.95%	24.95%	32.27%	34.40%	25.45%	37.68%	24.72%	43.10%	44.44%	52.29%
Percent Negative Ejecta	%	33.53%	46.44%	31.20%	26.50%	41.09%	52.08%	22.54%	31.83%	35.35%	32.10%	47.00%	12.87%	20.81%	10.36%

Item	Units														AVERAGE
Experiment ID	-	DLS19_De	DLS19_De	ESRF18_O	ESRF18_O	DLS19_Fe	DLS19_Fe	DLS19_Fe	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_De	DLS19_Dec_Run058	
Date of Experiment		12/12/19	12/14/19	10/29/18	10/29/18	02/15/19	02/15/19	02/15/19	12/13/19	12/13/19	12/13/19	12/14/19	12/14/19	12/14/19	
Trigger		Heater (N	Heater (N	Nail	Nail	Nail	Nail	Nail	Nail	Nail	Nail	Nail	Nail	Nail	
Cell failure Mechanism		Top and B	Top and B	Top and B	Top and B	Top and B	Top and B	Top Vent (	Top and B	Top and B	Top and B	Top and B	Top and B	Top and Bottom Ven	
Capacity	Ah	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5.00	5
OCV	V	4.123	4.156	4.134	4.137	4.112	4.138	4.157	4.107	4.150	4.170	4.175	4.146	4.015	4.149407
Initial Cell Mass	g	72.5700	72.8090	70.4409	70.6210	70.5562	70.6170	72.9619	72.8960	72.6000	72.5100	72.9000	72.7000	72.8090	72.14401
DPA Cell Mass	g	32.8000	29.6000	30.6400	28.6200	37.0000	31.4000	29.6000	34.6000	34.5000	30.4000	34.5000	35.5000	34.3000	34.88629
Post-Test-Mass-Positive-Ejecta-Mating-g	g	0.4000	6.3000	3.9800	3.7000	2.0000	2.9000	3.4000	2.6000	0.7000	0.5000	1.1000	2.3000	0.9000	2.442407
Post-Test-Mass-Positive-Ejecta-Bore-Baffles-g	g	3.1000	9.1000	6.2700	6.3000	8.0000	5.9000	11.3000	1.9000	2.9000	2.2000	0.9000	4.1000	2.6000	5.17463
Post-Test-Mass-Positive-Copper-Mesh-g	g	1.1000	0.5000	2.0600	0.9100	0.6000	0.8000	3.3000	0.4000	0.7000	0.5000	1.6000	0.3000	0.9000	1.01037
Post-Test-Mass-Negative-Ejecta-Mating-g	g	3.3000	1.8000	1.1200	0.0000	0.3000	0.8000	0.0000	1.4000	4.1000	2.4000	1.0000	2.4000	2.4000	2.048859
Post-Test-Mass-Negative-Ejecta-Bore-Baffles-g	g	8.9000	3.6000	8.2300	7.0800	1.5000	6.7000	0.0000	9.6000	9.4000	11.6000	7.1000	5.9000	8.5000	5.9901
Post-Test-Mass-Negative-Copper-Mesh-g	g	0.9000	1.4000	1.5100	0.0300	0.6000	2.0000	0.0000	0.0000	0.2000	1.1000	1.4000	1.3000	0.7000	0.8631
Post-Test-Mass-Unrecovered-g	g	22.0700	20.5090	16.6309	23.9810	20.5562	20.1170	25.3619	22.3960	20.1000	23.8100	25.3000	20.9000	22.5090	19.72826
Energy Trigger	kJ	110.4258	92.1650	-	-	-	-	-	-	-	-	-	-	-	84.42746
Heater Power	W	932.2597	940.2787	-	-	-	-	-	-	-	-	-	-	-	914.3696
Heater Time	s	118.5902	98.1402	-	-	-	-	-	-	-	-	-	-	-	109.6942
Ejected (Unrecovered) Mass Heat Loss Negative		1.9274	1.0139	1.3600	2.4391	0.3998	1.9023	0.0000	2.7960	2.9426	2.6584	2.3185	1.0837	0.5028	1.515318
Ejected (Unrecovered) Mass Heat Loss Positive	kJ	0.8588	1.9617	1.6298	2.1261	2.1461	1.4339	8.1902	0.3753	0.8272	0.4344	2.3853	2.1108	2.2907	1.576363
Heat Loss Corrected Total Energy Yield	**kJ**	**83.7022**	**84.4258**	**97.3381**	**98.9686**	**88.7318**	**96.0794**	**94.0338**	**91.9328**	**97.6396**	**99.0598**	**98.4240**	**97.9632**	**99.8301**	**89.3776**
Energy Fractio Cell Body	kJ	22.2240	24.8661	24.2284	25.1748	33.0421	28.6192	20.5016	26.4982	30.6448	27.3382	30.1139	33.8542	35.6732	27.90575
Energy Fraction Positive Ejecta	kJ	19.0843	38.2274	37.6961	37.4330	46.9709	31.1255	73.5309	7.1211	17.2436	9.1693	32.0053	40.0576	52.9562	31.77156
Energy Fraction Negative Ejecta	kJ	42.3939	21.3322	35.4137	36.3607	8.7189	36.3348	0.0013	58.3136	49.7511	62.5522	36.3047	24.0514	11.2007	29.7003
Percent Cell Body	%	26.55%	29.45%	24.89%	25.44%	37.24%	29.79%	21.80%	28.82%	31.39%	27.60%	30.60%	34.56%	35.73%	0.314178
Percent Positive Ejecta	%	22.80%	45.28%	38.73%	37.82%	52.94%	32.40%	78.20%	7.75%	17.66%	9.26%	32.52%	40.89%	53.05%	0.355982
Percent Negative Ejecta	%	50.65%	25.27%	36.38%	36.74%	9.83%	37.82%	0.00%	63.43%	50.95%	63.15%	36.89%	24.55%	11.22%	0.329839

ENERGY DISTRIBUTION (SAMPLE STDEV.S)



See more: Matthew Sharp et al. Thermal Runaway of Li-Ion Cells: How Internal Dynamics, Mass Ejection, and Heat Vary with Cell Geometry and Abuse Type, Journal of The Electrochemical Society, 2022 169 020526

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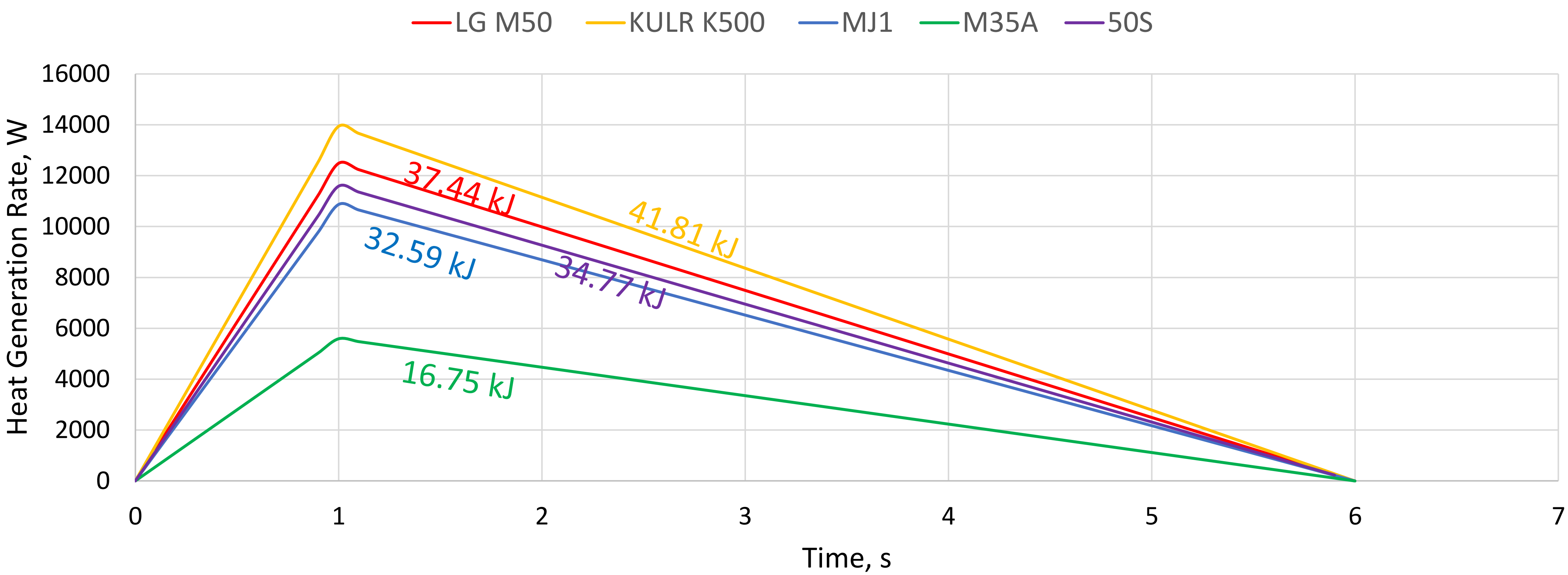
HEAT RATES


LG M50
KULR K500
MJ1
M35A
50S
16000
14000
12000
10000
8000
6000
4000
2000
0
Heat Generation Rate, W
37.44 kJ
41.81 kJ
32.59 kJ
34.77 kJ
16.75 kJ
0
1
2
3
4
5
6
7
Time, s

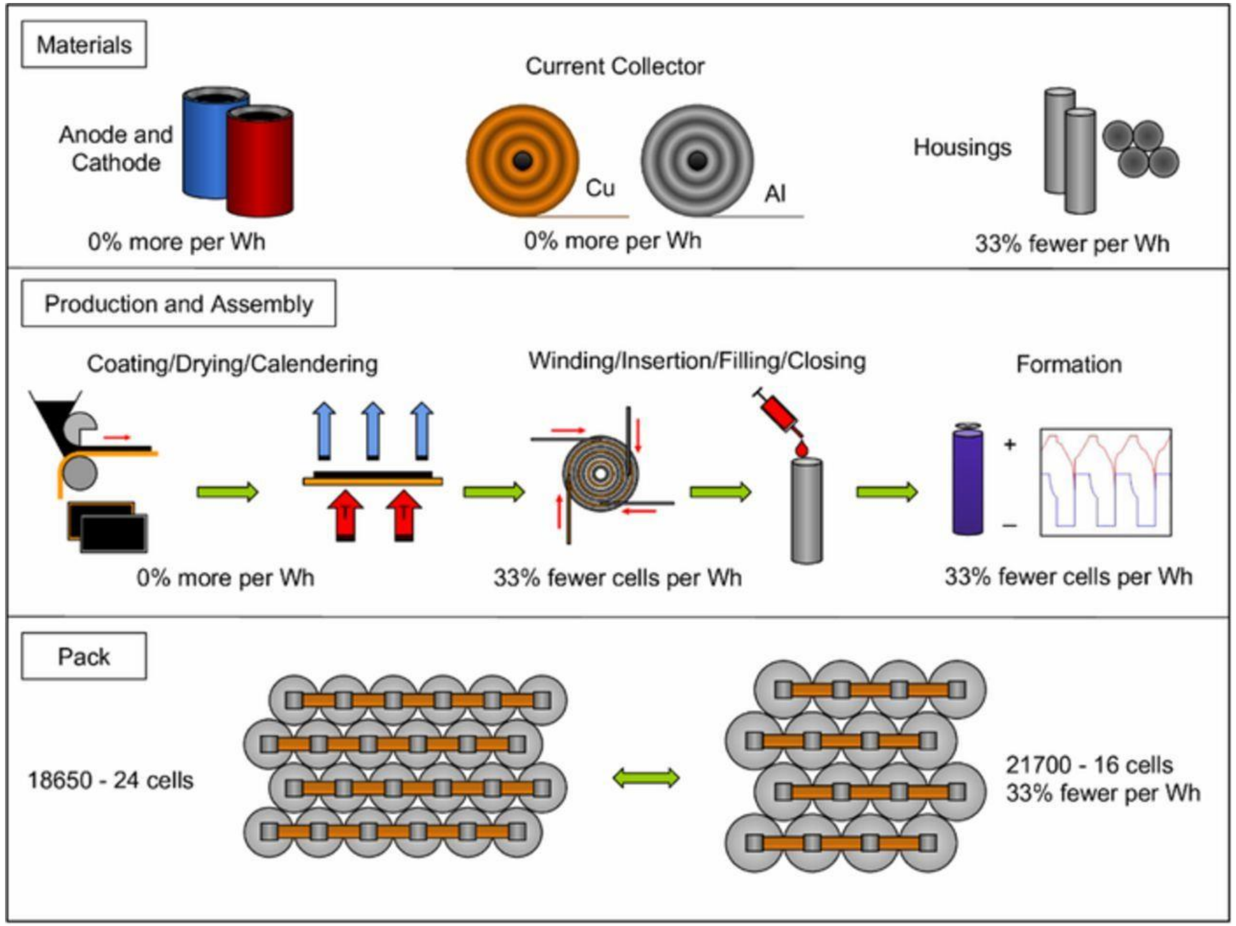
18650 - 21700

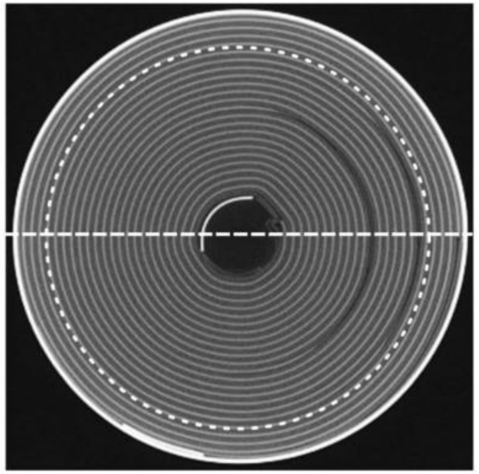
- LG MJ1 (18650)
  - 3.5Ah
  - 49 g
  - 3.6V
  - 12.6Wh
  - 257 Wh/kg
  - 711 Wh/L
- Moli M35A
  - 3.5Ah
  - 48 g
  - 3.6V
  - 12.6Wh
  - 262 Wh/kg
- KULR K500 (21700)
  - 5Ah
  - 72 g
  - 3.6V
  - 18Wh
  - 250 Wh/kg
  - 742 Wh/L
- LG M50 (21700)
  - 5Ah
  - 69 g
  - 3.6V
  - 18 Wh
  - 261 Wh/kg

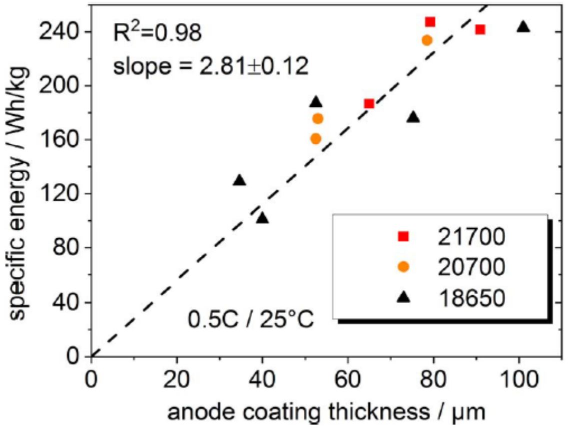
See more: Matthew Sharp et al. Thermal Runaway of Li-Ion Cells: How Internal Dynamics, Mass Ejection, and Heat Vary with Cell Geometry and Abuse Type, Journal of The Electrochemical Society, 2022 169 020526

[Battery Failure Databank | Transportation and Mobility Research | NREL]

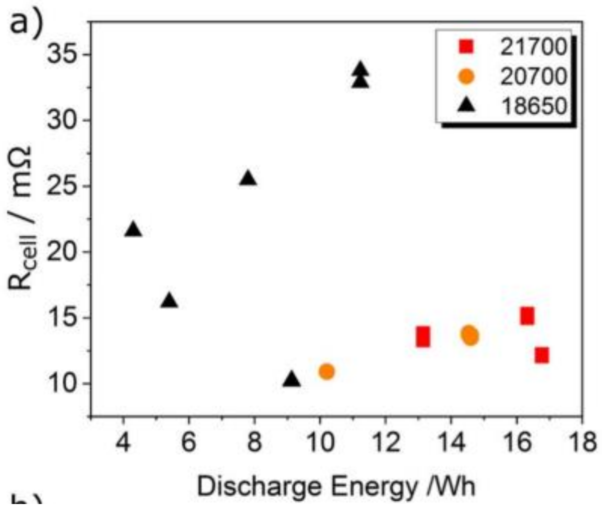
18650 - 21700







$$d\ [\mu m] = \frac{\text{specific energy [Wh/kg]}}{2.81 \pm 0.12}$$

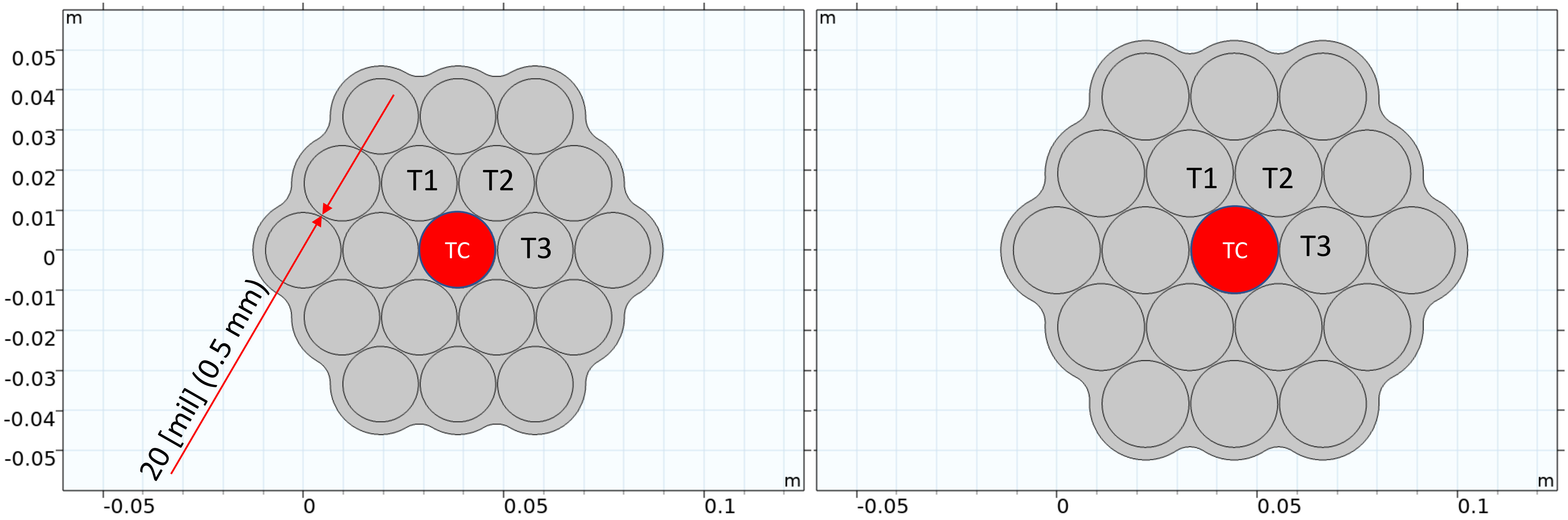


Jason B. Quinn, Thomas Waldmann, Karsten Richter, Michael Kasper and Margret Wohlfahrt-Mehrens, “Energy Density of Cylindrical Li-Ion Cells: A Comparison of Commercial 18650 to the 21700 Cells” Journal of The Electrochemical Society, Volume 165, Number 14

CASE 1 (ADIABATIC PACK)

m_{tot} = 1.23 kg
Q = 239.4 Wh
Q_m = 194 Wh/kg
Q_v = 525 Wh/L
LG MJ1 18650

m_{tot} = 1.75 kg
Q = 342 Wh (43%↑)
Q_m = 195 Wh/kg
Q_v = 539.48 Wh/L (3%↑)
KULR K500 21700



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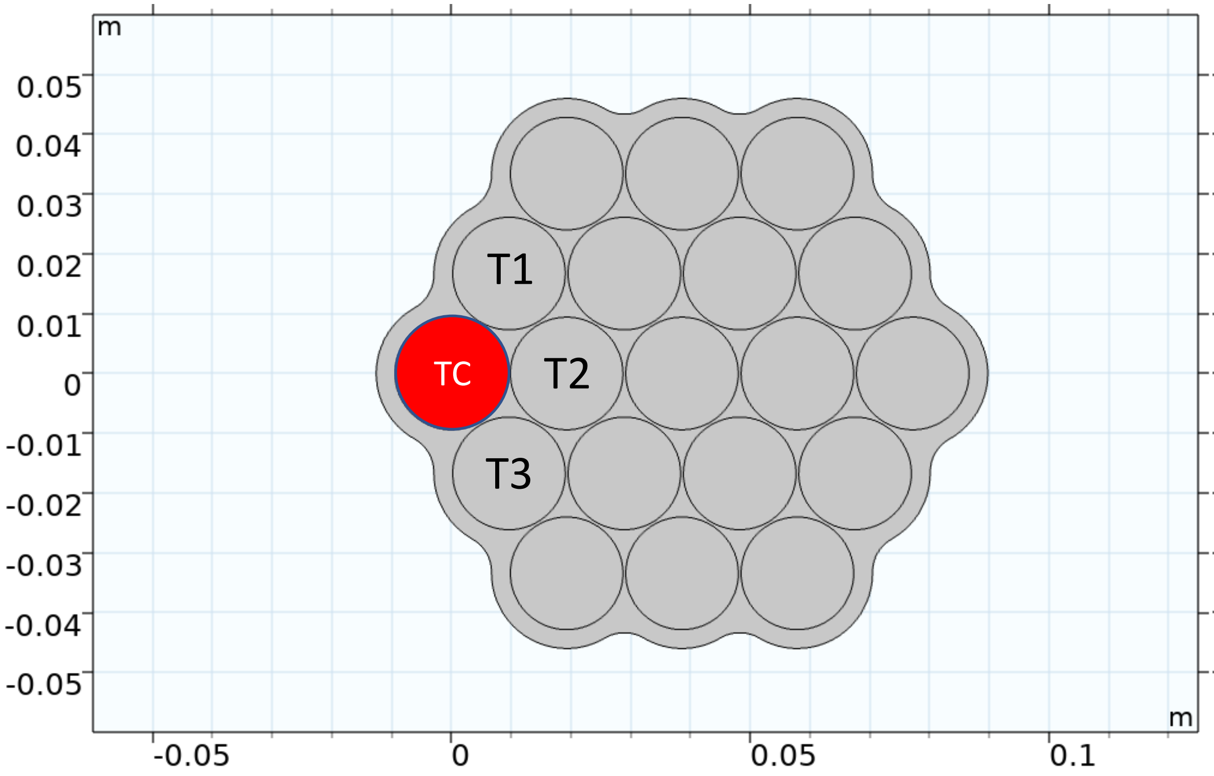
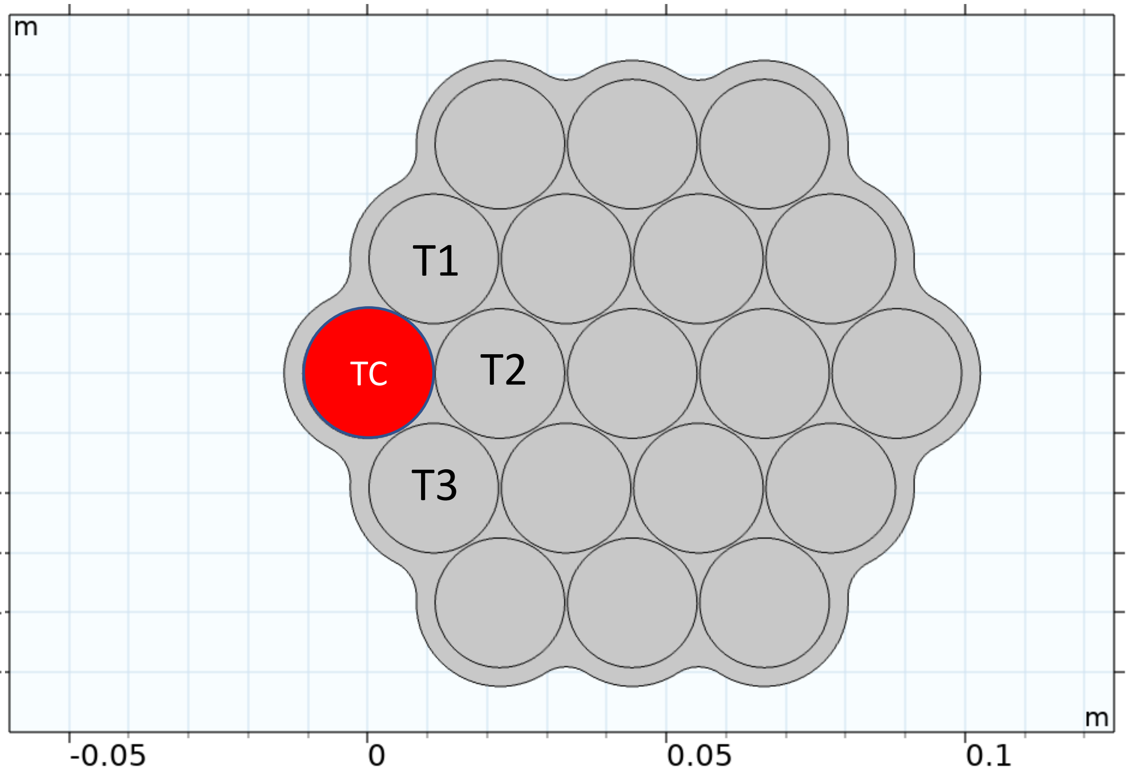
CASE 2 (ADIABATIC PACK)





MATERIALS USED

AL6061 Heat Sink

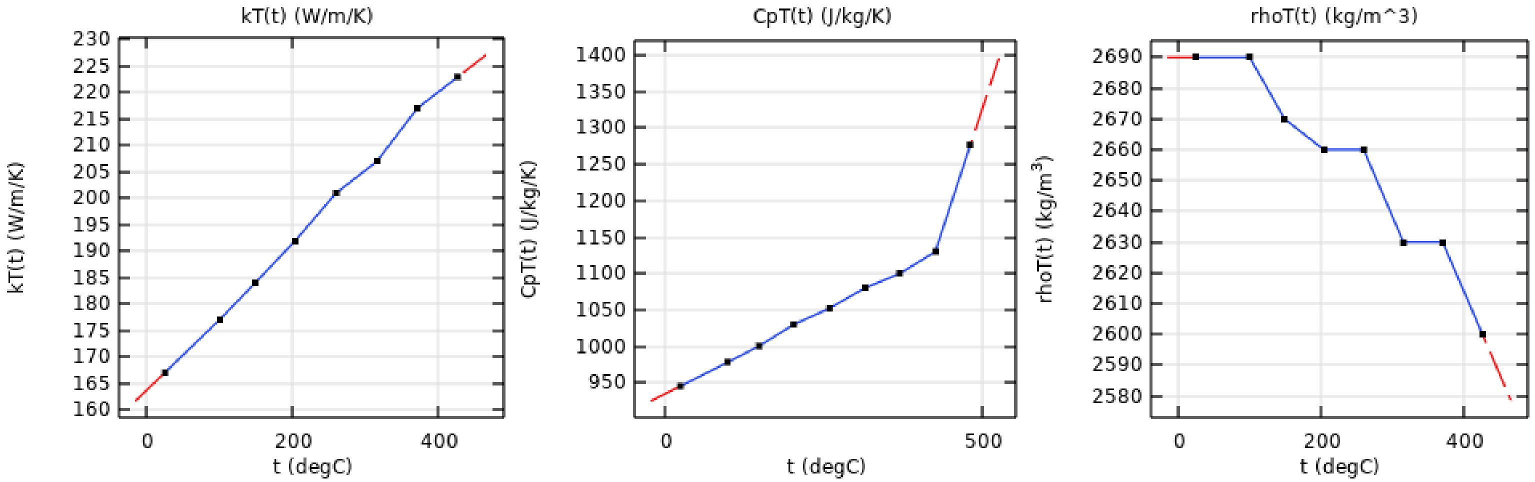
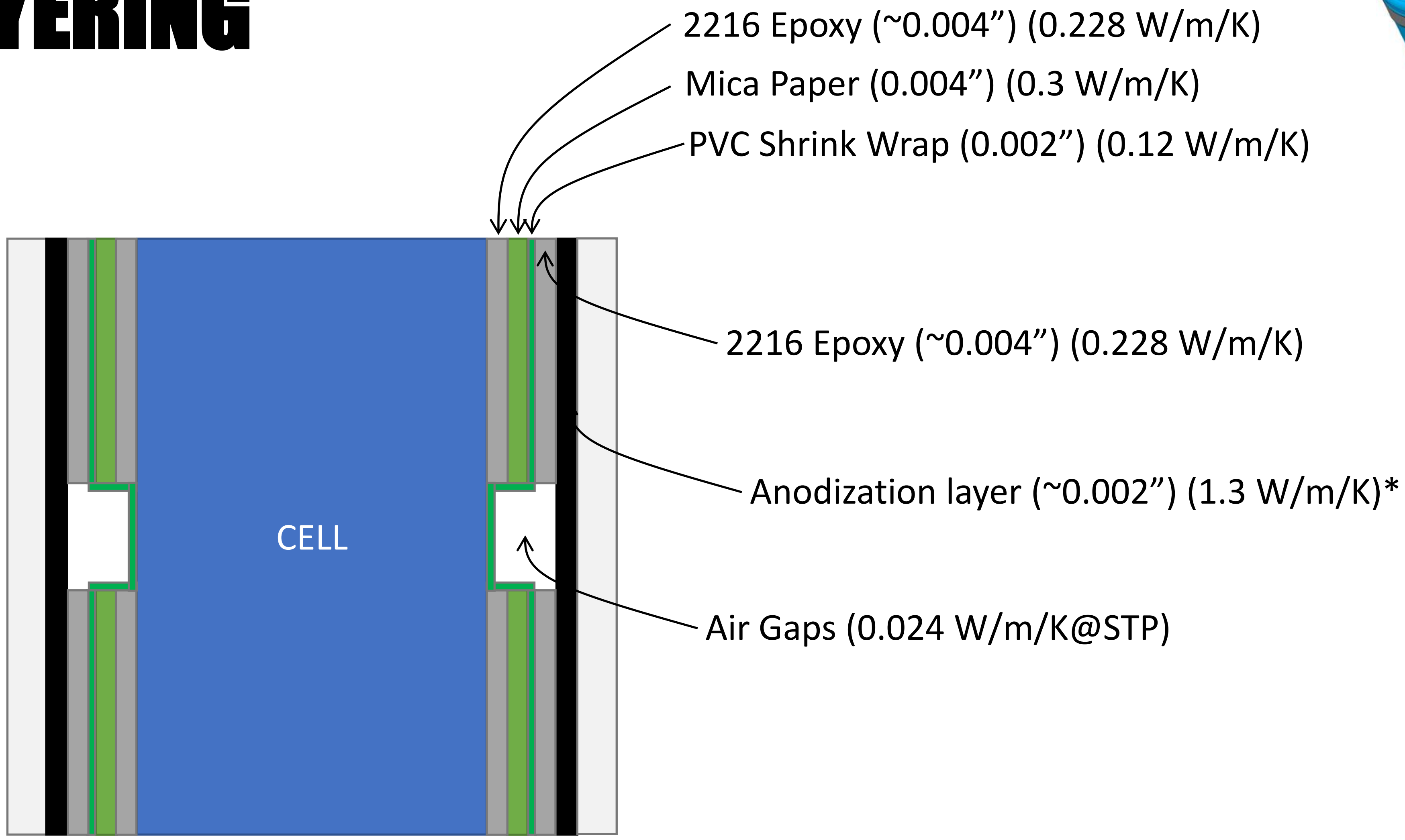


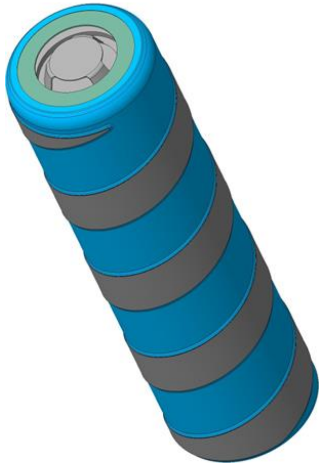
Table 1. Temperature-dependent material properties for Al6061-T6.

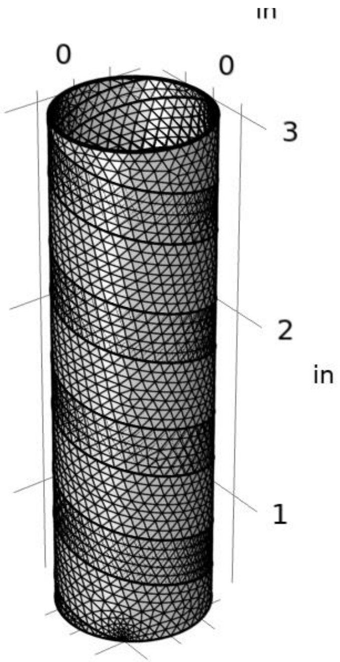
T [°C]	ρ [kg m^{-3}]	E [GPa]	v	α [10−6·°C−1]	C_P [J kg^{-1}·°C^{-1}]	λ [W m^{-1}·°C^{-1}]
25	2690	66.94	0.33	23.5	945	167
100	2690	63.21	0.334	24.6	978	177
149	2670	61.32	0.335	25.7	1000	184
204	2660	56.8	0.336	26.6	1030	192
260	2660	51.15	0.338	27.6	1052	201
316	2630	47.17	0.36	28.5	1080	207
371	2630	43.51	0.4	29.6	1100	217
427	2600	28.77	0.41	30.7	1130	223
482	-	20.2	0.42	-	1276	-

Zhi Zhu, Min Wang, Huijie Zhang, Xiao Zhang, Tao Yu and Zhenqiang Wu, A Finite Element Model to Simulate Defect Formation during Friction Stir Welding, Metals, **2017**, 7, 256

LAYERING







*Junghoon Lee, Yonghwan Kim, Uoochang Jung, Wonsub Chung - **Thermal conductivity of anodized aluminum oxide layer: The effect of electrolyte and temperature**, Materials Chemistry and Physics, 141 (2013) 680-685

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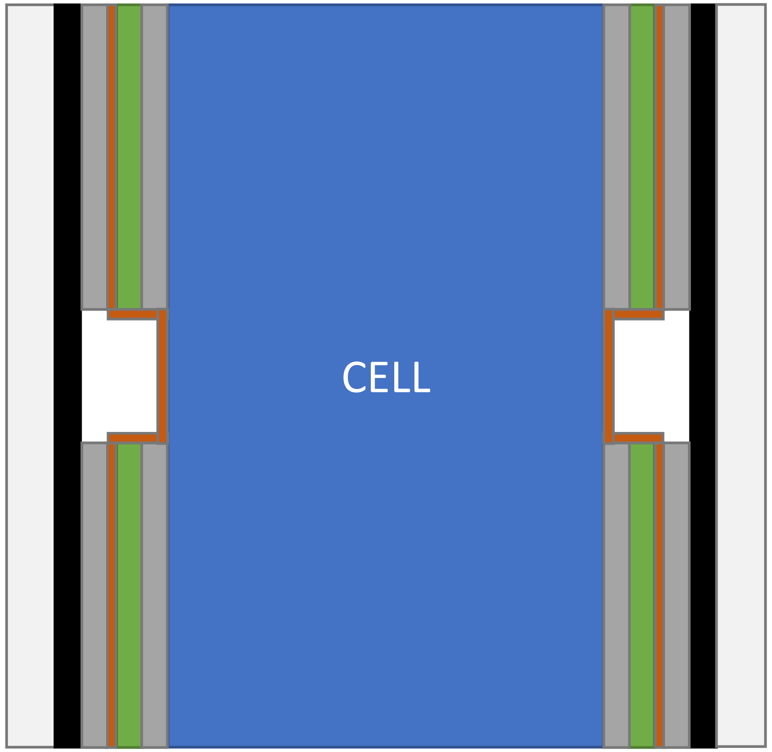
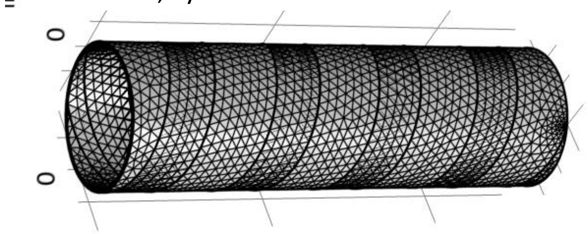
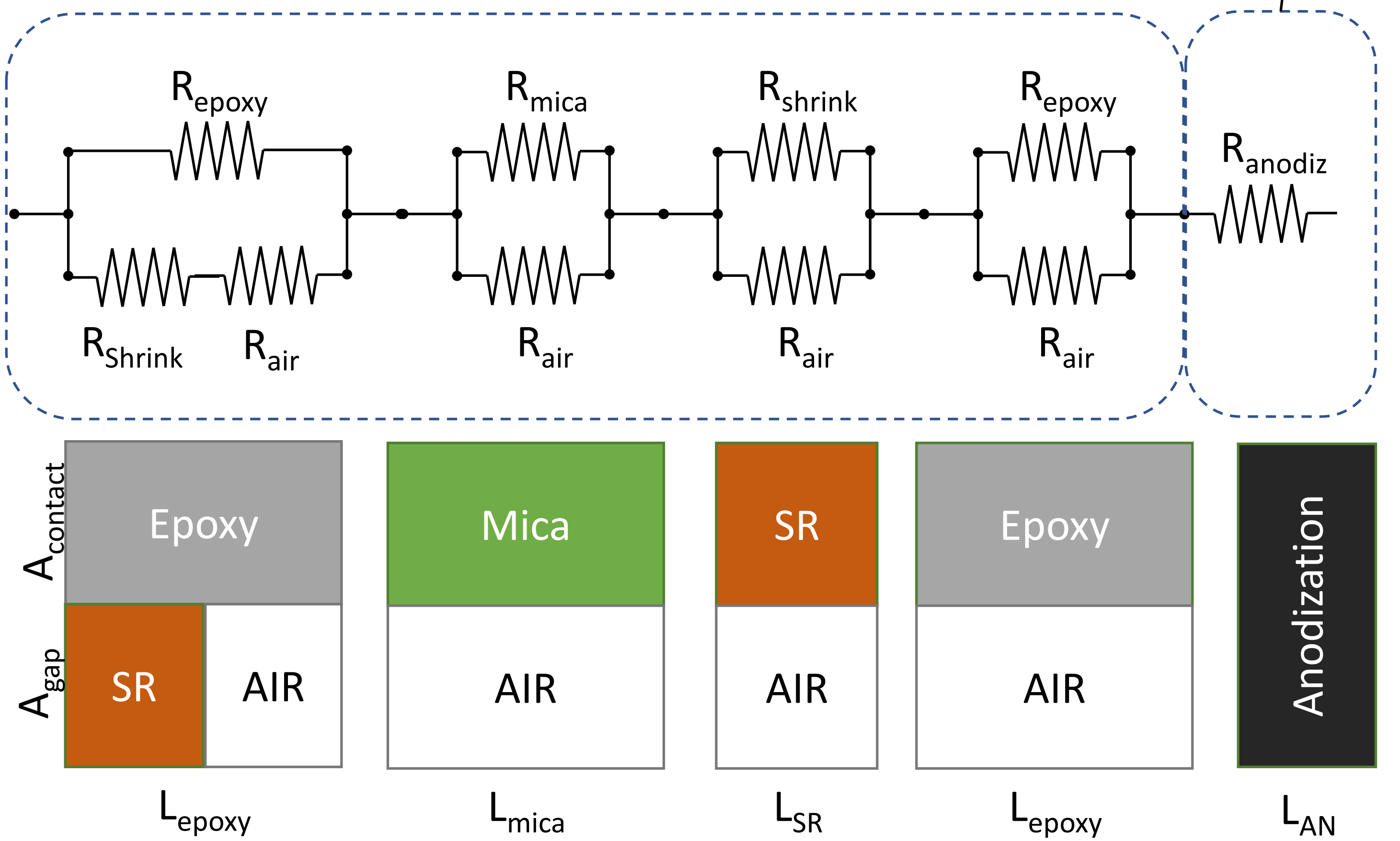
LAYERING



$k_{eff,layers}$ = 0.3 W/m/K





*Junghoon Lee, Yonghwan Kim, Uoochang Jung, Wonsub Chung - **Thermal conductivity of anodized aluminum oxide layer: The effect of electrolyte and temperature**, Materials Chemistry and Physics, 141 (2013) 680-685

MATERIALS USED

18650 M35A

Cell	Heat capacity [J/gK]		
	@ 0% SOC	@ 30% SOC	@ 100% SOC
AR46 (25 °C)	0.890	0.891	0.888
AR47 (25 °C)	0.880	0.884	0.872
AR48 (25 °C)	0.878	0.878	0.879
AR49 (50 °C)	-	0.859	-
AR50 (50 °C)	-	0.896	-
AR51 (50 °C)	-	0.909	-
AR52 (0 °C)	-	*	-
AR53 (0 °C)	-	*	-
AR54 (0 °C)	-	*	-

Table IVb. In-plane thermal properties of Sony US-18650 lithium-ion battery components with and without electrolyte [EC-DMC (1:1 wt %)/1 M $LiPF_6$].

Materials	ρ ($g\ cm^{-3}$)	C_p ($J\ g^{-1}\ K^{-1}$)	α ($cm^2\ s^{-1}$) $OCV = 2.45$ V	α ($cm^2\ s^{-1}$) $OCV = 3.75$ V	k ($W\ m^{-1}\ K^{-1}$) $OCV = 2.45$ V	k ($W\ m^{-1}\ K^{-1}$) $OCV = 3.75$ V
PE	3.121	0.602	0.115 ± 0.0040	0.116 ± 0.0010	21.57	21.75
NE	1.620	0.598	0.090 ± 0.00017	0.156 ± 0.0030	8.72	15.11
PE/Sp/NE	2.291	1.088	0.0071 ± 0.0040	0.099 ± 0.00150	17.69	24.66
PE/Sp/NE + electrolyte	2.78	1.278	0.058 ± 0.0010	0.079 ± 0.0004	20.06	28.05

Table IVa. Cross-plane thermal properties of Sony US-18650 lithium-ion battery components with and without electrolyte [EC-DMC (1:1 wt %)/1 M $LiPF_6$].

Materials	ρ ($g\ cm^{-3}$)	C_p ($J\ g^{-1}\ K^{-1}$)	α ($cm^2\ s^{-1}$): sd 4×10^{-4}		k ($W\ m^{-1}\ K^{-1}$)	
			$OCV = 2.45$ V	$OCV = 3.75$ V	$OCV = 2.45$ V	$OCV = 3.75$ V
PE	3.115	0.601	0.0124	0.0133	2.33	2.49
NE	1.622	0.623	0.0088	0.0119	0.89	1.20
PE/Sp/NE	2.290	1.089	0.0076	0.0095	1.90	2.36
PE/Sp/NE + electrolyte	2.680	1.280	0.0099	0.0100	3.39	3.40

$\rho = 2{,}780\ kg/m^3$

$C_p = 880\ J/g/K$

$k_{eff} = 11.62\ W/m/K$

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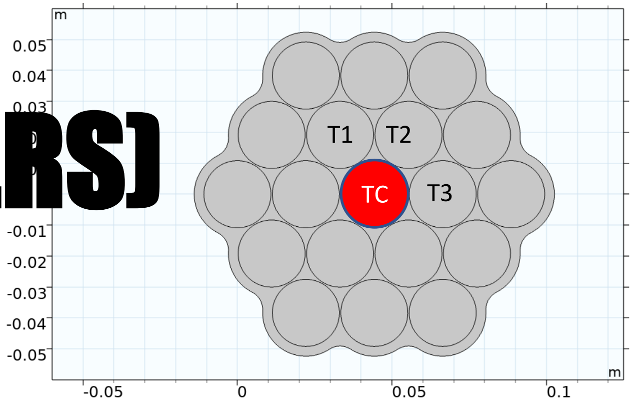
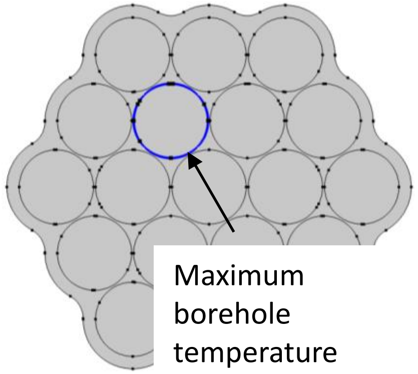
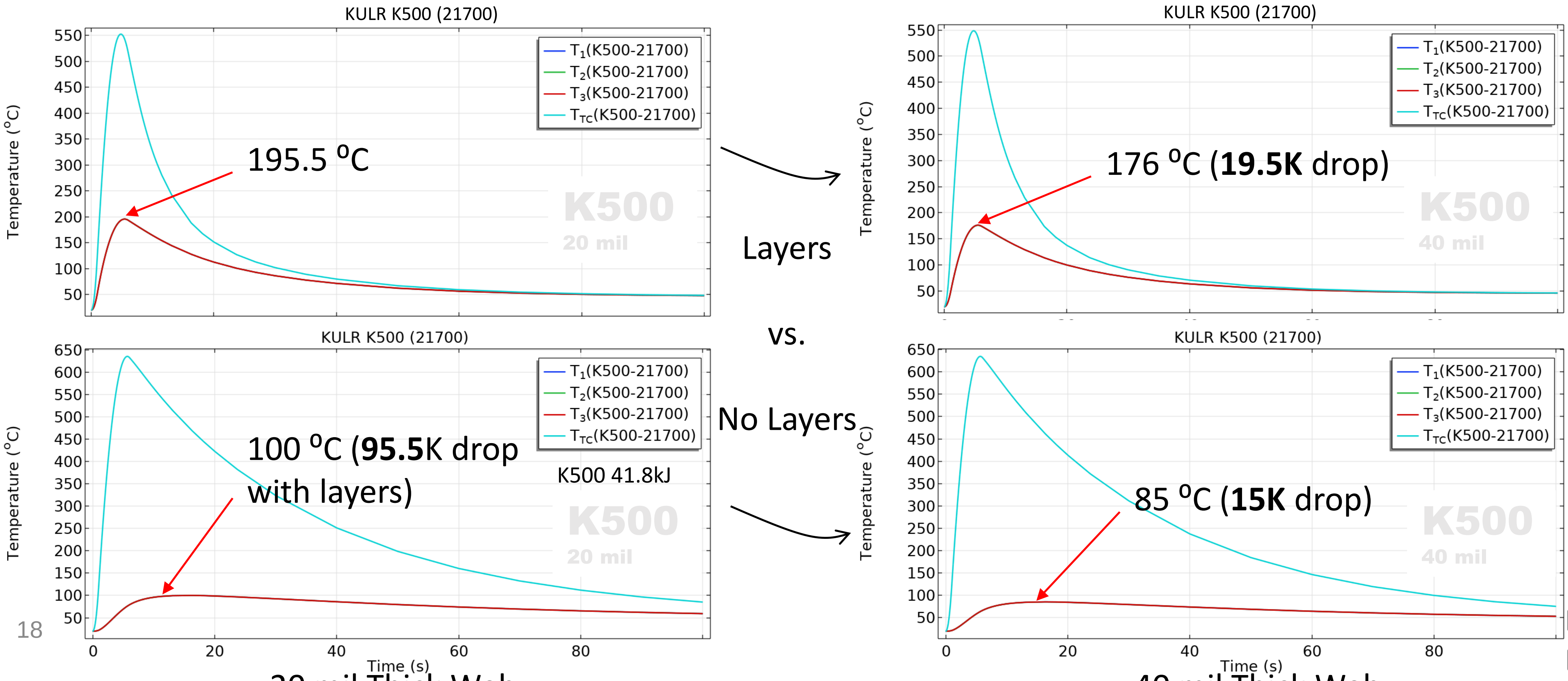
CASE 1 (LAYERS VS. NO LAYERS)

20 mil (left) vs 40mil (right) webbing, TC middle



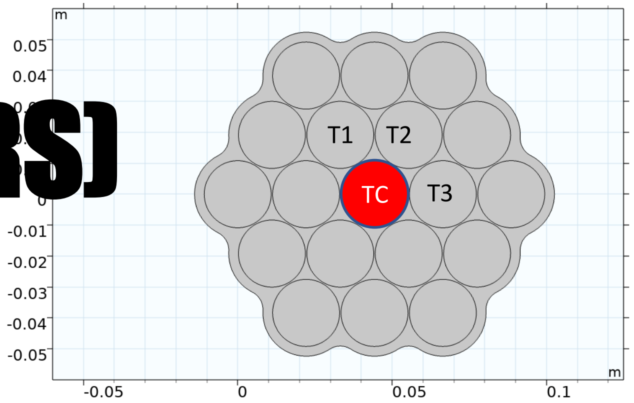


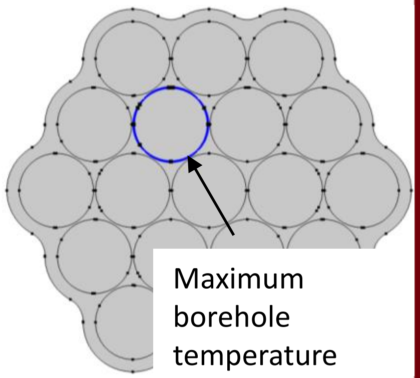


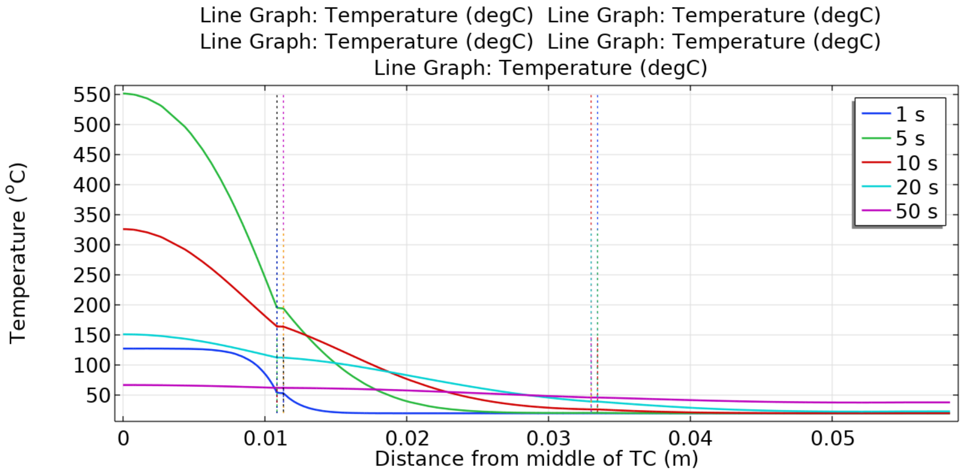
20 mil Thick Web

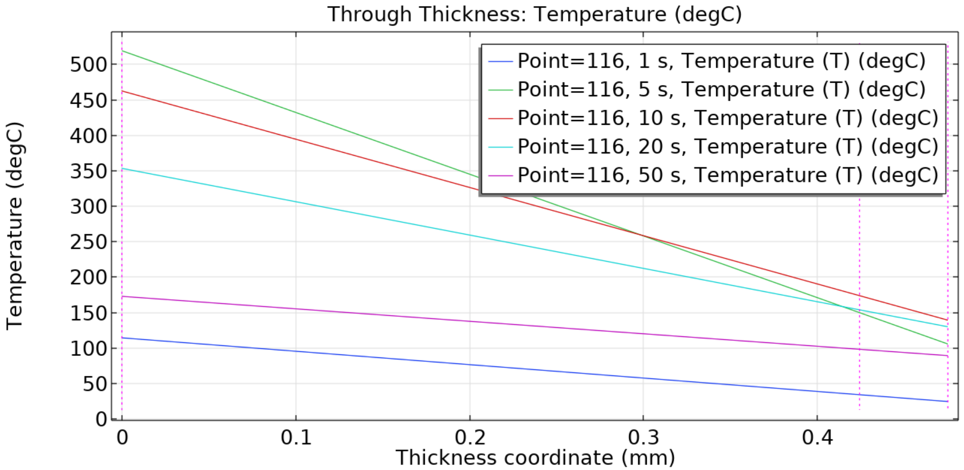
40 mil Thick Web

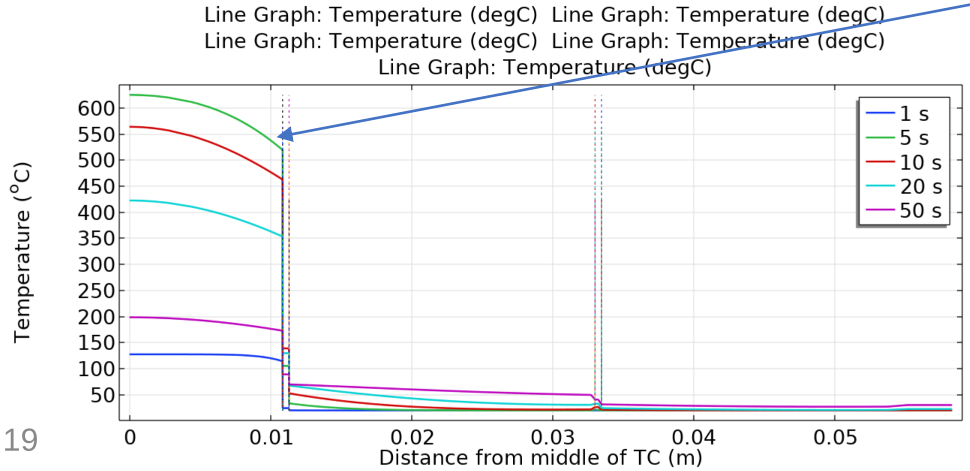
CASE 1 (LAYERS VS. NO LAYERS)

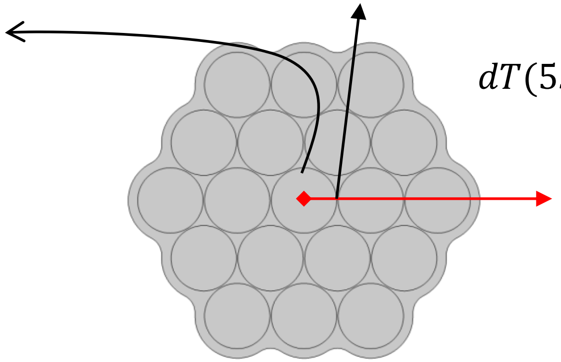












$$dT(5s) = q\,\frac{dx}{k} = 2.615e5\left[\frac{W}{m^2}\right]\frac{4.75e{-4}[m]}{0.3\left[\frac{W}{mK}\right]} = 414[K]$$

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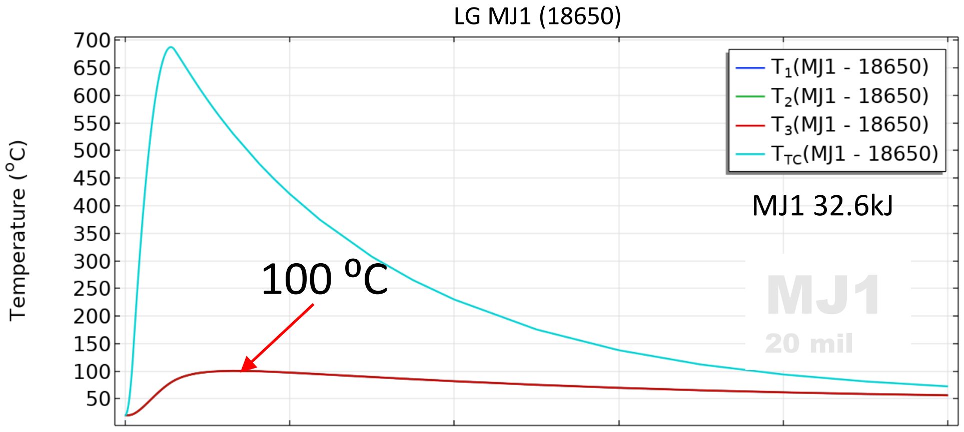
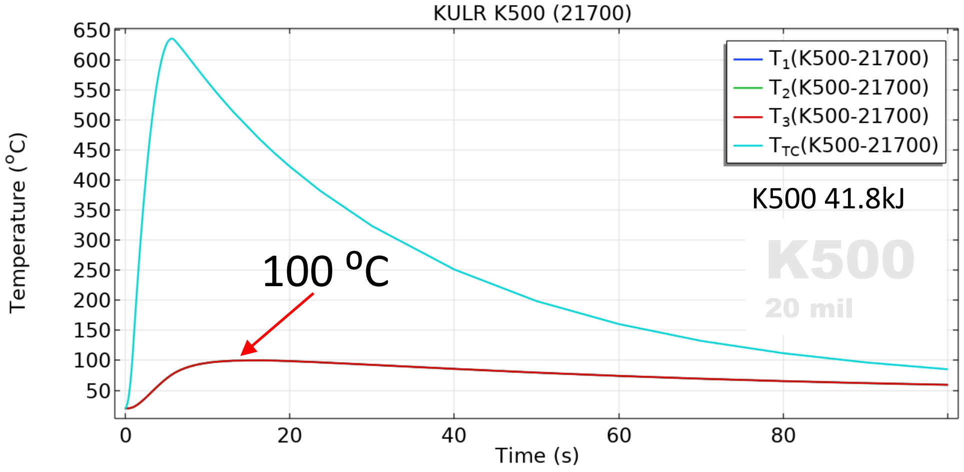
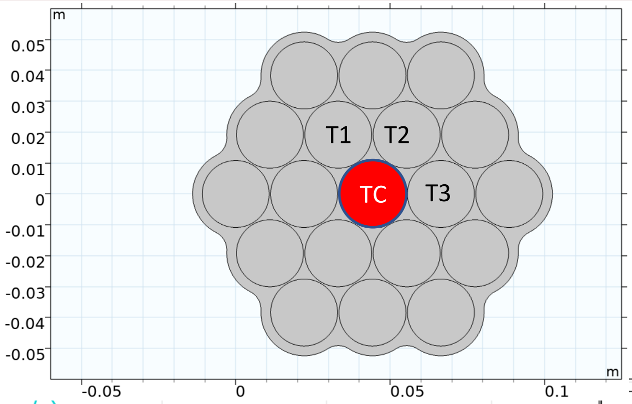
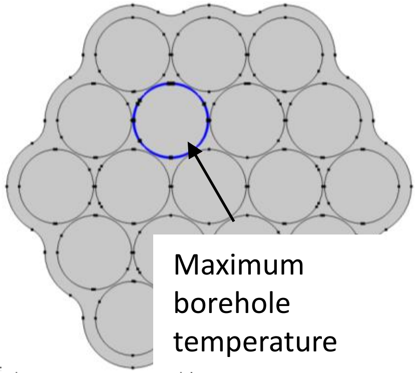
CASE 1

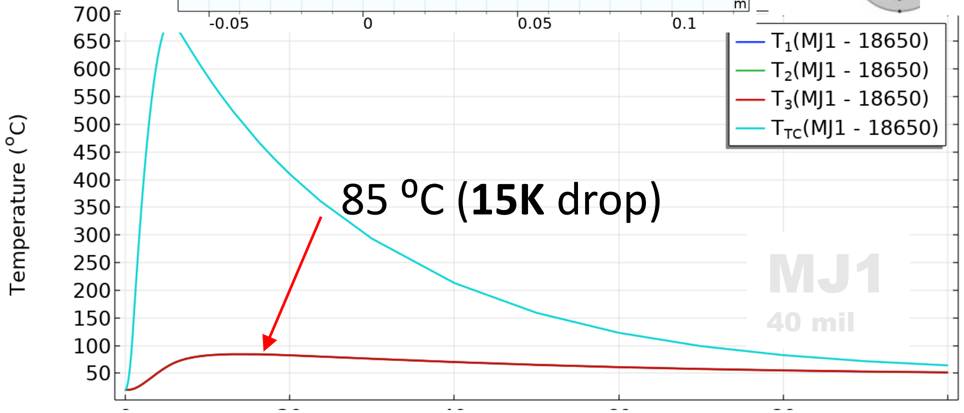
20 mil (left) vs 40mil (right) webbing, TC middle

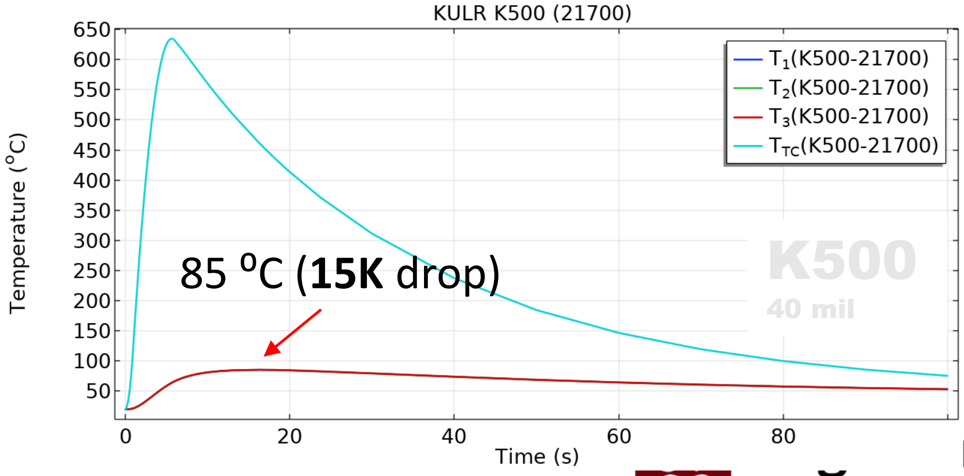










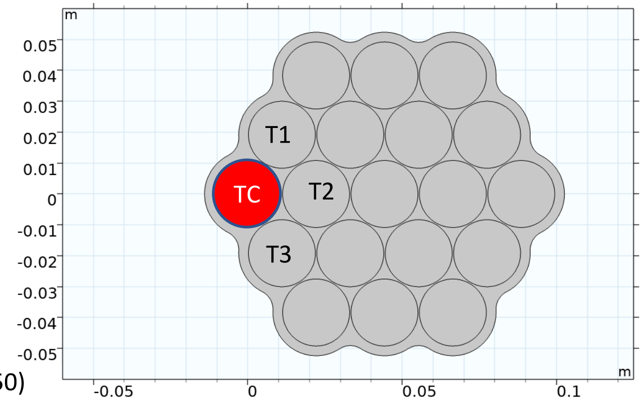


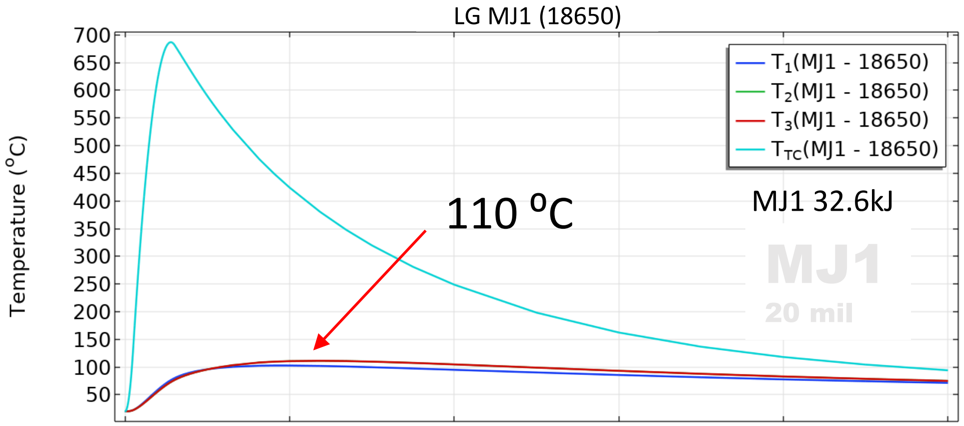
20 mil Thick Web

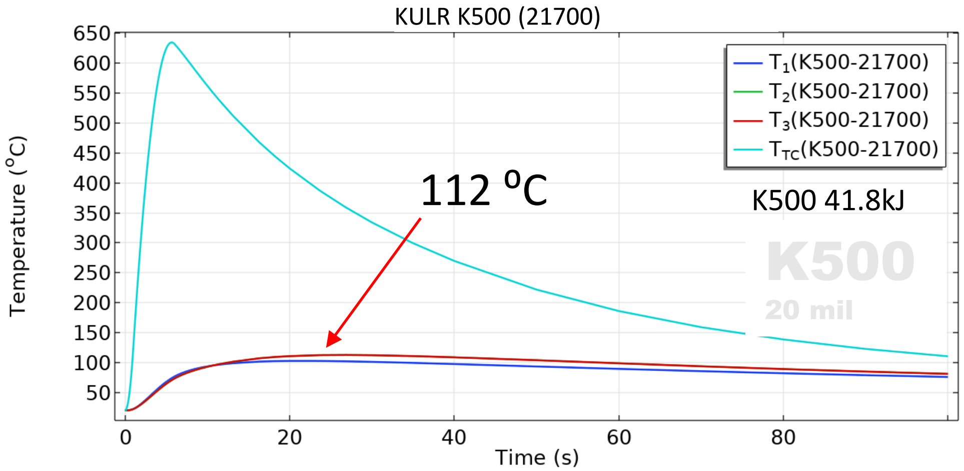
40 mil Thick Web

CASE 2

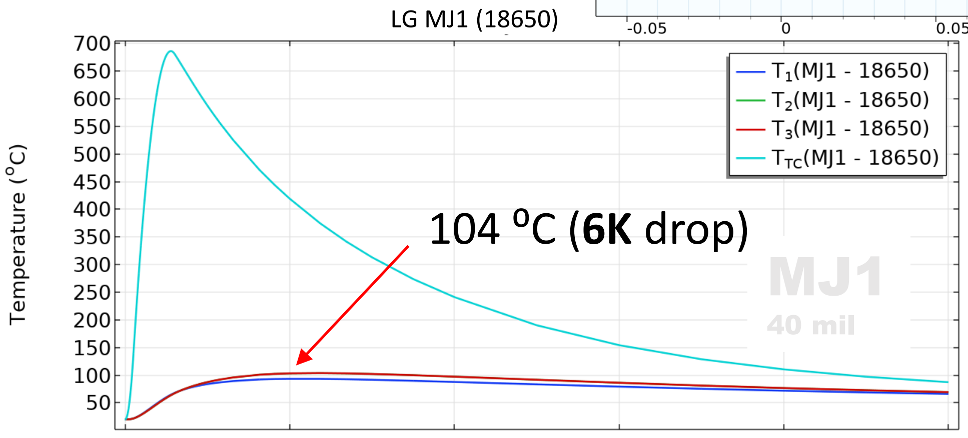
20 mil (left) vs 40mil (right) webbing, TC middle

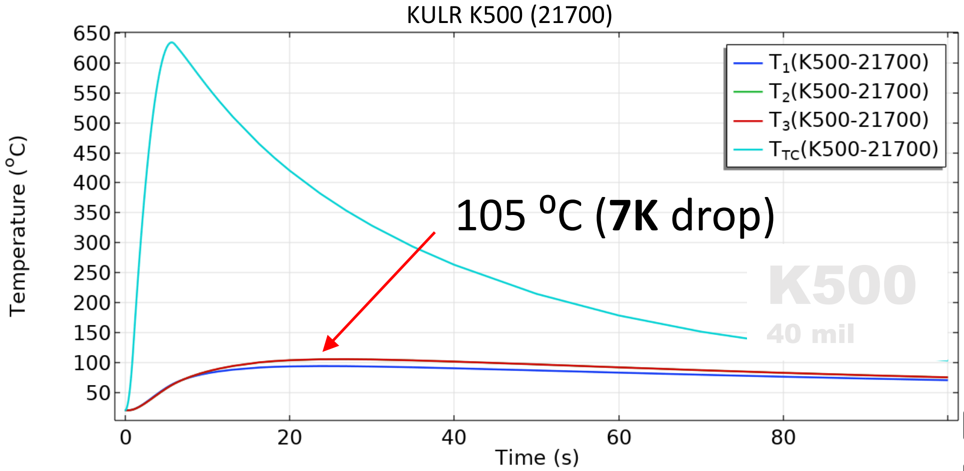






20 mil Thick Web





40 mil Thick Web

UPSCALING CONCLUSIONS

- Taking the worst-case scenario for 18650 (MJ1) vs worst case scenario 21700 (K500):
  - Upscaling leads to higher energy storage (~43% higher energy) in 21700 comparing to 18650, with small difference in terms of energy density at a pack level, but with a better volumetric energy density at a pack level (~3%)
  - Both cells have a similar behavior during thermal runaway, even though there is a higher difference in the energy released through the cell body (~28% higher energy release in K500, compared with MJ1 at 3σ)