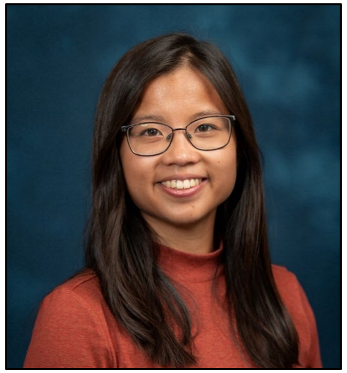
Towards Li-ion Battery Fire Mitigation and Reignition Prevention: Model-informed Fast Discharge Algorithm with Venting Constraints



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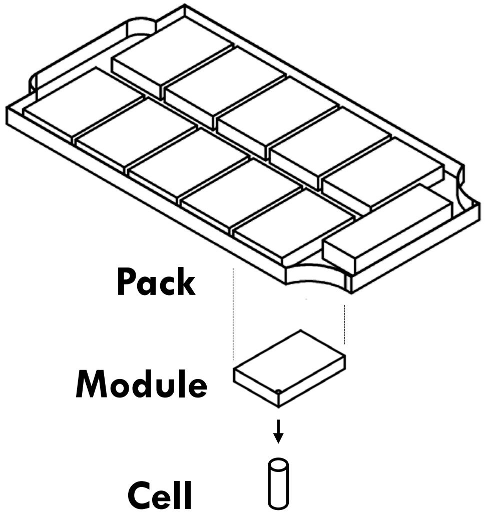
Baseed on: Tran, Vivian, et al. “Emergency Li-Ion Battery Discharge Using NMPC with Temperature and Venting Pressure Constraints.“ American Control Conference 2023.

Battery fires can be mitigated through discharging

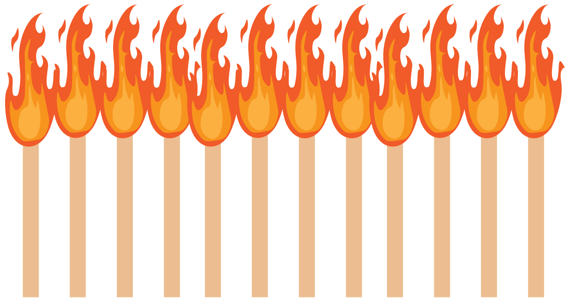
Early detection AND intervention can prevent battery fires from spreading throughout a battery system.



Batteries at low state-of-charge (SOC) are safer.

Intervention = Discharge

No energy dispersion



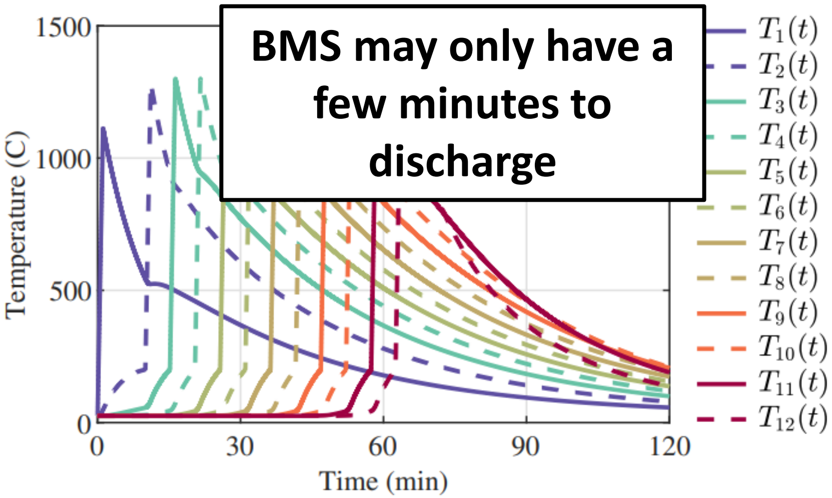
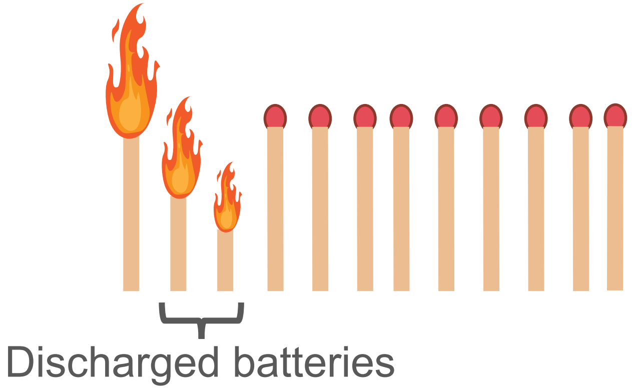


Fig. 3. Propagation Results with No Energy Dispersion

Discharging 1st and 2nd adjacent modules



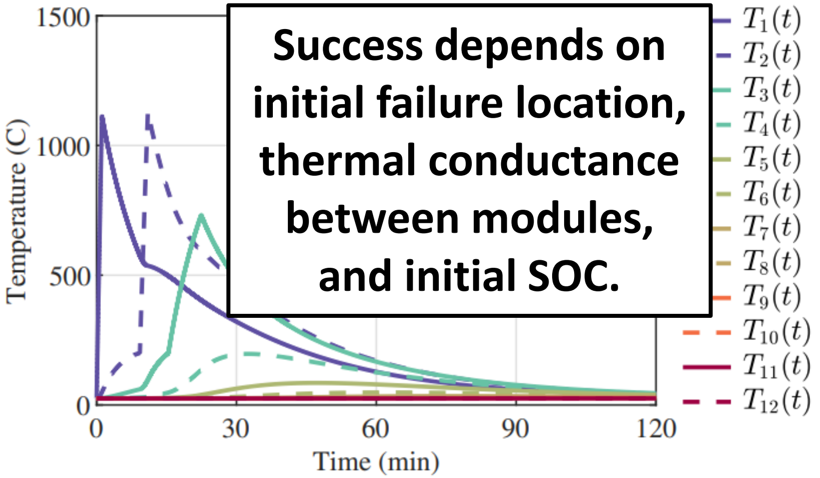
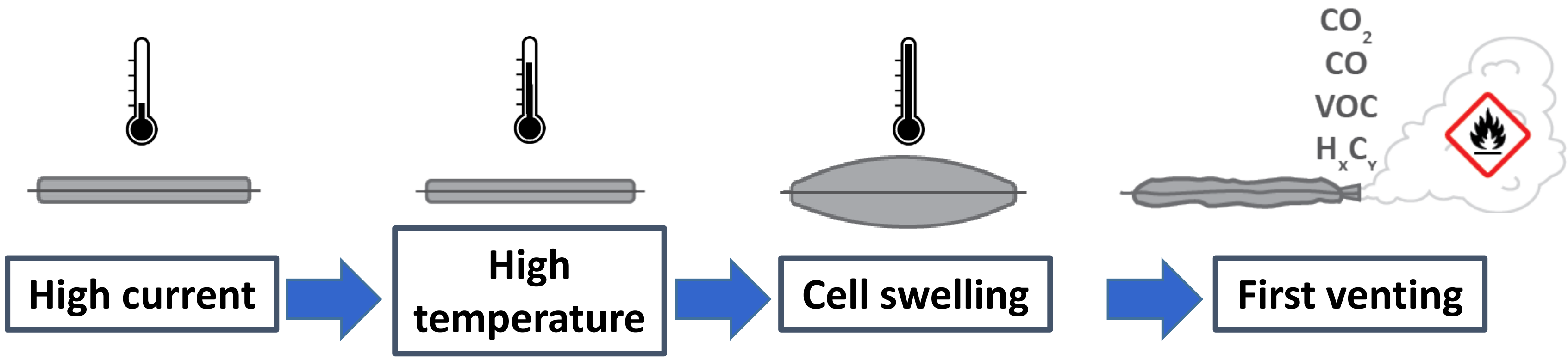


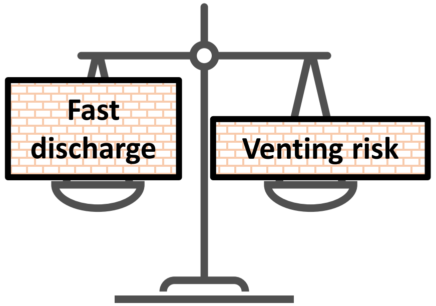
Fig. 6. Propagation Results with Energy Dispersed from 1st and 2nd Adjacent Modules

Mueller, Jacob A., et al. "Energy Redistribution as a Method for Mitigating Risk of Propagating Thermal Runaway." *2022 IEEE Energy Conversion Congress and Exposition (ECCE)*. IEEE, 2022.
Weng, Andrew, Eric Dufek, and Anna Stefanopoulou. "Battery passports for promoting electric vehicle resale and repurposing." *Joule* 7.5 (2023): 837-842.

Discharging too quickly can lead to unintended consequences

High temperatures cause venting of *hot, flammable gases* in a hot environment, creating a safety hazard.





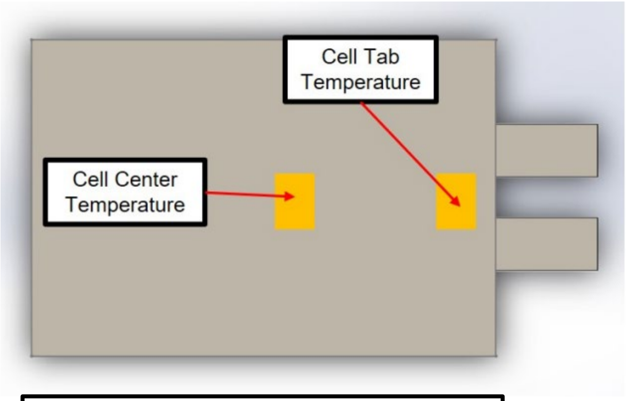
Approach:

1. Model the electrical, thermal, and venting behavior of a cell undergoing an external short circuit (ESC)
2. Formulate a constrained control problem that can balance competing objectives for a safe and fast discharge

Collecting experimental data at high discharge rates

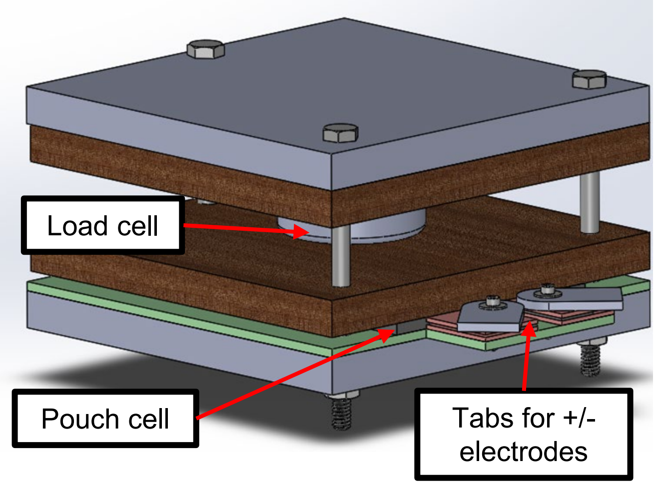
Cell external short circuit (ESC) experiment

1. Attached K-type thermocouples to a pouch cell

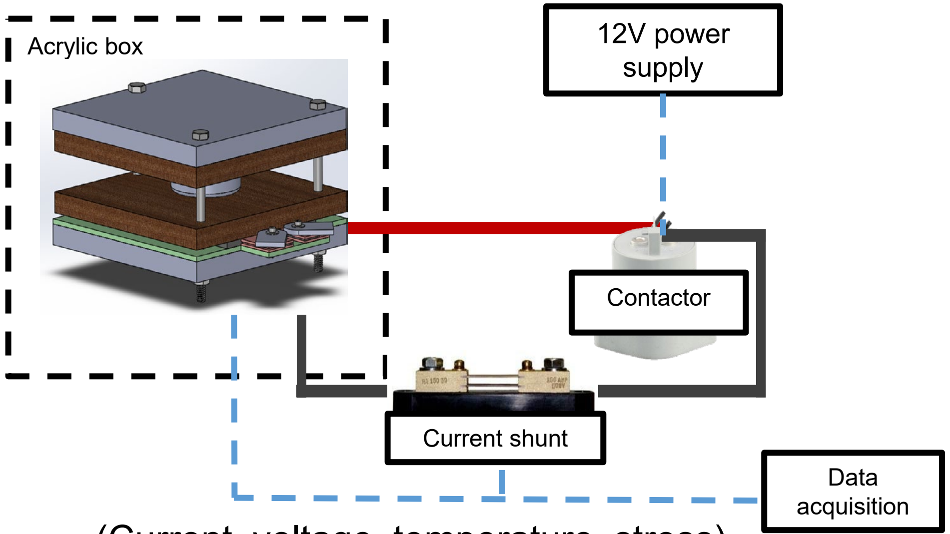


UMBL 4.6 Ah NMC/G

2. Secured the cell in the fixture instrumented with a load cell



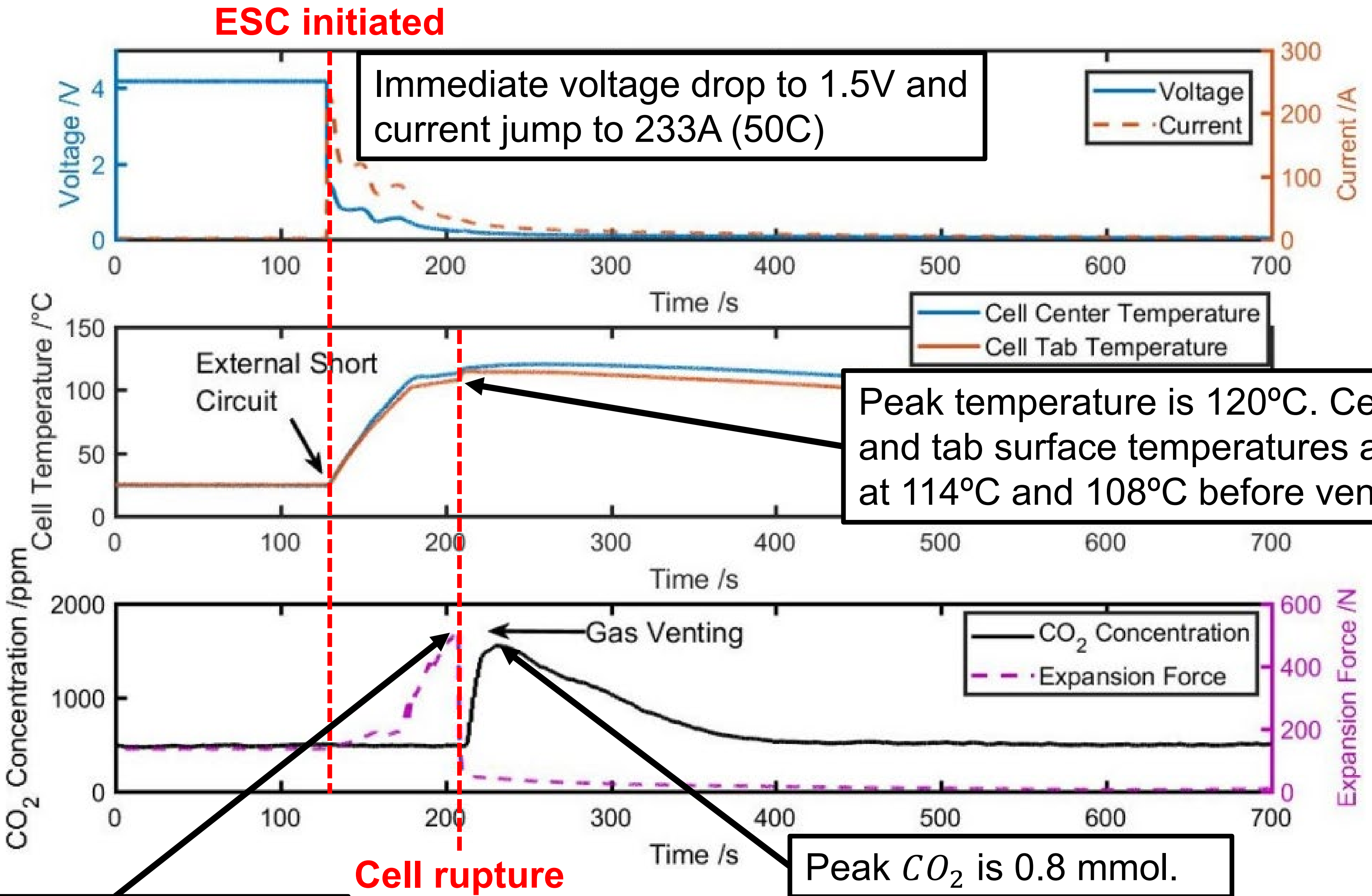
3. Connected the cell in series with a current shunt and open contactor ($R_{ext} = 6.7m\Omega$).



(Current, voltage, temperature, stress)

Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021.

Experiment: Cell electrical, thermal, and mechanical response to ESC



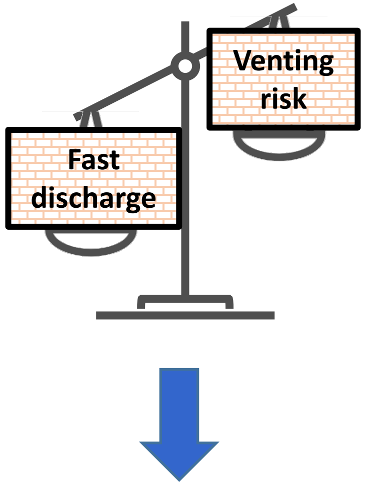
Immediate voltage drop to 1.5V and current jump to 233A (50C)

Peak temperature is 120ºC. Center and tab surface temperatures are at 114ºC and 108ºC before venting.

Peak CO_2 is 0.8 mmol.

P_{crit} is calculated from peak expansion of 517 N

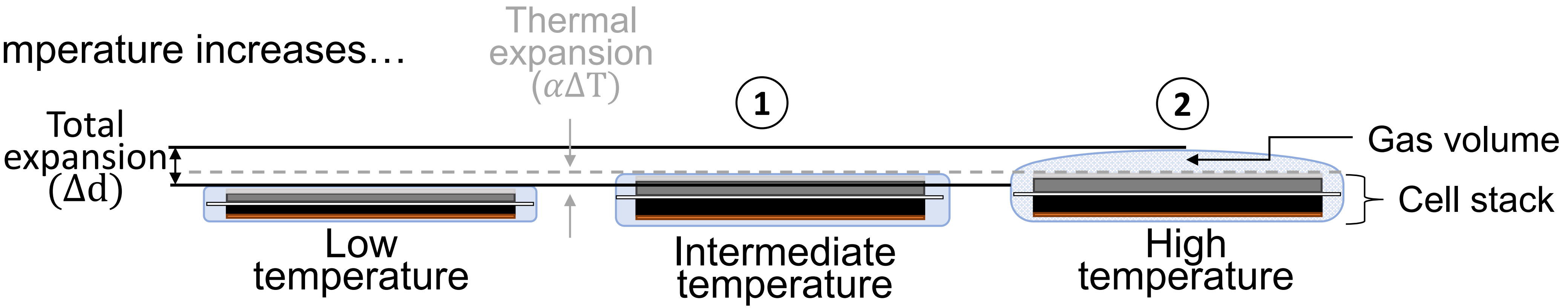
5-min ESC discharged a fully-charged cell to 42% SOC



Need to model and control venting

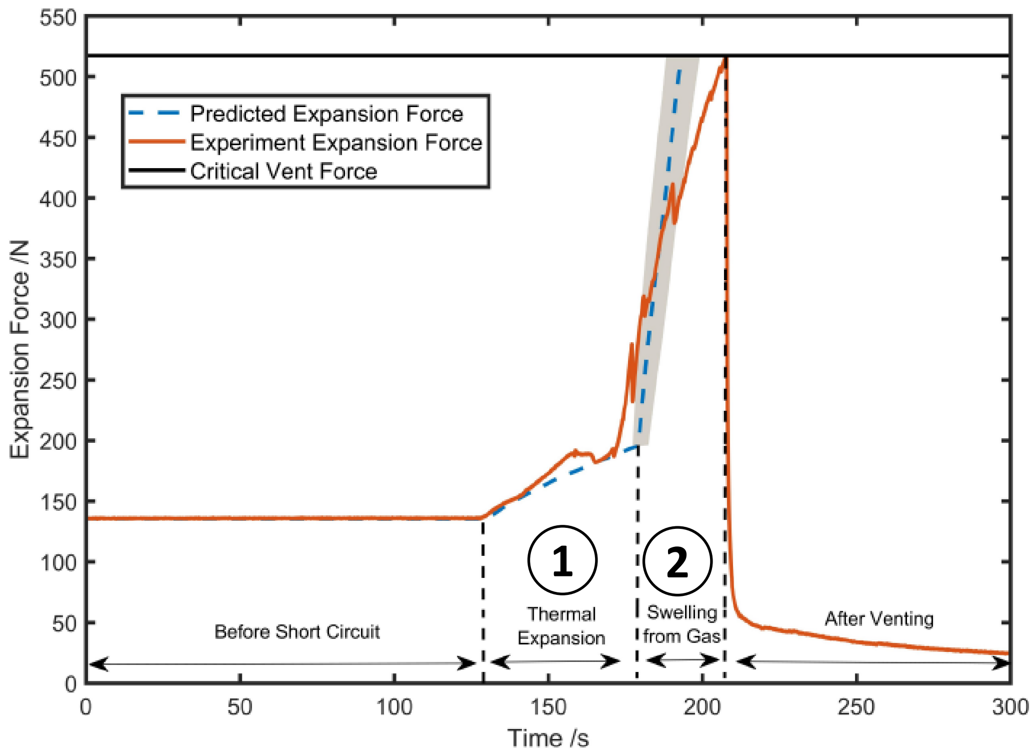
Overview of venting model

As the temperature increases…



2-staged expansion due to…

1. Thermal expansion of the active material
2. Cell swelling due to gas generation



Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021.

Modeling CO_2 gas generation from SEI decomposition

- At 80-120°C, the solid electrolyte interphase (SEI) decomposition can be described by

$$(CH_2OCO_2Li)_2 \rightarrow Li_2CO_3 + C_2H_4 + CO_2 + 0.5O_2$$

- Arrhenius reaction rate:

$$\dot{x}_{SEI} = -A_{SEI}x_{SEI}\exp\left(-\frac{E_{SEI}}{k_bT}\right)$$

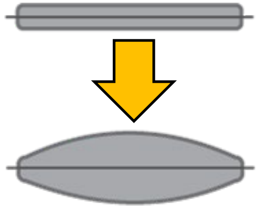
$$x_{SEI} = \frac{n(\text{Li in SEI})}{n_{C_6}}$$

- Amount of CO_2 gas generated:

$$n(CO_2) = \frac{m_{an}\left(x_{SEI,0} - x_{SEI}\right)}{2M_{C_6}}$$

Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021

Modeling cell internal pressure



Internal cell pressure:

$$P_{total} = P_{CO_2} + P_{sat}$$

$>$?

Critical venting pressure:

$$P_{crit} = \frac{F_{max}}{A_{surf}} + P_{atm}$$

Gas pressure from generated CO_2:

$$P_{CO_2} = \frac{n(CO_2)R\mathbf{T}}{V_h}$$

Electrolyte vapor saturation pressure:

$$P_{sat} = y_{EC}P_{sat,EC} + y_{DMC}P_{sat,DMC}$$

Amount of CO_2 from SEI decomposition model:

$$\dot{x}_{SEI} = -A_{SEI}x_{SEI}\exp\left(-\frac{E_{SEI}}{k_b\mathbf{T}}\right)$$

$$n(CO_2) = \frac{m_{an}(x_{SEI,0} - x_{SEI})}{2M_{C_6}}$$

Electrolyte component saturation pressure:

$$\log_{10}(P_{sat}) = c_1 - \frac{c_2}{\mathbf{T} + c_3}$$

Antoine coefficients

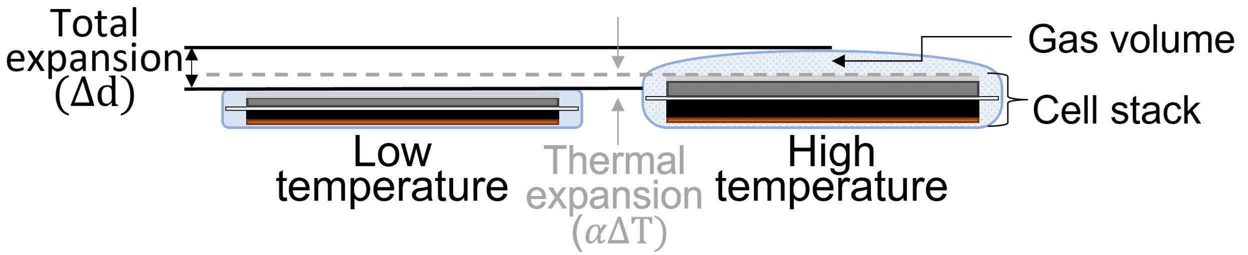
Component	c_1	c_2	c_3
DMC	6.3438	1413.0	-44.25
EC	6.4897	1836.6	-102.23

Cell head volume from expansion:

$$V_h = V_{h,0} + A_{surf}(\Delta d - \alpha_{cell}\mathbf{\Delta T})$$

$$\Delta d = \frac{L\Delta\sigma}{E}$$

$$\Delta\sigma = \max\left(P_{total} - \sigma_0 - P_{atm}, \frac{E\alpha_{cell}\mathbf{\Delta T}}{L}\right)$$



Cai, Ting, et al. "Modeling Li-ion Battery First Venting Events Before Thermal Runaway." Modeling, Estimation and Control Conference 2021

Thermal and electrical models

LUMPED THERMAL MODEL

Heat generation / Convection

$$m_{cell}C_{p,cell}\dot{T}_{cell} = \dot{Q}_{ohmic} + \dot{Q}_{SEI} - hA(T_{cell} - T_{amb})$$

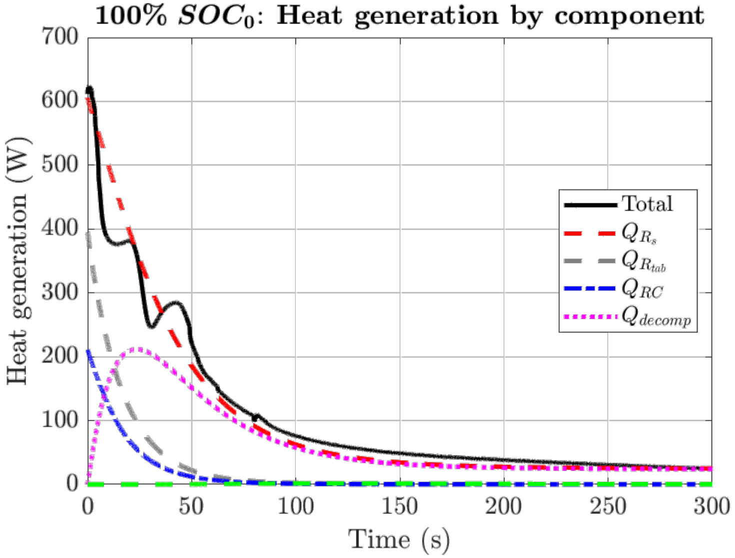
SEI decomposition heating:

~~$\dot{Q}_{SEI} = -m_{an}h_{SEI}\dot{x}_{SEI}$~~

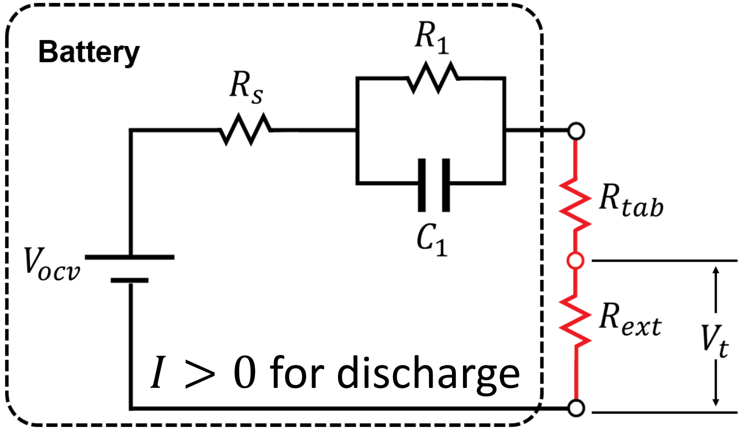
Ohmic heating:

$$\dot{Q}_{ohmic} = I(V_t - V_{OCV})$$

$$= I^2(R_{tab} + R_s) + IV_1$$



MODIFIED SINGLE RC EQUIVALENT CIRCUIT MODEL



$$I(t) = \frac{V_{OCV}(SOC) - V_1}{R_{ext} + R_{tab} + R_s}$$

$$V_t(t) = V_{OCV}(SOC) - V_1 - (R_s + R_{tab})I(t)$$

$$\dot{V}_1 = -\frac{1}{(\alpha\tilde{R}_1)(\beta\tilde{C}_1)}V_1 + \frac{1}{(\beta\tilde{C}_1)}I(t)$$

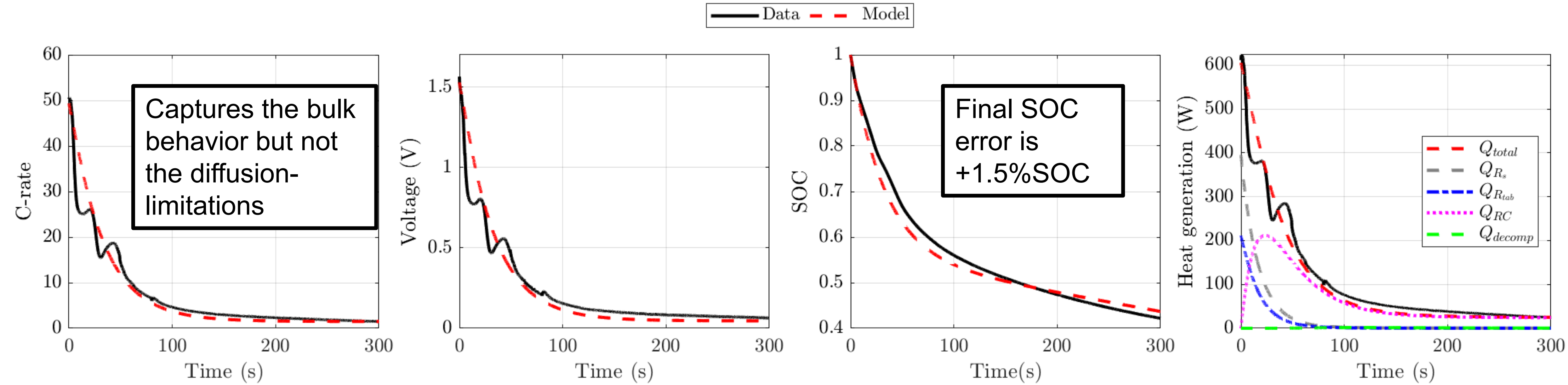
$$\dot{SOC} = -\frac{1}{Q}I(t)$$

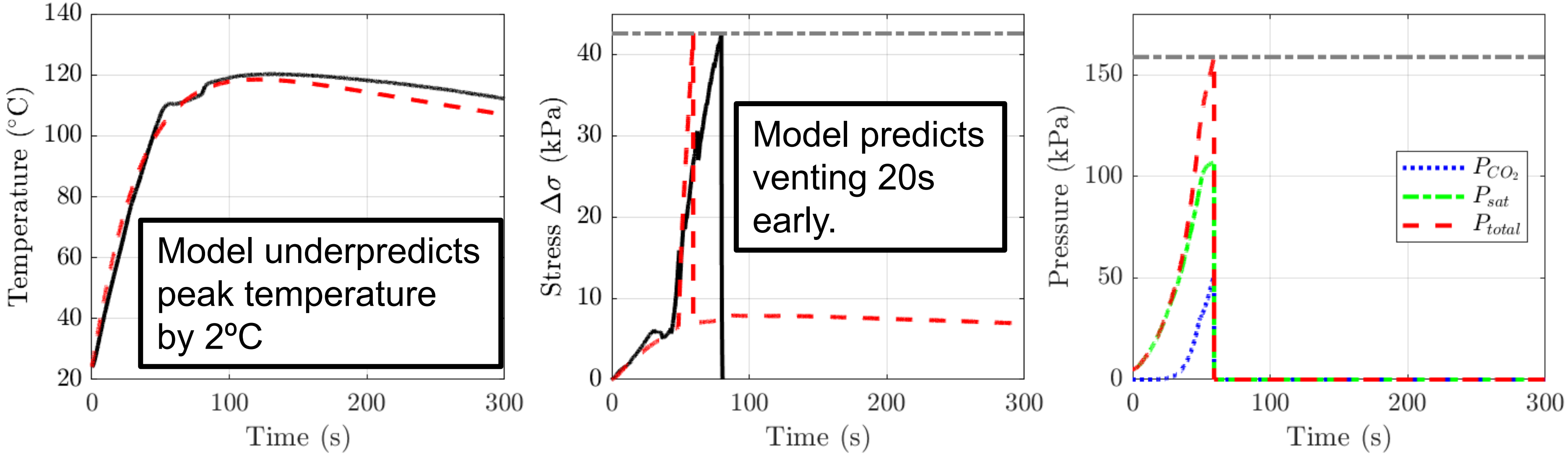
Tran, Vivian, et al. "Equivalent Circuit Model for High C-Rate Discharge with an External Short Circuit." *2022 American Control Conference (ACC)*. IEEE, 2022.

Hatchard, T. D., et al. "Thermal model of cylindrical and prismatic lithium-ion cells." *Journal of The Electrochemical Society* 148.7 (2001): A755.

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 device using an efficiency factor and arrhenius formulations," Journal of The Electrochemical Society, vol. 164, no. 4, pp. A587–A593, 2017.

Electro-thermo-mechanical model validation





- Captures main characteristics
- Should still be conservative with pressure constraint to avoid venting

MPC set up to "track" a safe and fully-discharged cell

$$J_N = \Delta x_N^T \bar{V}_N \Delta x_N + \sum_{k=0}^{N-1} \frac{u_k^T \bar{R} u_k}{||u_{max}||^2} + \left(\frac{\Delta x_k^T \bar{Q} \Delta x_k}{||x_{max}||^2} + \gamma_x s_k \right) + \left(\frac{\Delta y_k^T \bar{W} \Delta y_k}{||y_{max}||^2} + \gamma_y s_{y,k} \right)$$

Terminal cost

Input current

Deviation from nominal state

Deviation from nominal pressure

Variables from the models:	$u_k = \mathrm{I}$	$x_k = [SOC \quad V_1 \quad T_{cell} \quad x_{SEI}]^T$	$y_k = \mathrm{P}$
Reference representing a safe and fully-discharged cell:	–	$x_{ref} = [0 \quad 0 \quad T_{amb} \quad x_{SEI,0}]^T$	$y_{ref} = \mathrm{P}_0$
What is penalized:	u_k	$\Delta x_k = x_k - x_{ref}$	$\Delta y_k = y_k - y_{ref}$

MPC optimization problem

$$\min_{u,x,y,s,s_y} J_N = \Delta x_N^T \bar{V}_N \Delta x_N + \sum_{k=0}^{N-1} \frac{u_k^T \bar{R} u_k}{||u_{max}||^2} + \left(\frac{\Delta x_k^T \bar{Q} \Delta x_k}{||x_{max}||^2} + \gamma_x s_k\right) + \left(\frac{\Delta y_k^T \bar{W} \Delta y_k}{||y_{max}||^2} + \gamma_y s_{y,k}\right)$$

Terminal cost

Input current

Deviation from nominal state

Deviation from nominal pressure

subject to:

$x_{k+1} = f(x_k, u_k), \quad k = [0, N-1]$ Electrical, thermal, and SEI decomp. state equations

$y_k = f_2(x_k), \quad k = [1, N]$ Cell internal pressure equations

$I_{min} \leq I_k \leq I_{max}, \quad k = [0, N-1]$ Hard current input constraint (0-10C)

$T_{min} - s_k \leq T_k \leq T_{max} + s_k, \quad k = [1, N]$ Soft temperature state constraint

$P_{min} - s_{y,k} \leq P_k \leq P_{max} + s_{y,k}, \quad k = [0, N-1]$ Soft pressure output constraint

$s_k > 0, \quad k = [1, N]$

$s_{y,k} > 0, \quad k = [1, N]$

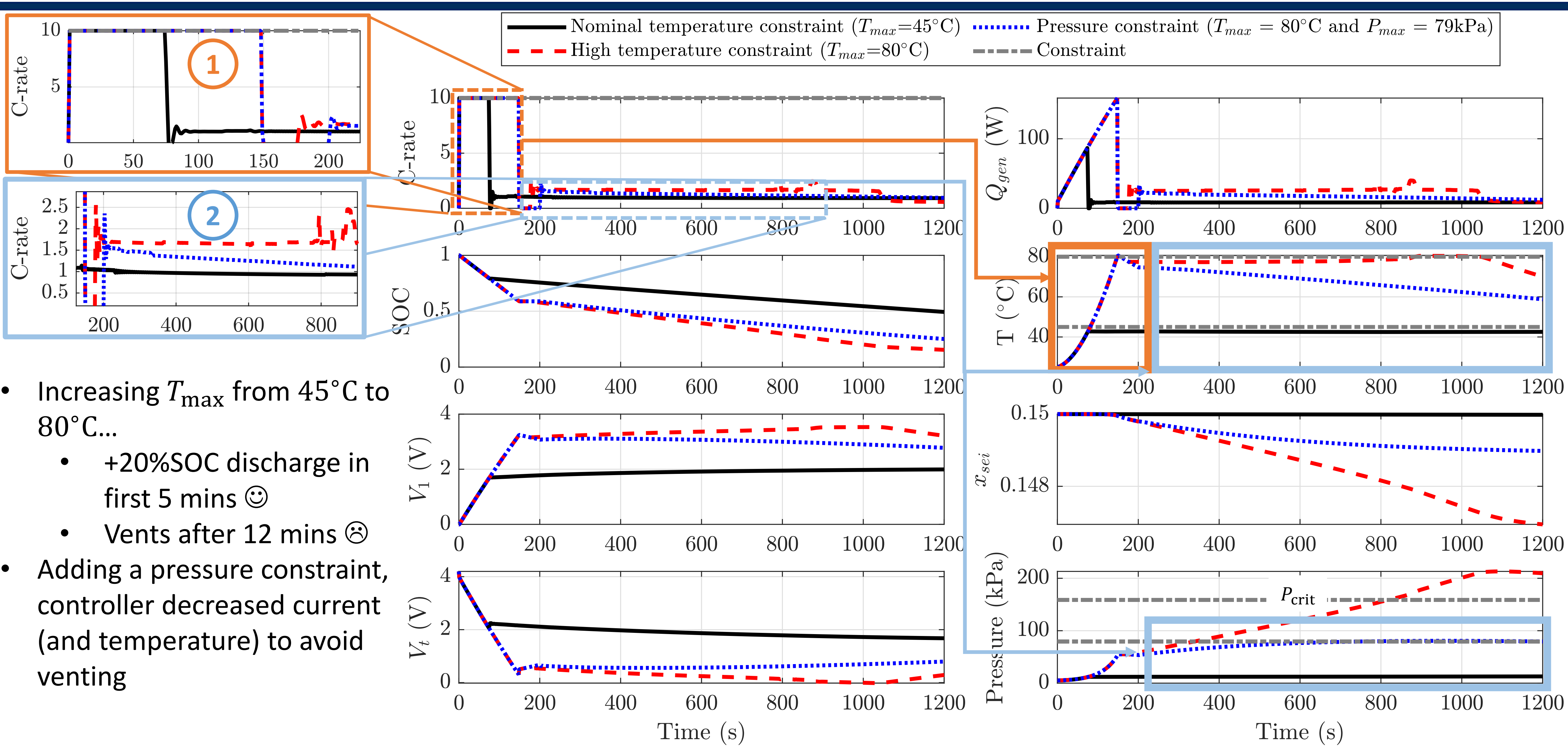
Positive slack constraints

Solved using SQP with $N = 90$ and $\Delta t = 1s$.

Simulations for a 20-minute discharge under 3 scenarios

Scenarios	T_{max} (°C)	P_{max} (kPa)
1. Nominal	45	—
2. High temperature constraint	80	—
3. High temperature and pressure constraints	80	79 $\left(\frac{1}{2}P_{\text{crit}}\right)$

20-minute fast discharge simulation



- Increasing T_{max} from 45°C to 80°C…
  - +20%SOC discharge in first 5 mins ☺
  - Vents after 12 mins ☹
- Adding a pressure constraint, controller decreased current (and temperature) to avoid venting

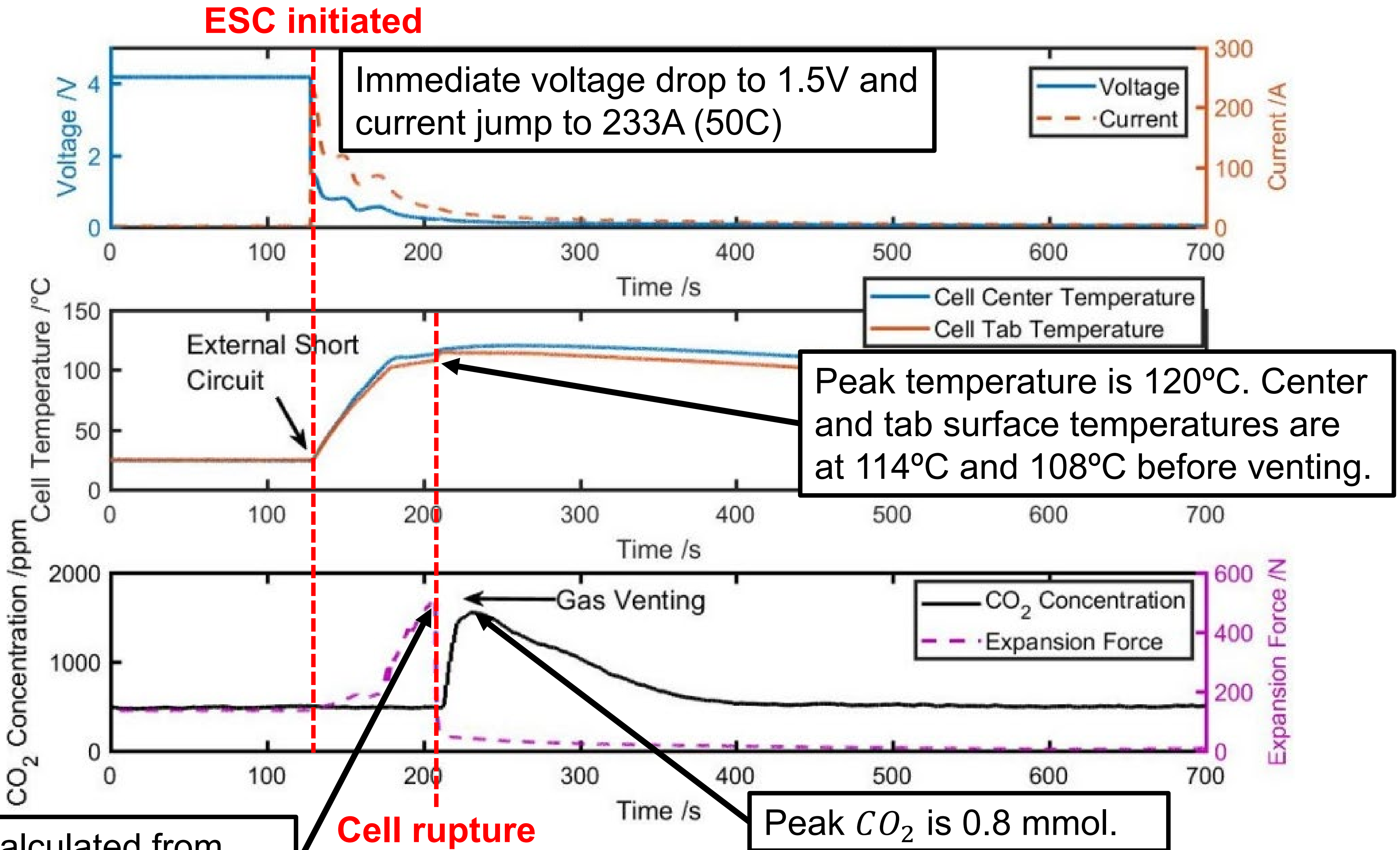
Conclusions

- A 4-state, electro-thermo-mechanical model captured the behavior of a cell undergoing an ESC.
- From the 3 discharge scenarios, we showed that
  1. Raising the maximum temperature from 45°C to 80°C allowed the controller to discharge the cell an extra 20%SOC in the first 5 minutes but allowed the cell to vent.
  2. When x_{SEI} and pressure are penalized and pressure is constrained, venting was prevented at the expense of 2%SOC in the first 5 minutes of discharge.
- Future work:
  - Improve the model to **predict the diffusion-limited discharge behavior** in the plant model
  - Incorporate **parameter estimation** and **adaptive control** strategies to handle model mismatch

Thank you for listening!

Questions?

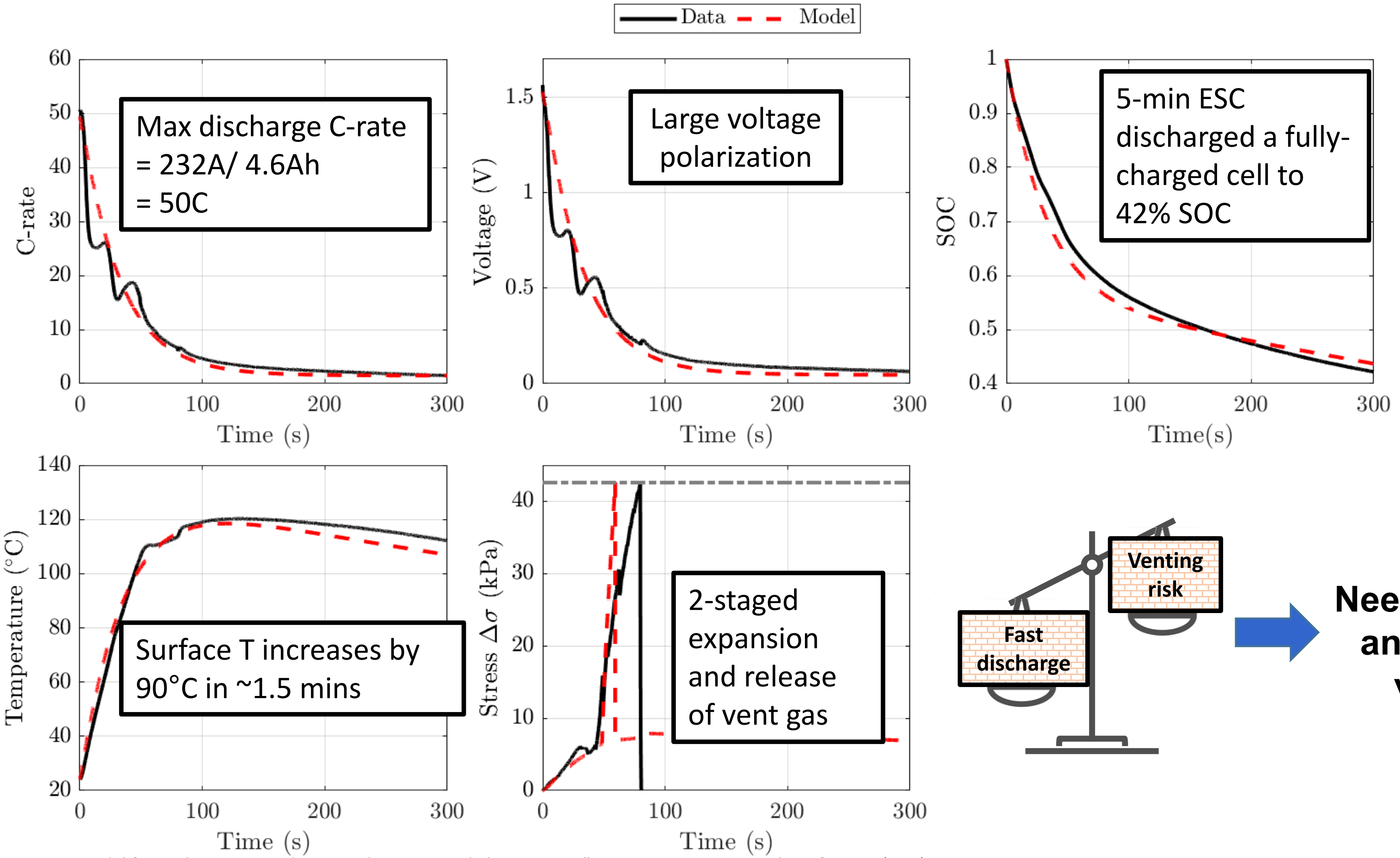
Experiment: Cell electrical, thermal, and mechanical response to ESC



P_{crit} is calculated from peak expansion of 517 N

Peak CO_2 is 0.8 mmol.

Capturing external short circuit (ESC) behavior with a simple model



Need to model and control venting

Tran, Vivian, et al. "Equivalent Circuit Model for High C-Rate Discharge with an External Short Circuit." *2022 American Control Conference (ACC)*. IEEE, 2022.

Summary stats

Summary metrics	Scenario		
	N	HT	HTP
5-min SOC	0.73	0.53	0.55
20-min SOC	0.49	0.25	0.15
Vented?	No	Yes	No