OpenFOAMを用いた
リチウムイオン電池の解析事例

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東京大学本郷キャンパス

0. About Us

- Science Solutions DIvision ,
  Mizuho Information and Research Institute Inc.

  - Computer Aided Engineering consultation in wide fields over 30 years
    - ・fluid dynamics ・structural analysis ・energy technology ・fuel cells
    - ・electronics ・nano-technology ・biomolecular simulations

  - Use of OpenFOAM for 3 years
    - ・aero dynamics around vehicles
    - ・VOF simulations
    - ・gas diffusion / mixing
    - ・...etc

Contents

1. Introduction

- Objective: modeling of Lithium ion Cell in OpenFOAM

Prismatic cell

Cylindrical cell

K.-J. Lee*, G.-H. Kim, K. Smith
NREL/PR-5400-49795

- Due to large energy content, Lithium ion cells are used in many products
- Heat management is very important for safety issues

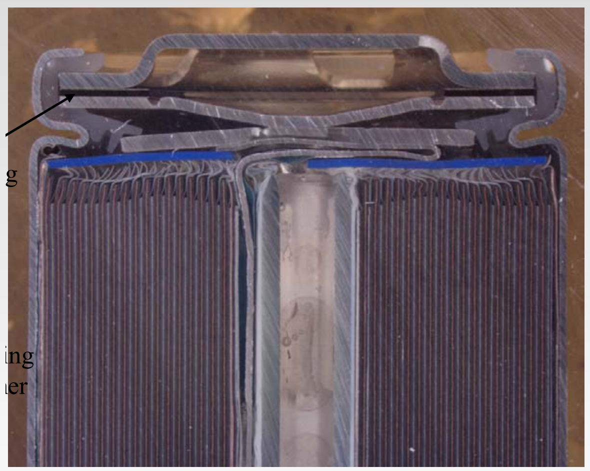
  under abused conditions, thermal run-away takes place

abuse: over-charging, neil penetration, crush, short → Lithium plating, decomposition, internal short, excessive reaction → **thermal run-away** → smoke, leak, flame

1. Introduction

■ structure and modeling approaches of Lithium-ion cell

• Cell level



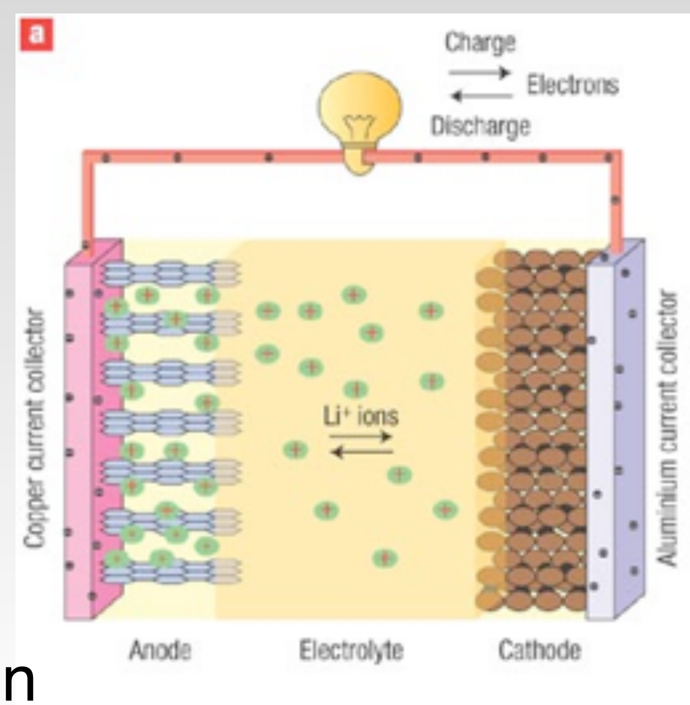
Moli ICR-18650J

- macro scale
- current and heat distributions
  (+ electrochemistry)
- continuum approximation

E. C. Darcy, NREL/PR-540-45388
G.-H. Kim and K. Smith, NREL/PR-540-46076

• Electrode level

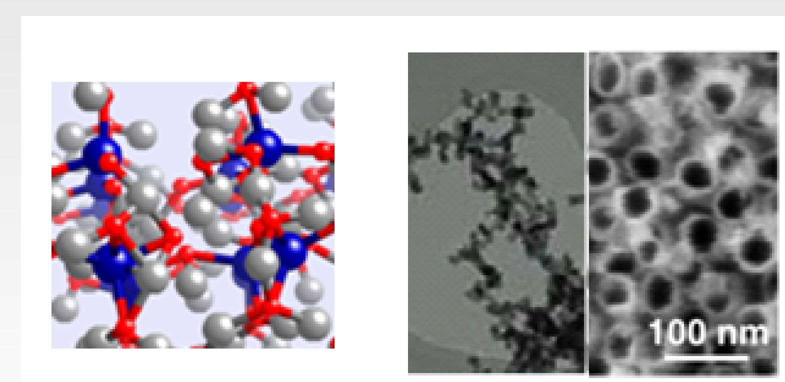
- mili-to-micro scale
- electrochemical
  reactions
- continuum approximation



B. Scrosati, Nature Nanotechnology 2, 598 - 599 (2007)

• Nano level

- micro-to-nano scale
- molecular dynamics



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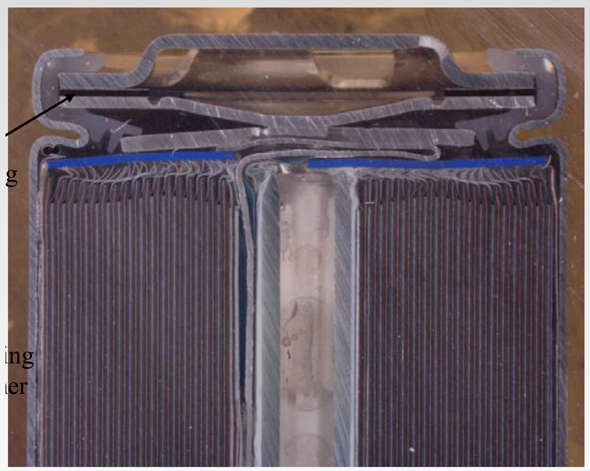
NREL/PR-5400-49795

1. Introduction

■ structure and modeling of Lithium-ion cell

our work

● Cell level



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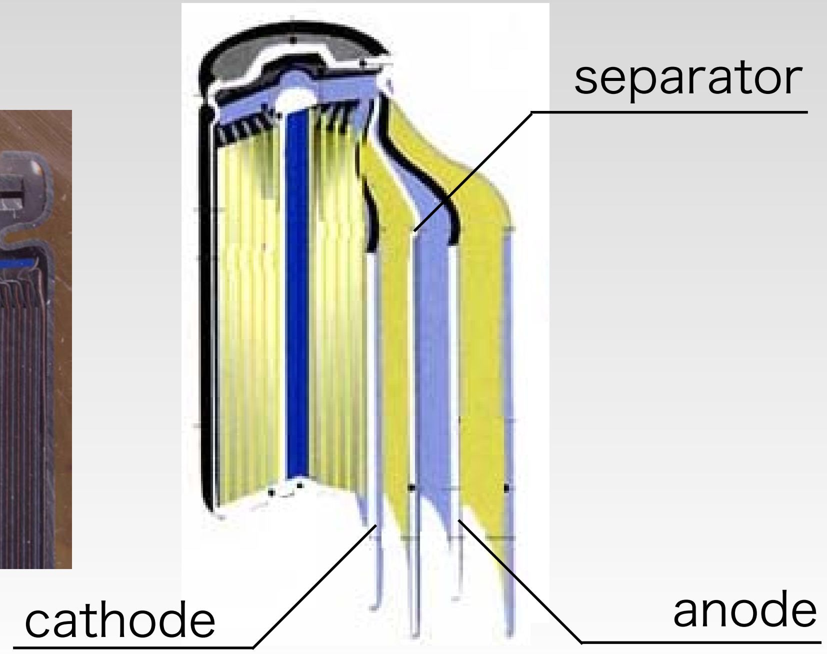

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● Electrode level

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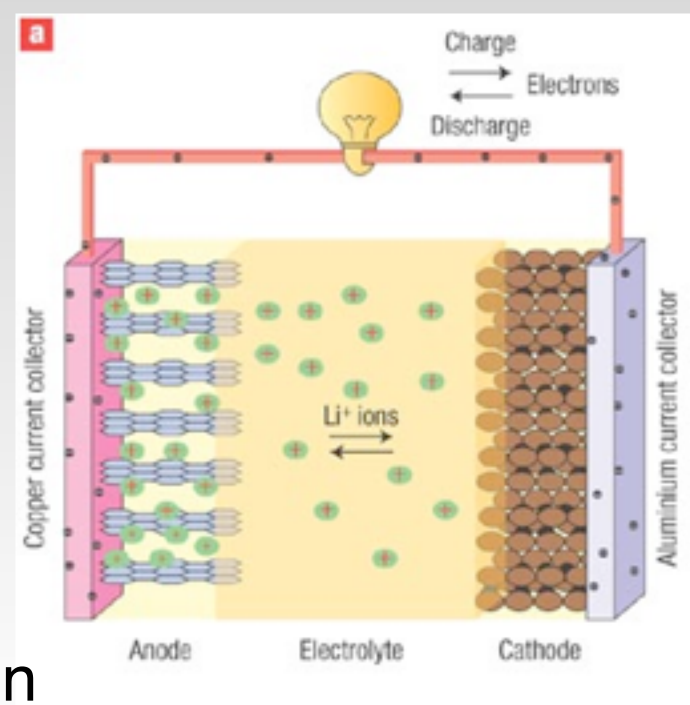

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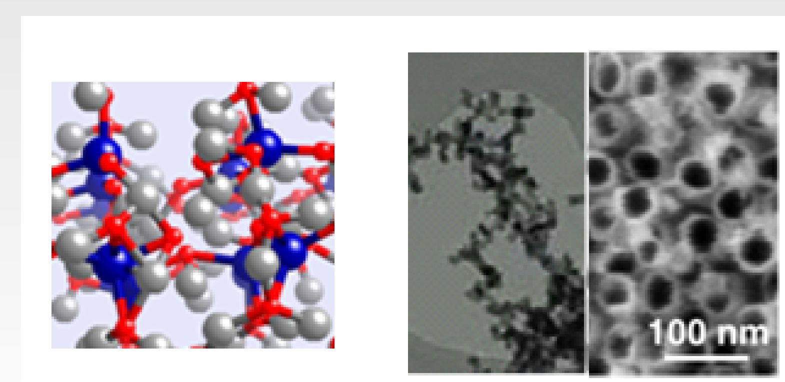
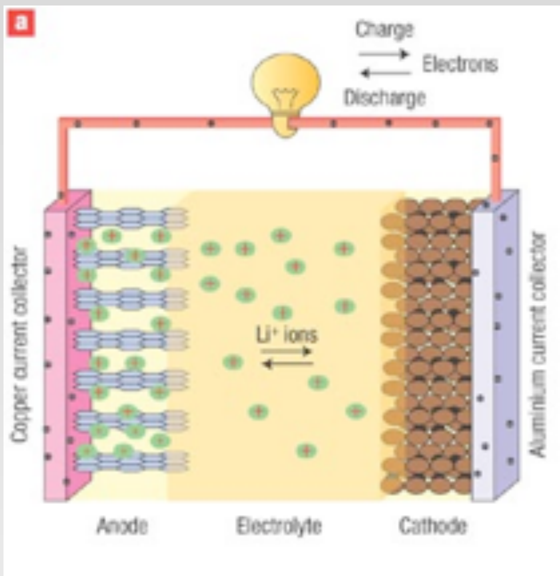


K.-J. Lee*, G.-H. Kim, K. Smith
NREL/PR-5400-49795

2. Cell-level (macro) Modeling of Lithium-ion Cell

■ macroscopic modeling

electrodes and electrolytes, electrochemical reactions	(continuum) resistors and capacitors



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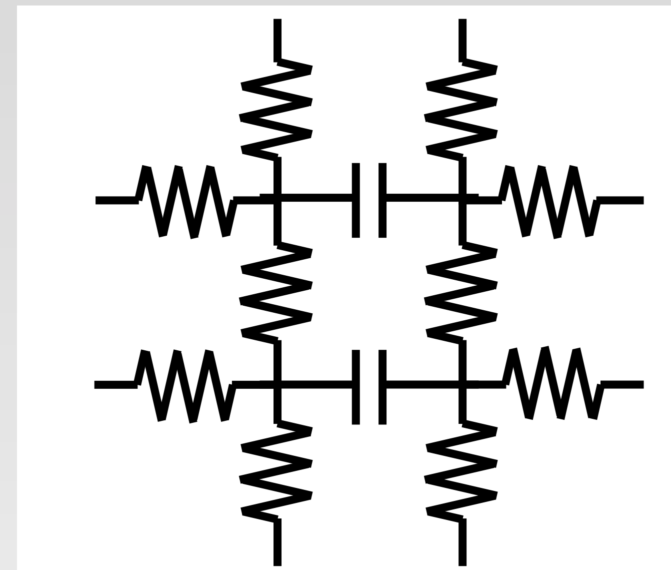
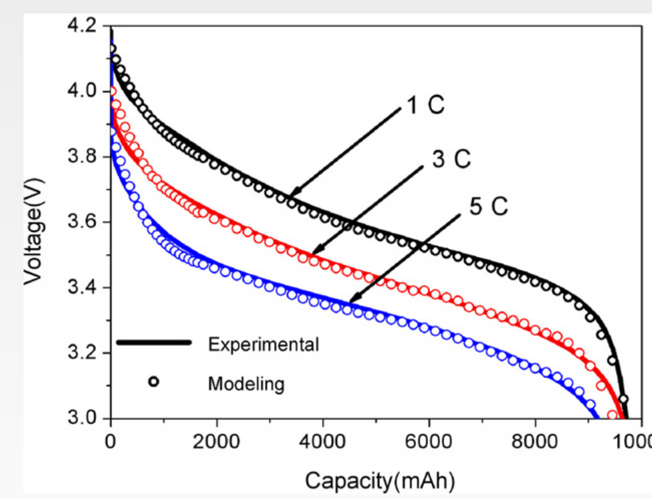


ΔV

- only electric potential V and temperature T are solved
- electrochemical reactions are not considered
- in this model, cell (capacitor) has zero-thickness
- capacitor has surface resistivity



U.S.Kim, C.B.Shin, C.S.Kim, J.Power.Sources 180 (2008) 909-916

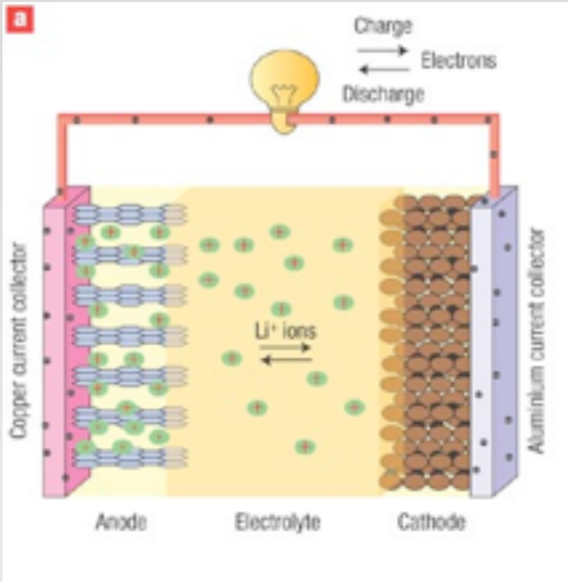
cell characteristics are represented by $\Delta V(j, Q)$

input data

2. Cell-level (macro) Modeling of Lithium-ion Cell

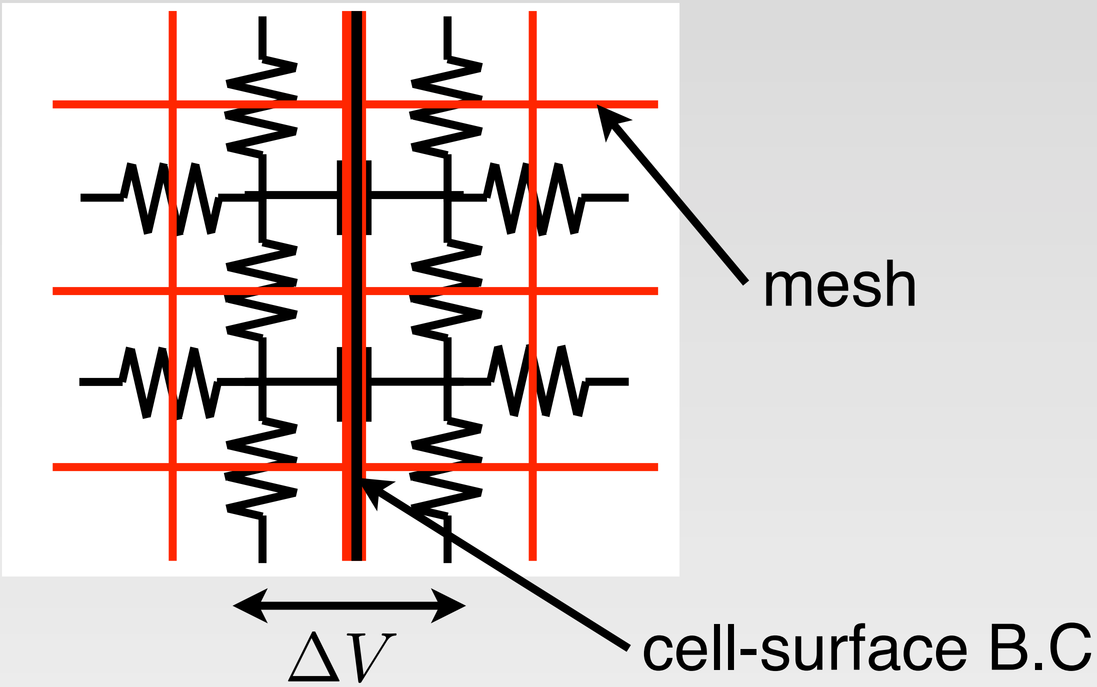
■ macroscopic modeling

electrodes and electrolytes,
electrochemical reactions



Bruno Scrosati, Nature Nanotechnology 2, 598 - 599 (2007)

(continuum)
resistors and capacitors



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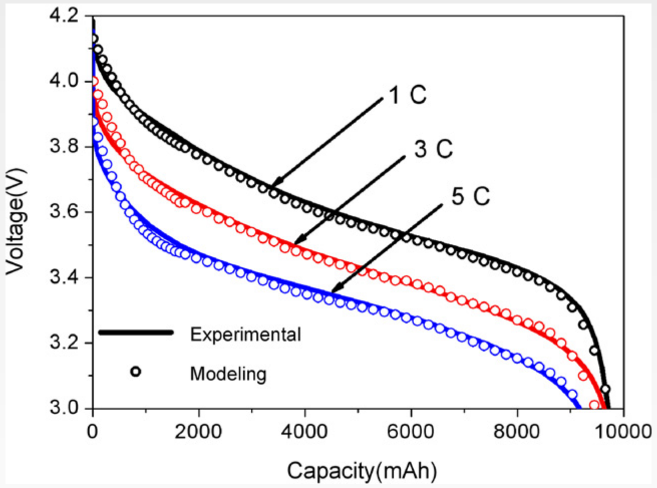

U.S.Kim, C.B.Shin, C.S.Kim,
J.Power.Sources 180 (2008) 909-916

cell characteristics are represented by $\Delta V(j, Q)$

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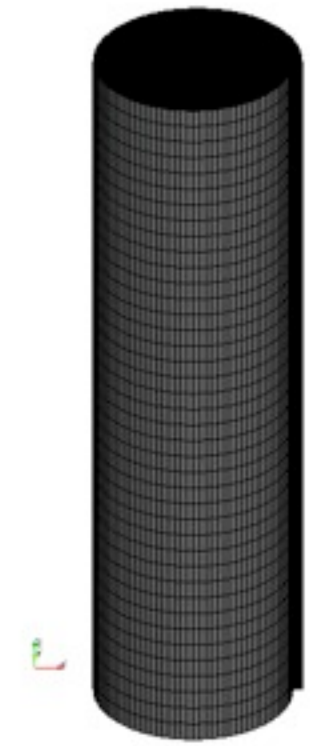
2. Cell-level (macro) Modeling of Lithium-ion Cell

- Basic procedure

G.-H. Kim and K. Smith,
NREL/PR-540-46076



- Laplace equation is solved with “cell-surface” boundary conditions

$$\triangle(\sigma V) = 0$$

- Current distribution is determined by $\mathbf{j} = \sigma \nabla V$

- Update charge on “Cell-surface” by $\Delta Q = \mathbf{j} \cdot \mathbf{n} \Delta t$

- Heat diffusion equation is solved with Joule heating

$$\rho c_p \frac{dT}{dt} = \triangle(kT) + \sigma |V|^2$$

time loop

2. Cell-level (macro) Modeling of Lithium-ion Cell

- implementation of "Cell-surface" boundary condition

・basically, capacitor gives "jump" of electric potential $\Delta V(j,Q)$ $j \equiv \mathbf{j} \cdot \mathbf{n}$

⟶ jumpCyclic boundary condition with $\Delta V(j,Q)$?

- following explicit scheme does not work!

$$\Delta V(j^n, Q^n) \xrightarrow{\triangle(\sigma V)=0} V^{n+1}$$

$$\longrightarrow \begin{cases} j^{n+1} &= \sigma \nabla V \cdot \mathrm{n} \\ Q^{n+1} &= Q^n + j^{n+1}\Delta t \end{cases}$$

n : time step

・in real cells, function $\Delta V(j,Q)$ is non-linear,

determined by experiments or electrochemical simulations

⟶ solution deviates from given $\Delta V(j,Q)$ curve in a few time-steps

2. Cell-level (macro) Modeling of Lithium-ion Cell

• iterative scheme

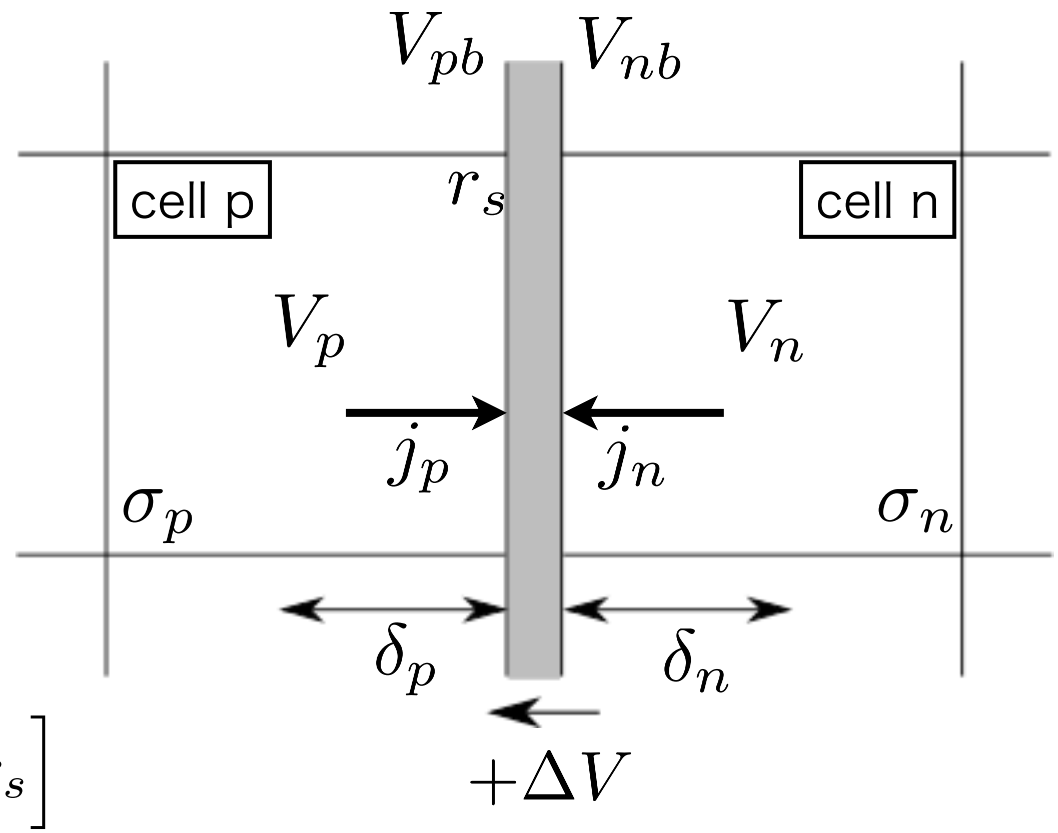
continuity: $j_p = -j_n = j$

definition of jump:

$\star\ j[\mathrm{A/m^2}]$
$r_s[\Omega \cdot m^2]$

$$V_{pb} = V_{nb} + \Delta V(j, Q) + \underline{j r_s}$$

surface resistivity



・solve j and Q implicitly, simultaneously with V

$$j_{k+1}^{n+1} = \tilde{\sigma}\left[V_{p,k+1}^{n+1} - V_{n,k+1}^{n+1} - \underline{\Delta V(j_{k+1}^{n+1}, Q_{k+1}^{n+1})} - j_{k+1}^{n+1} r_s\right]$$

invert →

$$j_{k+1}^{n+1} = \beta\left[V_{p,k+1}^{n+1} - V_{n,k+1}^{n+1} - \Delta V(j_k^{n+1}, Q_k^{n+1}) + \left(\frac{\partial \Delta V}{\partial j} + \frac{\partial \Delta V}{\partial q}\Delta t\right) j_k^{n+1}\right]$$

matrix coefficients   extra source terms

→gradientInternalCoeffs, gradientBoundaryCoeffs, updateInterfaceMatrix, based on cyclicFvPatchField

$$\tilde{\sigma} \equiv \frac{\frac{\sigma_p \sigma_n}{\delta_p \delta_n}}{\frac{\sigma_p}{\delta_p} + \frac{\sigma_n}{\delta_n}} \qquad \beta \equiv \frac{\tilde{\sigma}}{1 + \tilde{\sigma}\left(\frac{\partial \Delta V}{\partial j} + \frac{\partial \Delta V}{\partial q}\Delta t + r_s\right)}$$

・introduce sub-cycle k with under-relaxation

$$V^n, j^n, Q^n = V_0^{n+1}, j_0^{n+1}, Q_0^{n+1} \xrightarrow{\text{relax}} \cdots\cdots$$

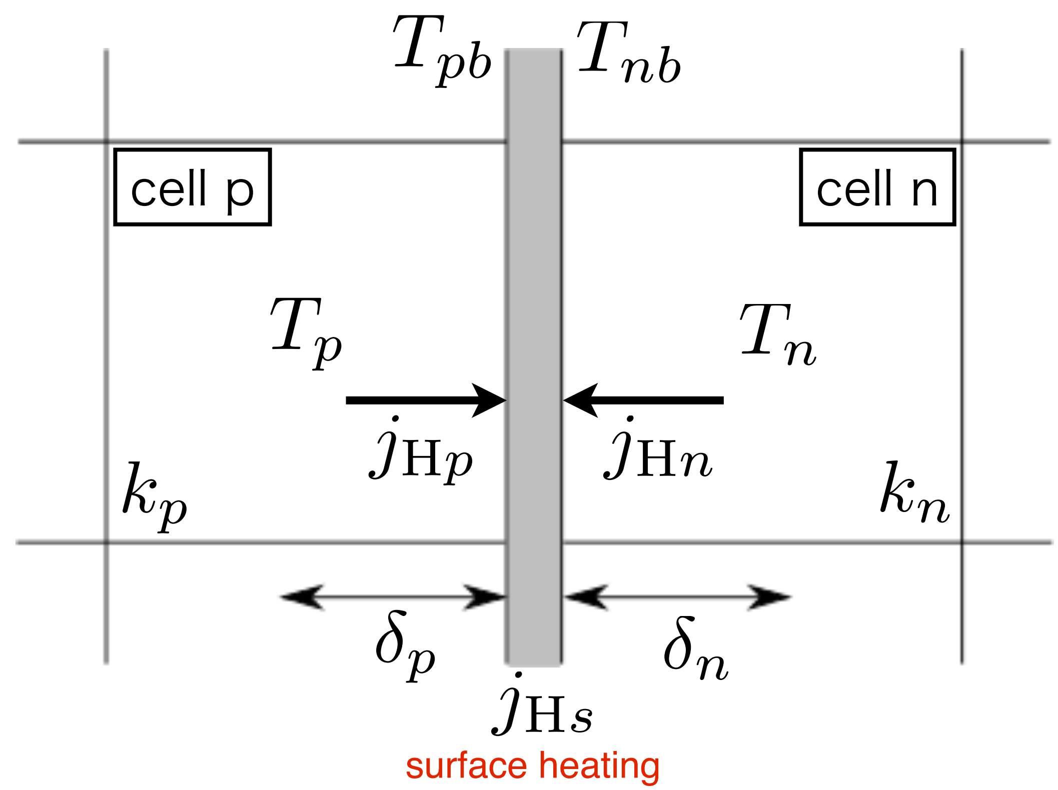
$$\sum |V_{k+1}^{n+1} - V_k^{n+1}| < \epsilon$$

$$\cdots\cdots \xrightarrow{\text{relax}} V_k^{n+1}, j_k^{n+1}, Q_k^{n+1} \xrightarrow{\text{relax}} V_{k+1}^{n+1}, j_{k+1}^{n+1}, Q_{k+1}^{n+1} = V^{n+1}, j^{n+1}, Q^{n+1}$$

convergence

2. Cell-level (macro) Modeling of Lithium-ion Cell

- heat transfer with surface heating at cell



continuity: $j_{Hs} + j_{Hp} + j_{Hn} = 0$

surface heating: $j_{Hs} = j^2 r_s$

•evaluation of thermal current

$$j_{Hp} = \tilde{k}\left[T_p - T_n - \frac{\delta_n}{k_n} j_{Hs}\right]$$

$$j_{Hn} = \tilde{k}\left[T_n - T_p - \frac{\delta_p}{k_p} j_{Hs}\right]$$

$$\tilde{k} \equiv \frac{\frac{k_p k_n}{\delta_p \delta_n}}{\frac{k_p}{\delta_p} + \frac{k_n}{\delta_n}}$$

matrix coefficients

extra source terms

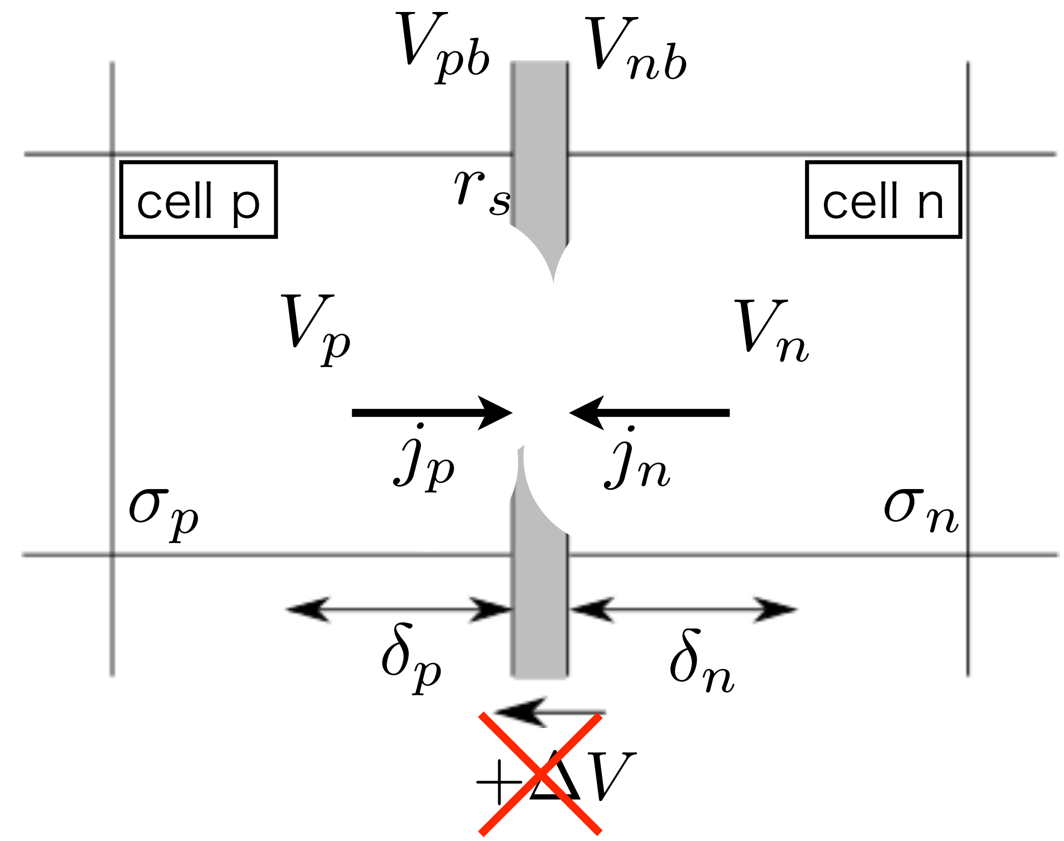
2. Cell-level (macro) Modeling of Lithium-ion Cell

- modeling internal short circuit

  - if internal short circuit takes place, current can flow freely through cell-surface

    ↓

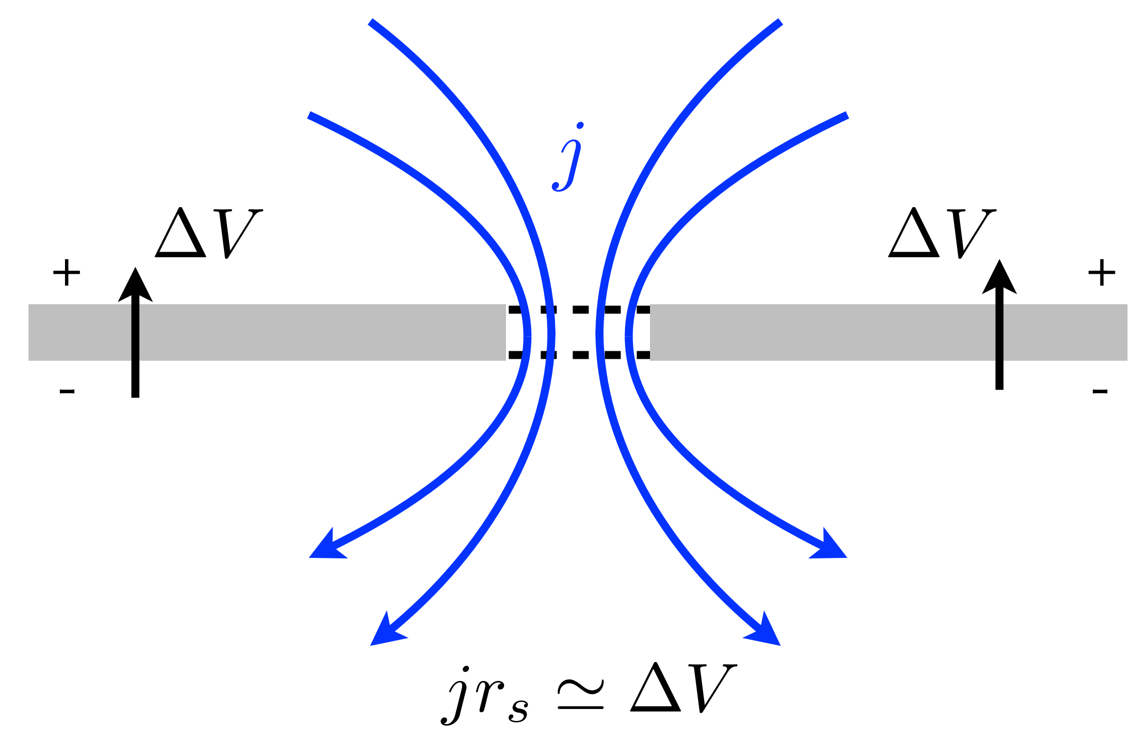
    short circuit can be modeled by simply “turning-off” potential jump



  - at the short circuit, large current is required to compensate potential jump

  - cell surface resistivity r_s

    → highly concentrated Joule heating from short current

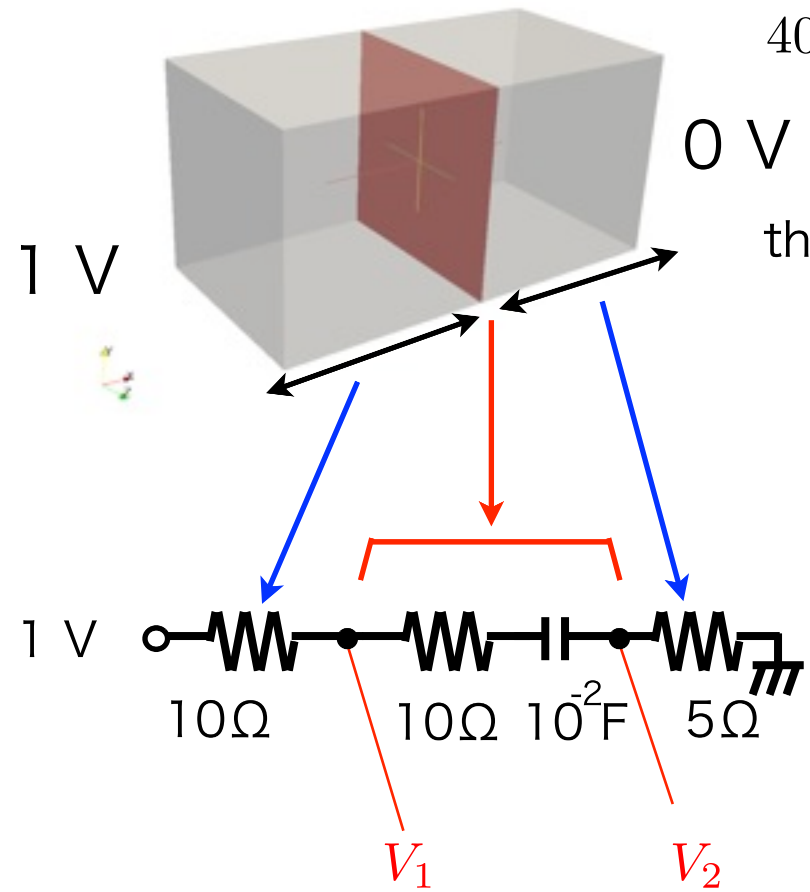


3. Basic validations

▪simple capacitor

$\sigma = 1[\mathrm{A/Vm}]$ $\sigma = 2[\mathrm{A/Vm}]$ $0.2[\mathrm{m}] \times 0.1[\mathrm{m}] \times 0.1\mathrm{m}]$

$40 \times 20 \times 20$ cells



the other B.C.: zeroGradient

- analytically,

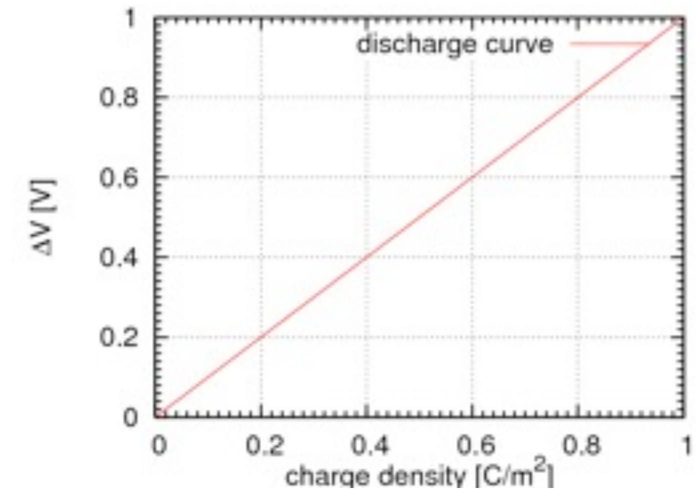
$$I = 0.04e^{-\frac{t}{0.25}}$$

$$Q = 0.01\left(1 - e^{-\frac{t}{0.25}}\right)$$

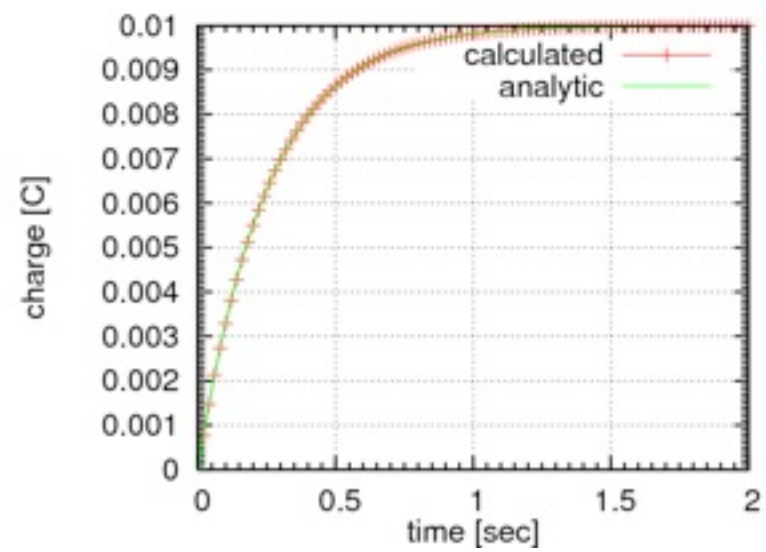
$$V_1 = 1 - 0.4e^{-\frac{t}{0.25}}$$

$$V_2 = 0.2e^{-\frac{t}{0.25}}$$

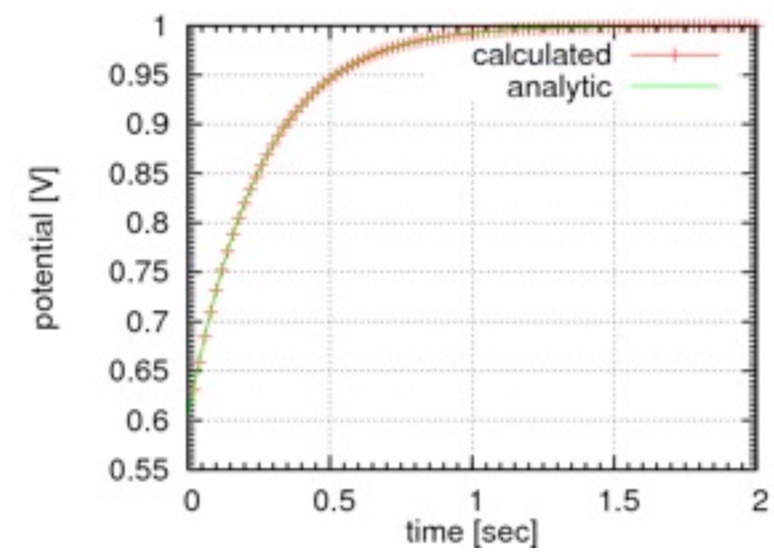
- input discharge curve



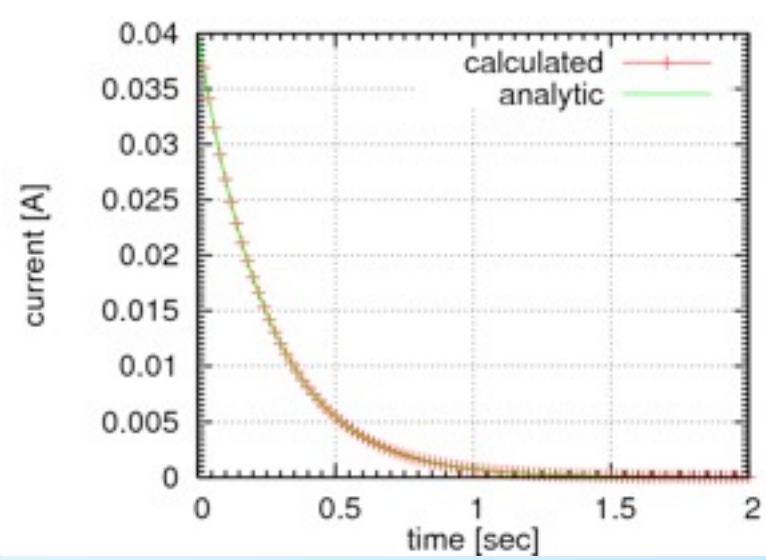
- total charge



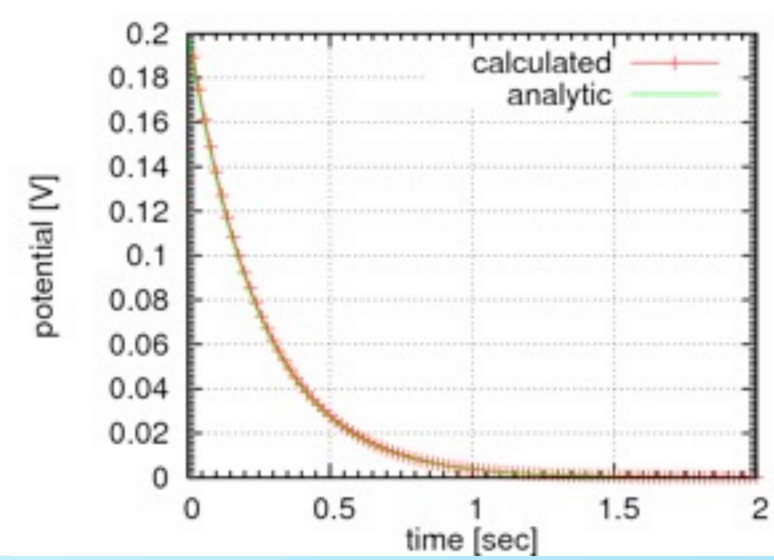
- potential V_1



- total current



- potential V_2



3. Basic validations

■1-layer flat cell

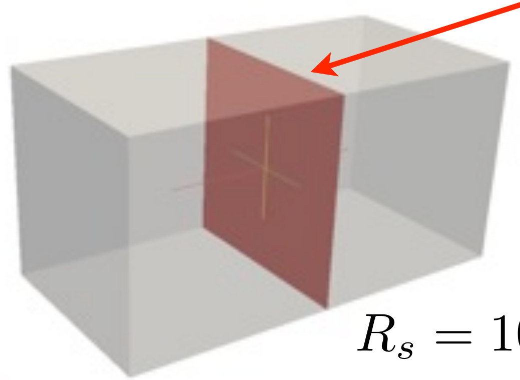
- input discharge curve

$\sigma = 10^5 [\mathrm{A/Vm^2}]$

4.2V

↓

3.0V
(2000sec)



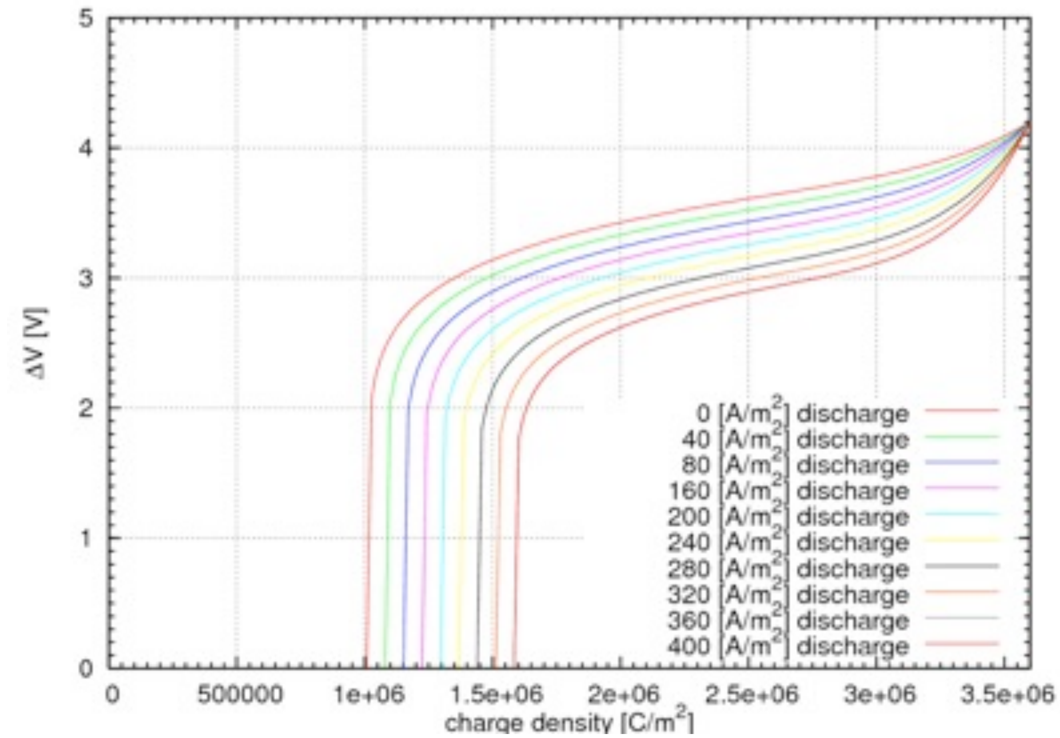
0 V

$\sigma = 2 \times 10^5 [\mathrm{A/Vm^2}]$

$R_s = 10^{-4} [\Omega]$

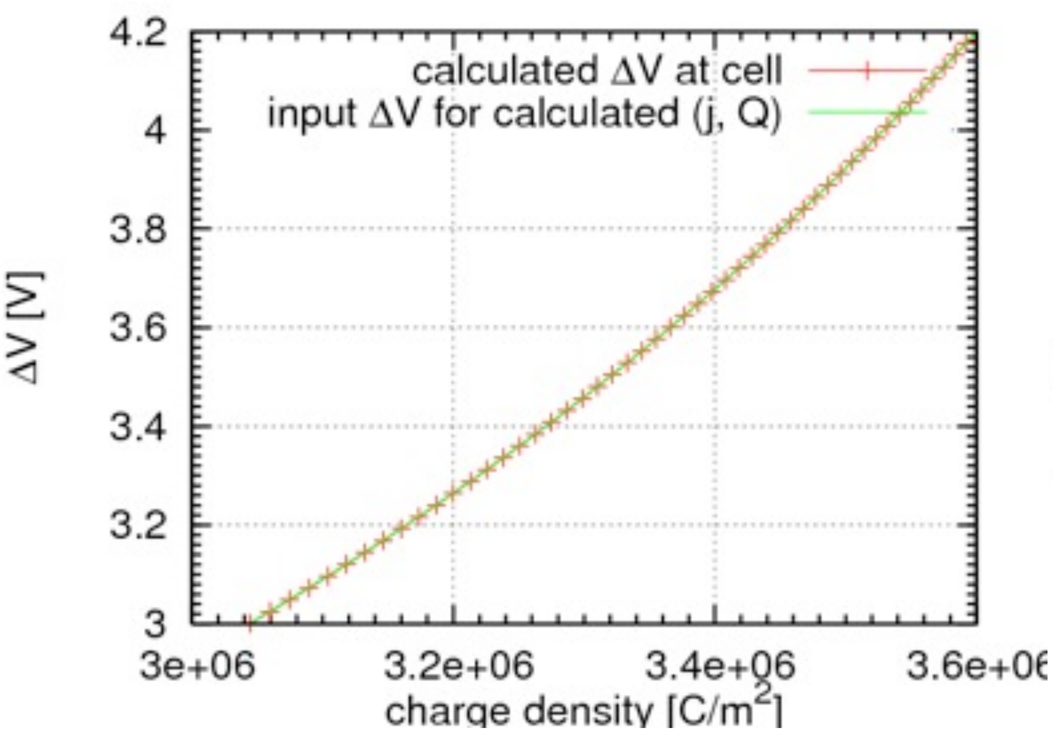
$q = 3.6 \times 10^6 [\mathrm{C/m^2}]$

total: $10 [\mathrm{Ah}]$

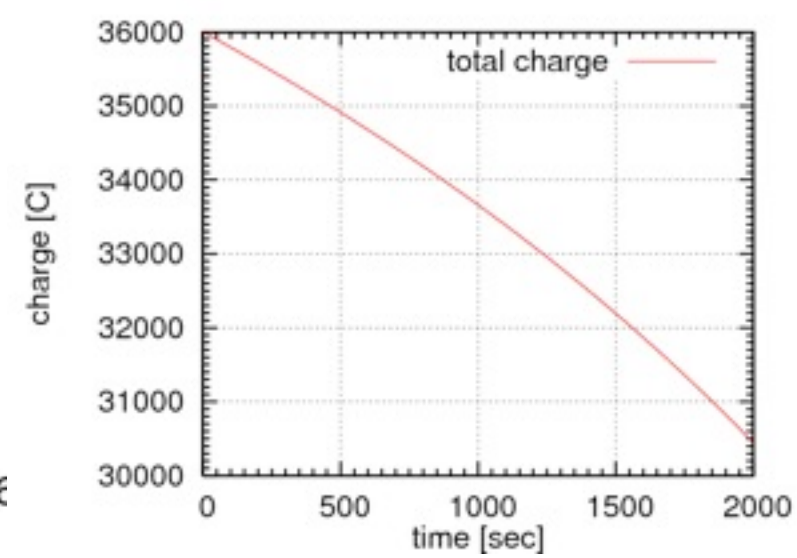


*imaginary cell: this discharge curve was artificially produced for test calculation, mimicking real cell discharge curve

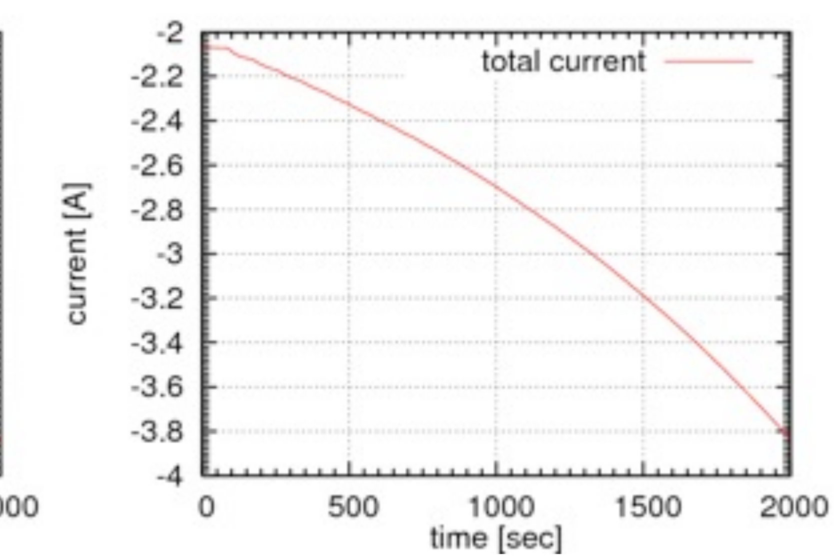
- $V_{pb} - V_{nb} - jr_s$ .vs. $\Delta V(j, Q)$



- total charge



- total current



input discharge curve is followed correctly!

3. Basic validations

■1-layer flat cell (broken cell)

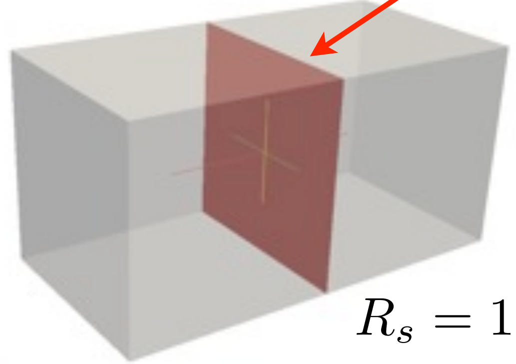
$\sigma = 10^5[\mathrm{A/Vm^2}]$

4.2V

↓

3.0V

(2000sec)



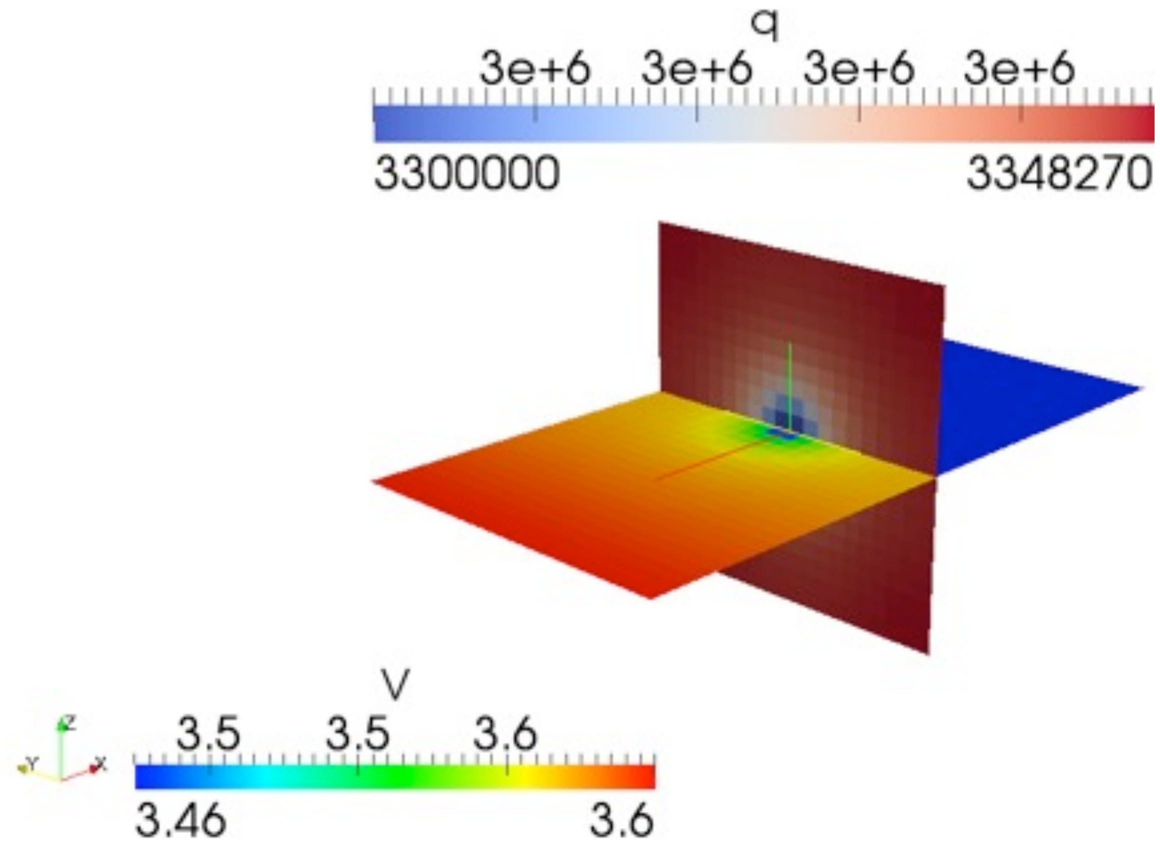
discharge curve:
same as previous result

0 V

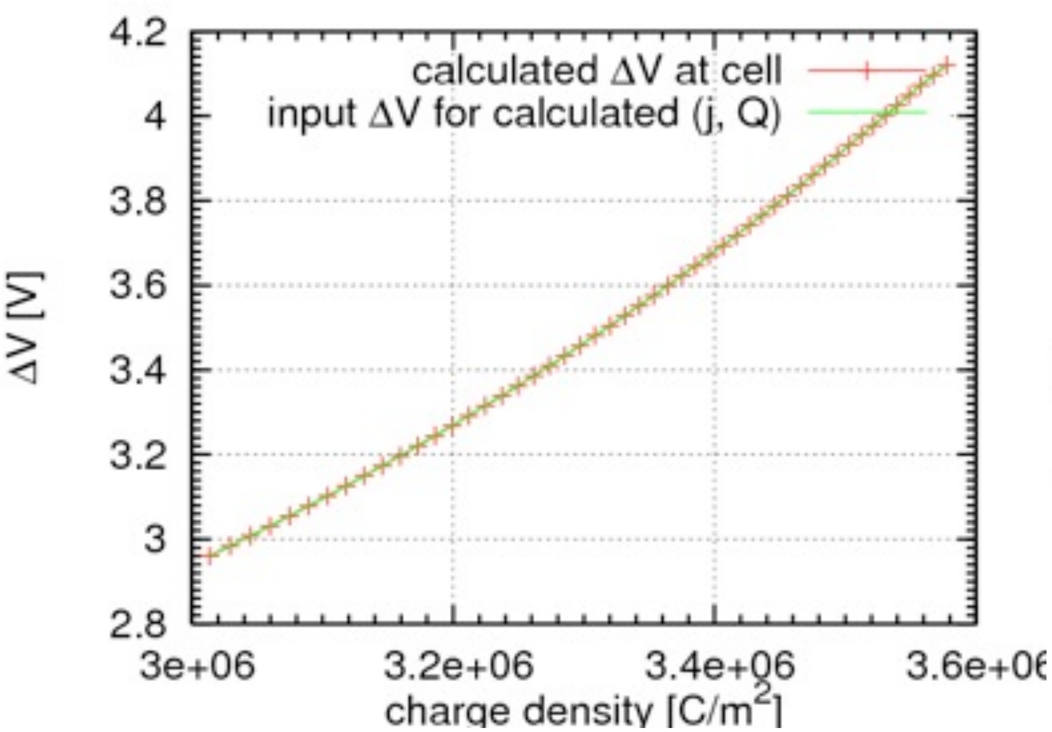
$\sigma = 2 \times 10^5[\mathrm{A/Vm^2}]$

$R_s = 10^{-4}[\Omega]$

●1[mm] x 1[mm] short circuit at center of cell

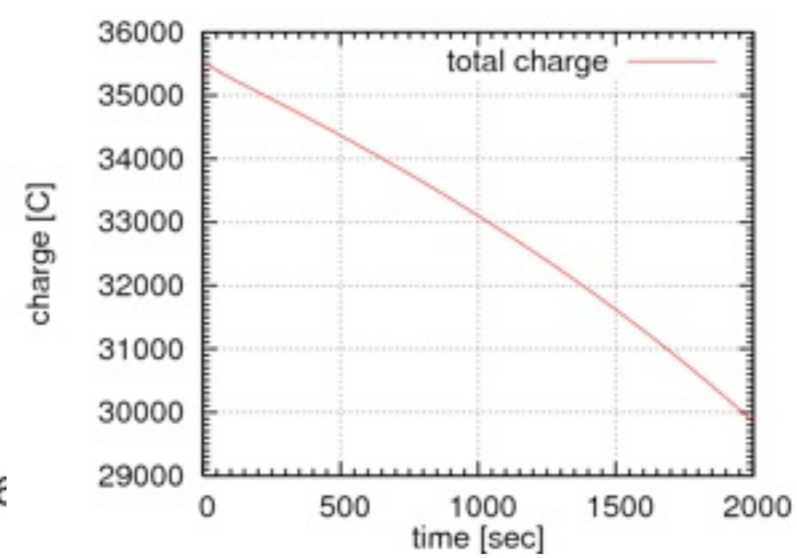


- $V_{pb} - V_{nb} - jr_s$ .vs. $\Delta V(j, Q)$

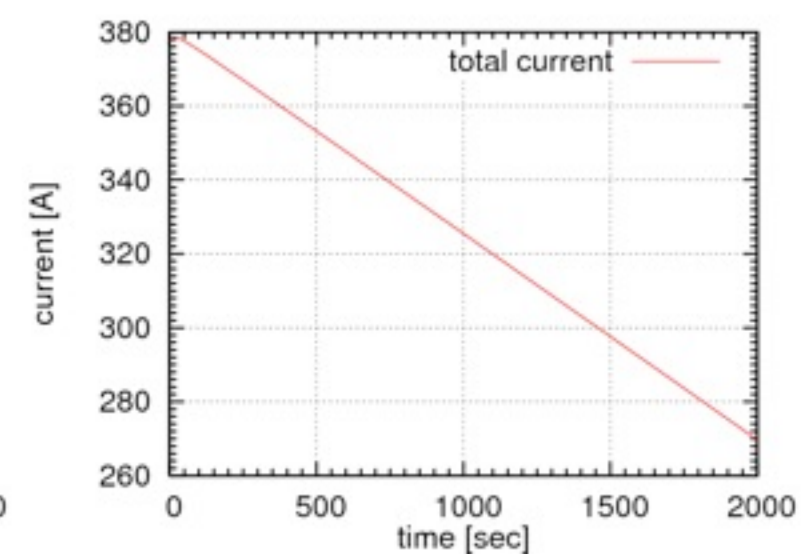


input discharge curve is followed correctly!

- total charge



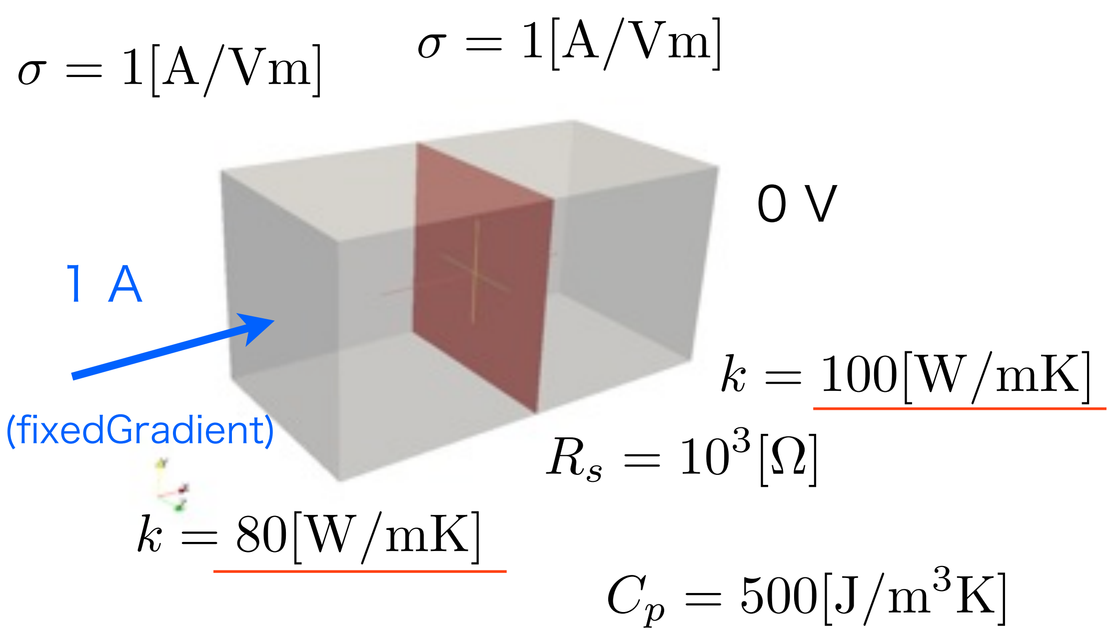
- total current

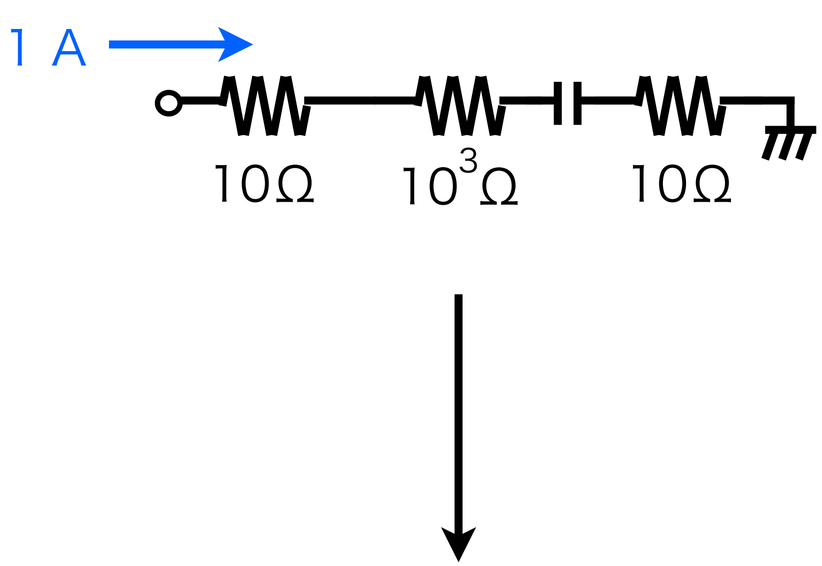


short current

3. Basic validations

■1-layer flat cell with fixed current

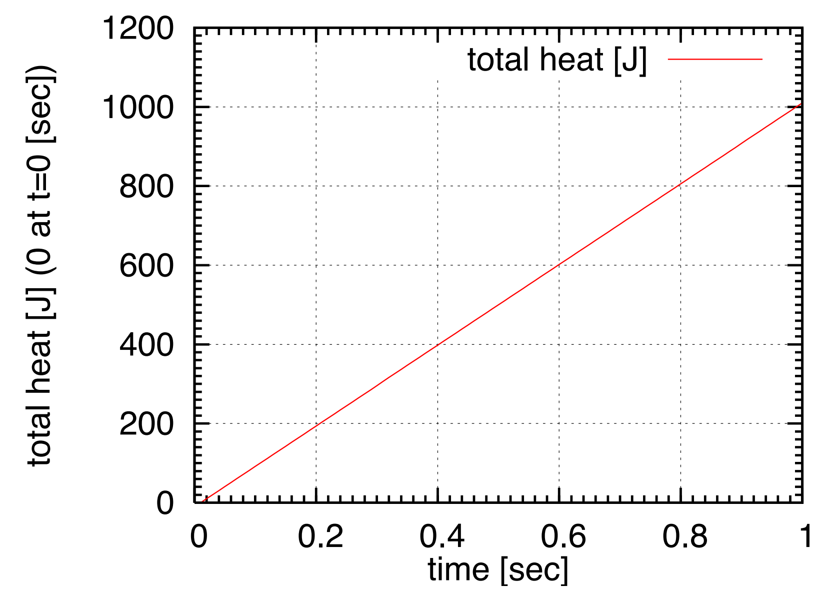




1020W heating

- test 1: growth of total heat $\int_V C_p T d\Omega$

all boundary for T : adiabatic (zeroGradient)

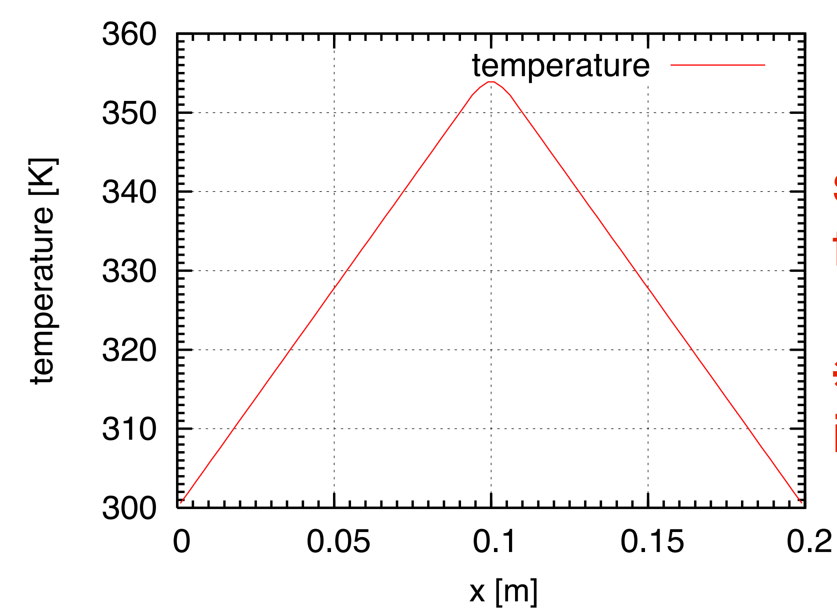


← 1020J in 1sec

- test 2: temperature distribution on x-axis

$\min(x), \max(x)$ boundary for T: 300K fixed

the other boundaries for T : adiabatic (zeroGradient)

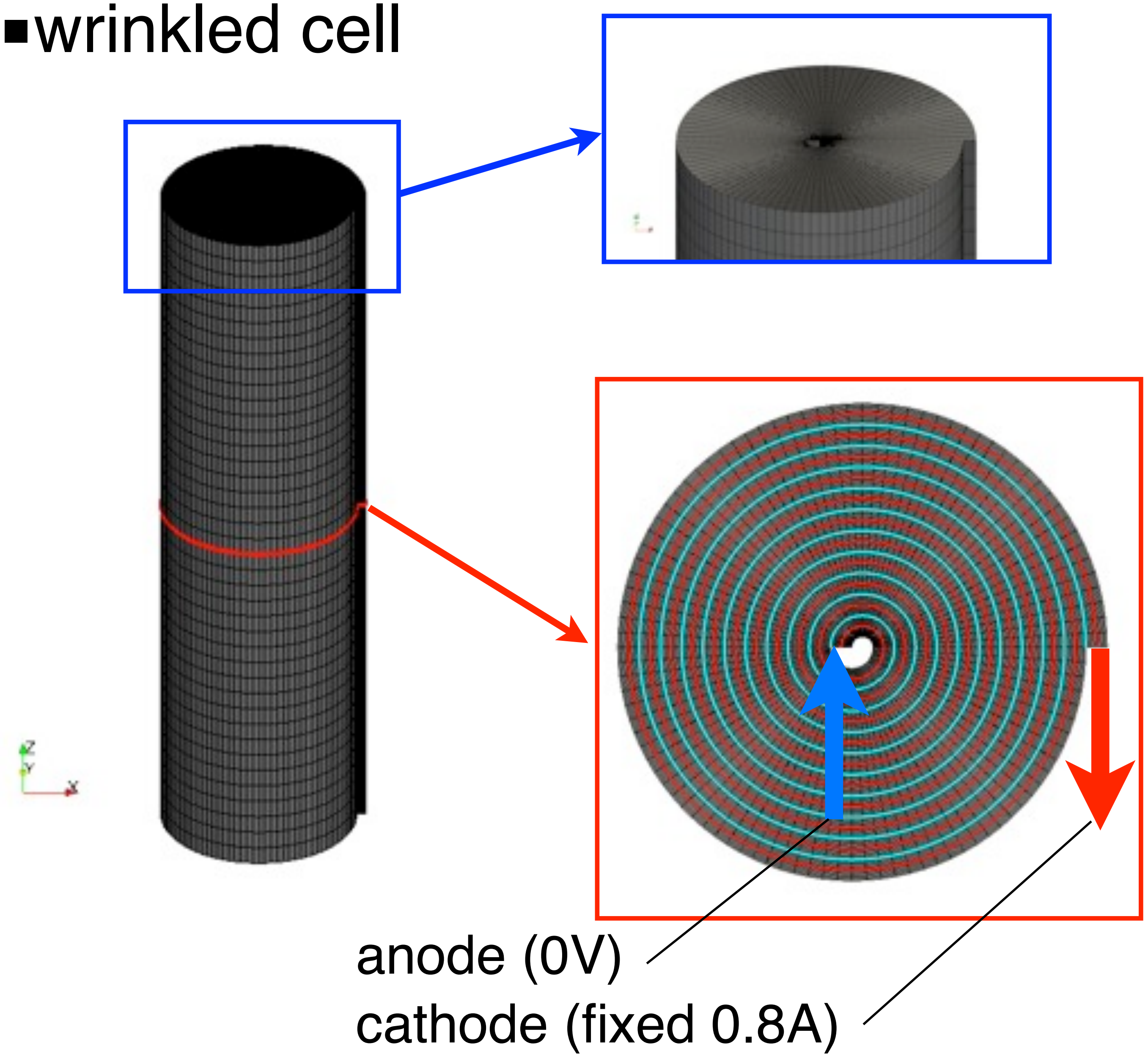


same linear distribution for different k

※volume Joule heating is turned-off

4. Demonstration Results of Cell-level simulations

▪wrinkled cell



- diameter: 11.5mm
- length: 40mm
- layer thickness: 500µm
- 10.5 rolled
- 420,000cell (hexahedra)

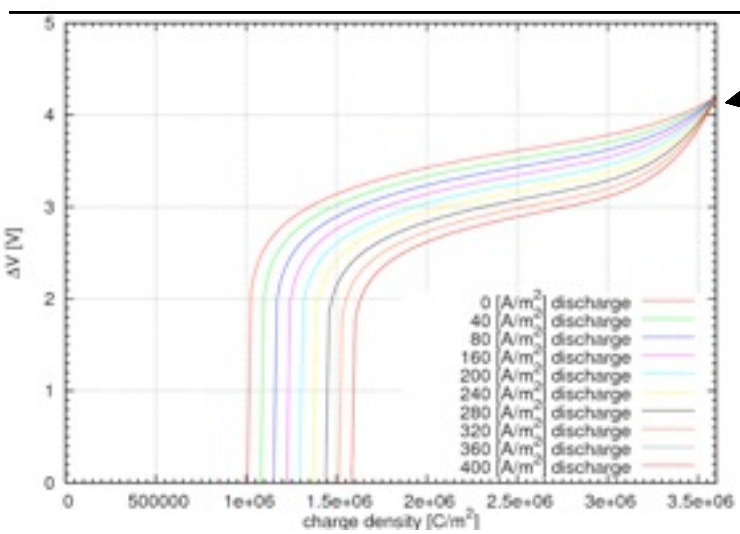
- red B.C.: cell surface
  - V : cell model $R_s = 10[\mathrm{m}\Omega]$
  - T : surface heating
- blue B.C.: insulation
  - V : zeroGradient
  - T : heat exchange
- the other B.C. for T

  heat transfer with $h = 5[\mathrm{W/m^2 \cdot K}]$

  $T_{\mathrm{ext}} = 300[K]$
- materials

	cathode	anode
$\sigma[\mathrm{A/m \cdot V}]$	5.9×10^5	3.74×10^5
$k[\mathrm{W/m \cdot K}]$	0.4	0.3
$\rho c_p[\mathrm{J/m^3}]$	1.35×10^6	1.0×10^6

※ assumption: 10% thickness of corrector metal (Cu and Al)
other material is polymer



- initial condition

  100% charged (about 8Ah)

  $q = 3.6 \times 10^6 [\mathrm{C/m^2}]$

4. Demonstration Results of Cell-level simulations

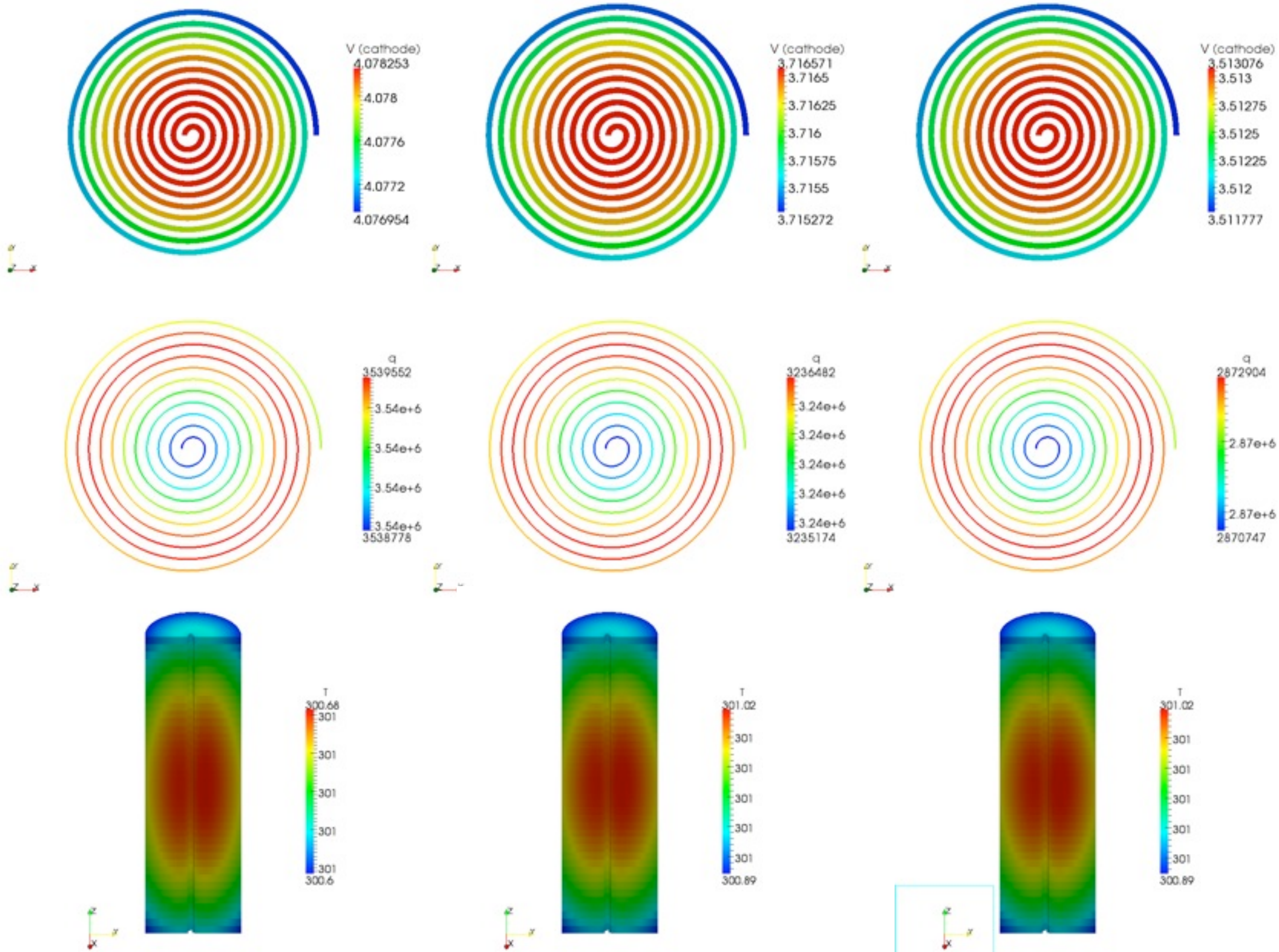
- wrinkled (no internal short, 0.8A discharge)

600 [sec] | 3600 [sec] | 7200 [sec]

V (cathode)

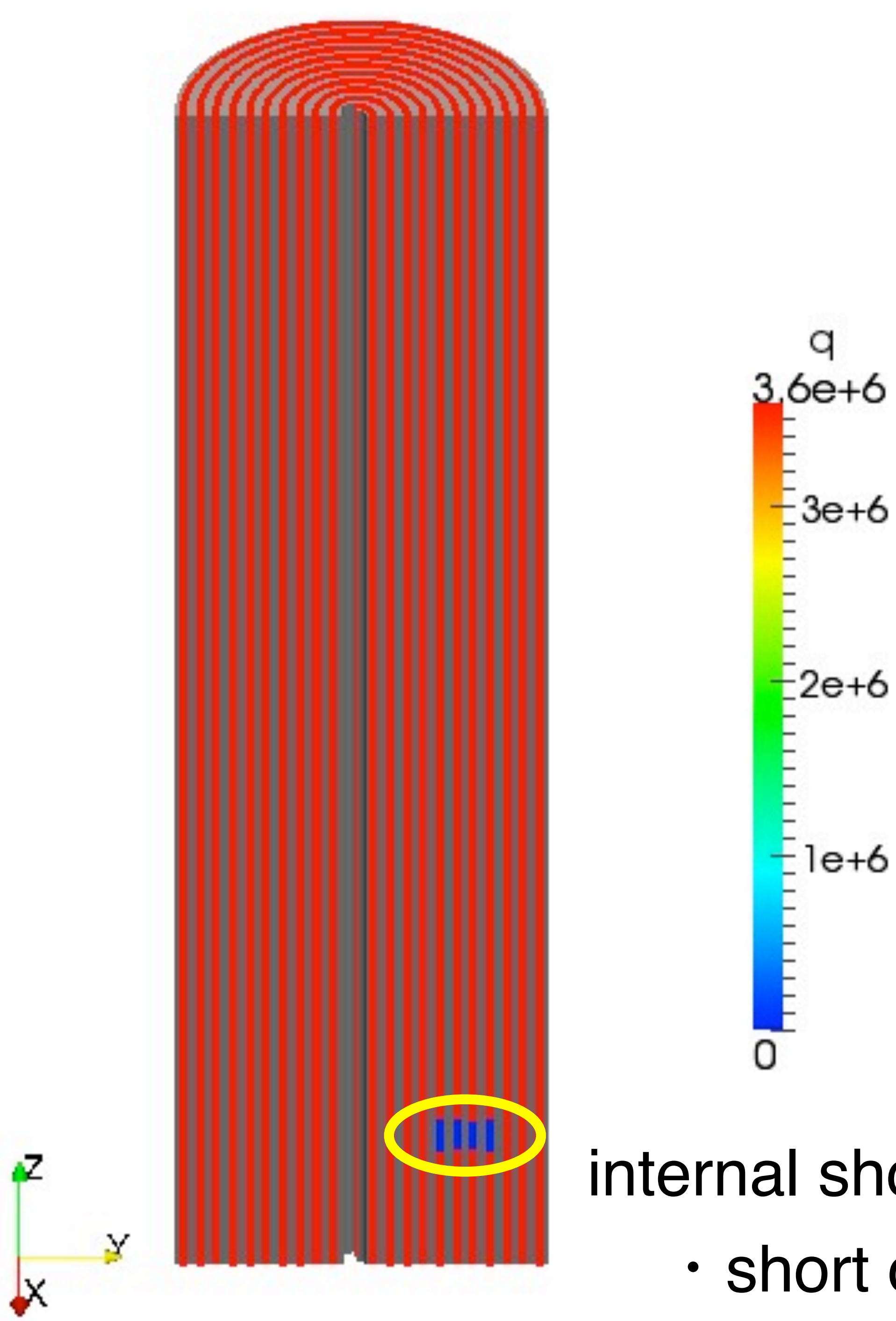
q [C/m^2]

T [K]



4. Demonstration Results of Cell-level simulations

- wrinkled (with internal short, 0.8A discharge. ※ visualized slice includes short)



internal short circuit

- short circuit region bounding box:

  (-0.5 2.0 4.0) (0.5 4.0 5.0) [mm]

- 4 layers (in this case, insulation remains safe)

4. Demonstration of Cell-level simulations

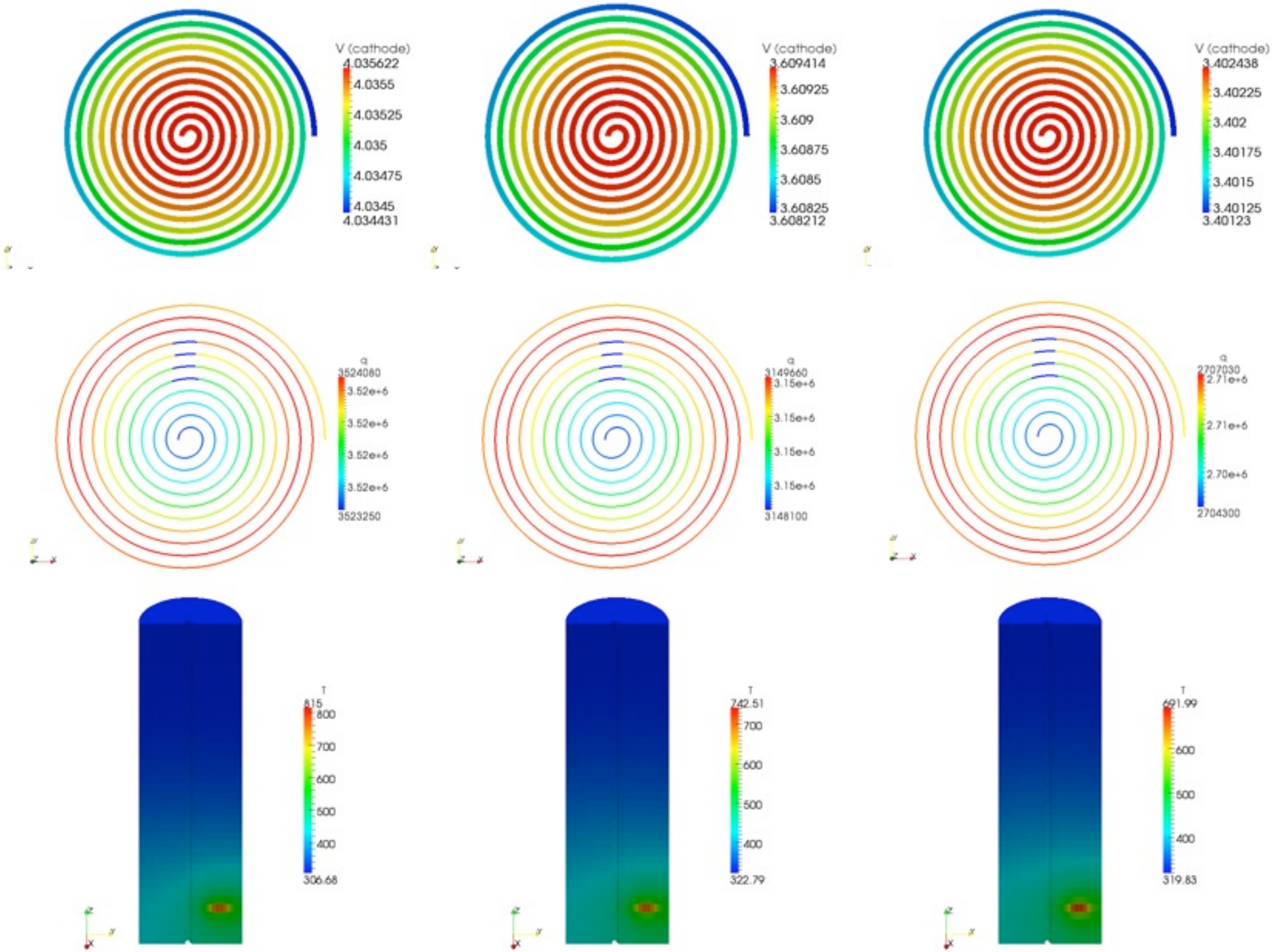
- wrinkled (with internal short, 0.8A discharge. ※ visualized slice includes short)

600 [sec] | 3600 [sec] | 7200 [sec]

V (cathode)

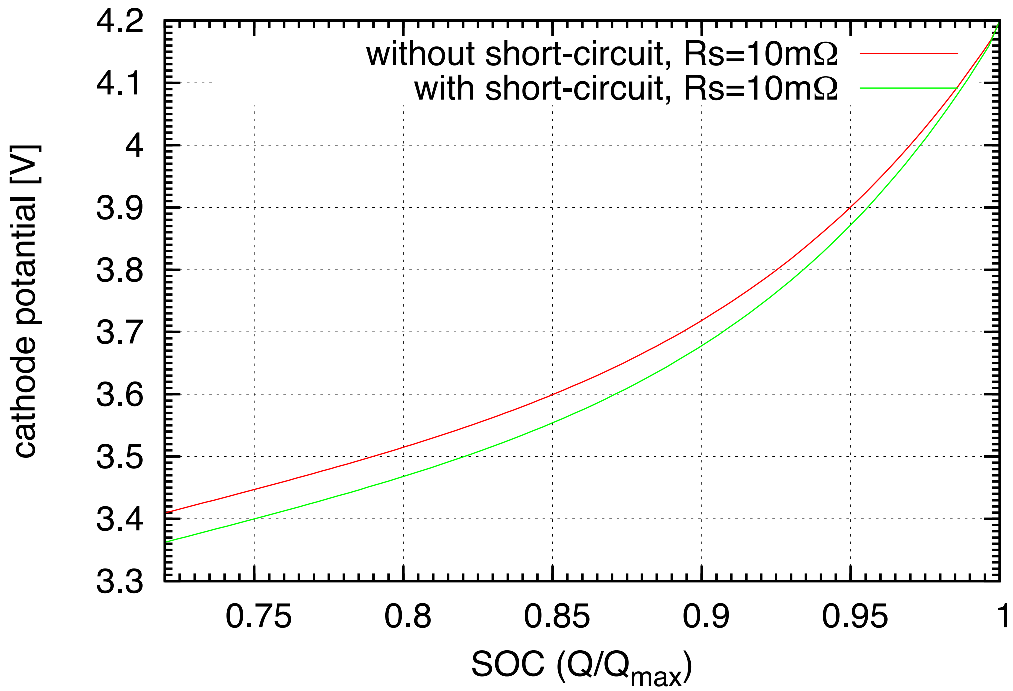
q [C/m^2]

T [K]



4. Demonstration of Cell-level simulations

- discharge curve



cathode potential loss
by short circuit

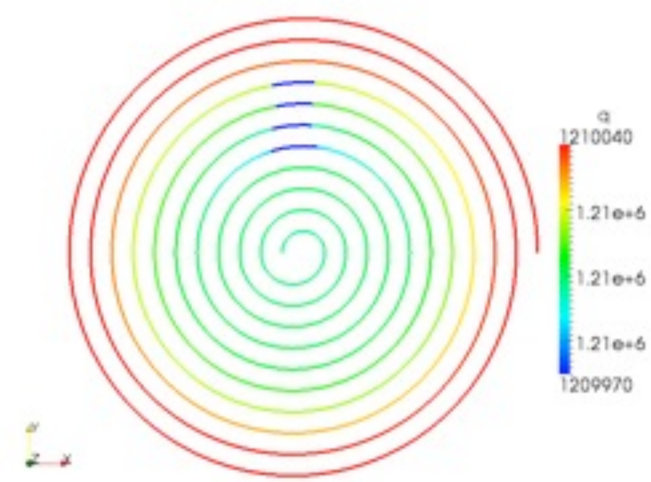
$\sigma \times 10^{-1}$

7200 [sec]

- V and q distribution is insignificant, because of high σ
- q difference around short circuit is small due to high R_s
  (potential difference is compensated by short current)

$R_s = 10^{-1} [\mathrm{m}\Omega]$

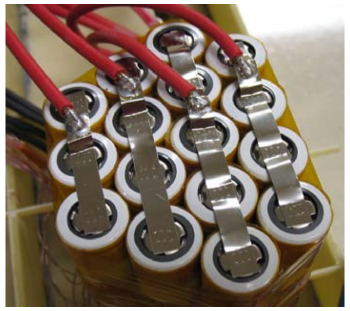
3600 [sec]



5. Summary and Future work

- cell-level model of Lithium-ion cell is implemented
  - works well in basic tests
- several parameter studies can be done
  - charge balance, temperature distribution, discharge curve, etc
- comparison with experiments is important

  (however, our company can not do experiments by ourselves)



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- more realistic and complicated configurations (full unit simulation)
  - robustness and good convergence are necessary, and to be tested
- model improvement
  - material properties (anisotropic electric or thermal conductivity)
  - reaction heat
  - temperature dependence ⟶ bidirectional coupling (V→T to V↔T)
- electrochemical modeling (now beyond our scope)
- [support of internal boundary conditions in OpenFOAM is desirable]