COMSOL CONFERENCE
2015 BOSTON

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

B. Rajabloo[1], M. Désilets[1], Y. Choquette[2]

[1]Département de génie chimique et de génie biotechnologique, Université de Sherbrooke, QC, CANADA

[2]Institut de recherche d'Hydro-Québec, Varennes, QC, CANADA

UNIVERSITÉ DE SHERBROOKE

Hydro Québec

COMSOL CONFERENCE 2015 BOSTON

Hydro Québec

UNIVERSITÉ DE SHERBROOKE

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

Single Particle Model

Parameter Estimation

R solution

Conclusion

October 2015

COMSOL CONFERENCE 2015 BOSTON

Hydro Québec

UNIVERSITÉ DE SHERBROOKE

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

Single Particle Model

Parameter Estimation

R solution

Conclusion

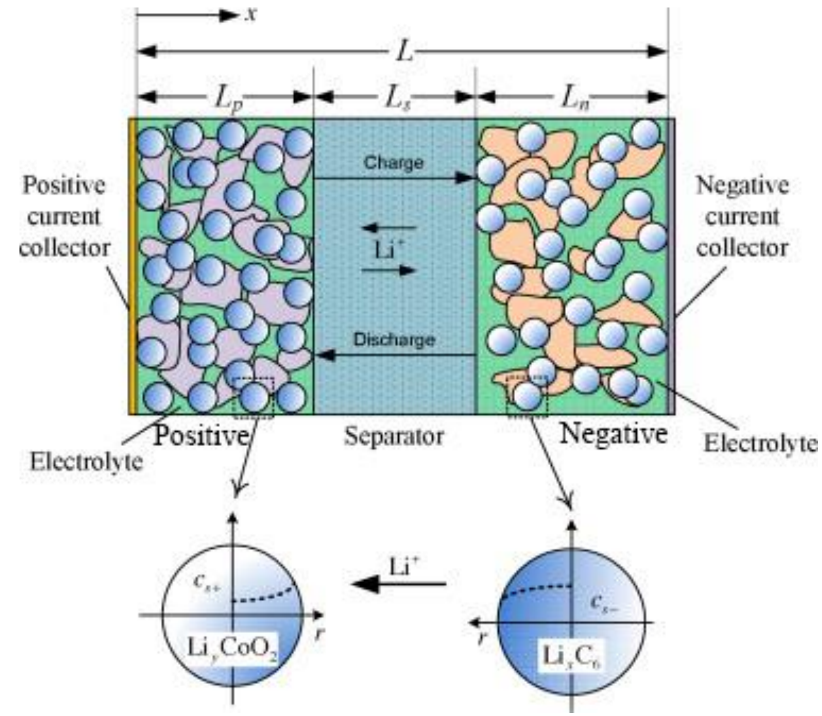
October 2015

SPM Single Particle Model

➢ Uniform current distribution

➢ Ignore variation of electrolyte concentration and potential

➢ Assume a lumped solution resistance



Dao, T. S. *et. al.*, *J. Power Sources* **198**, 329-337 (2012)

Positive points:

➢ High speed solution

Parameter estimation	Inverse method	Dynamic optimization	Pack	Aging

Reasonable when:

➢ Highly conductive electrodes ➢ Low applied current density ➢ Thin electrodes

SPM

Local current density

$$i_{loc} = I/S$$

I: total current
S: total electroactive surface area

Solid concentration

$$\frac{\partial Cs}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial Cs}{\partial r}\right)$$

$$\left.\frac{\partial Cs}{\partial r}\right|_{r=0} = 0 \qquad D\left.\frac{\partial Cs}{\partial r}\right|_{r=R} = -\frac{i_{loc}}{F}$$

Open circuit potential

$$Eq(SOC_{neg})$$

Overpotential negative electrode (Butler – Volmer equation)

$$\eta_{neg} = \frac{RT}{\beta F} a\sinh\left(\frac{i_{loc}}{2i_0}\right)$$

Potential negative electrode

$$\varphi_{s,neg} = \eta_{neg} + Eq(SOC_{neg})$$

$$E_{cell} = \varphi_{s,pos} - \varphi_{s,neg} - i_{app} R_{solution}$$

Adjustable parameter

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

Single Particle Model

Parameter Estimation

R solution

Conclusion

October 2015

Parameter estimation

Why?

1. It is not convenient to find all physical and chemical parameters that are needed for the simulation of lithium-ion cells

(porosity, particle size, diffusion coefficients, electrical conductivity, contact resistance, transfer coefficients, etc.)

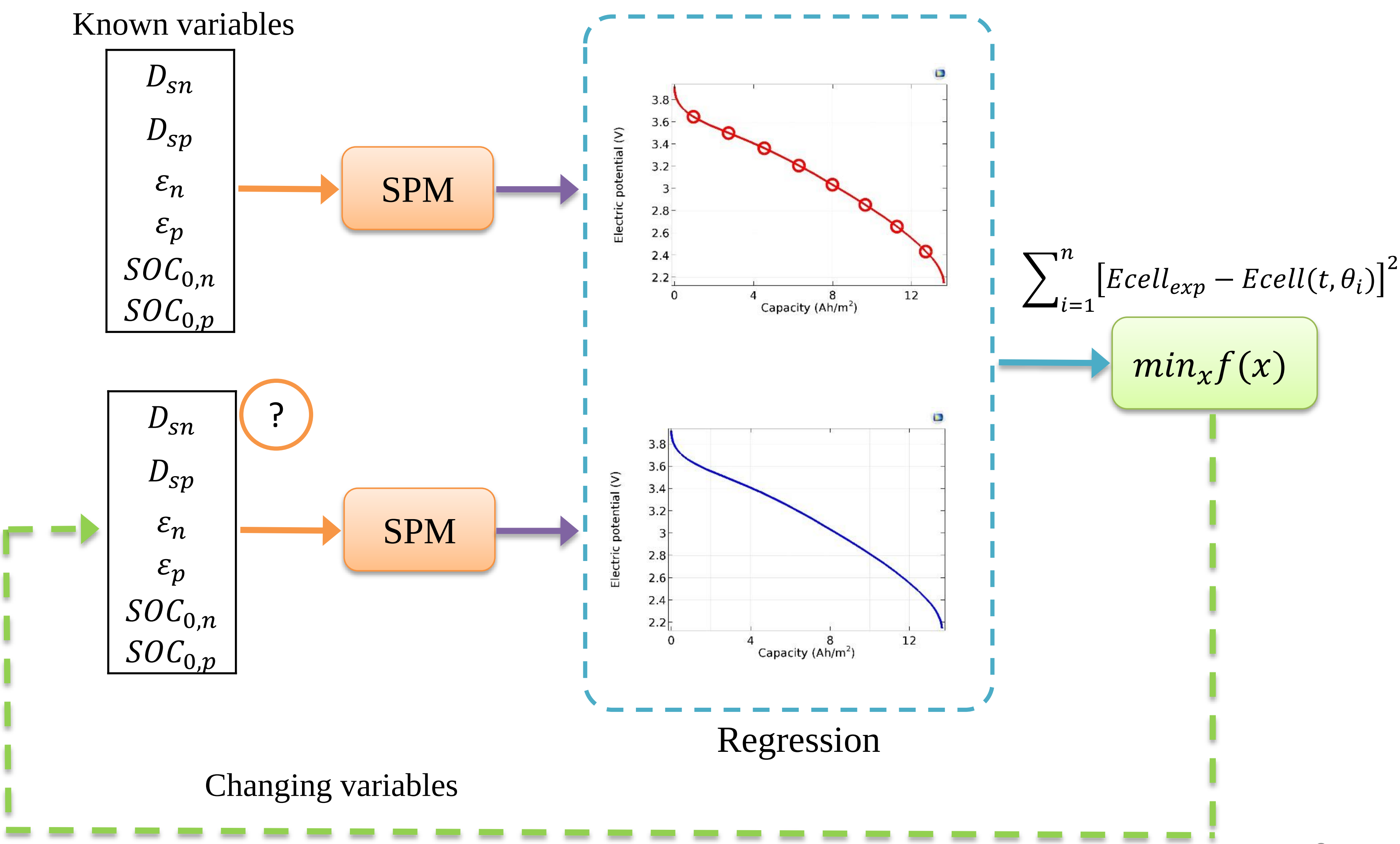
2. Parameter estimation might be a useful approach to find these parameters from the experiment charge/discharge data

How?

Minimization of the sum-of-squared differences between the model outputs and their experimentally measured values at time t_j for each cycle *i*

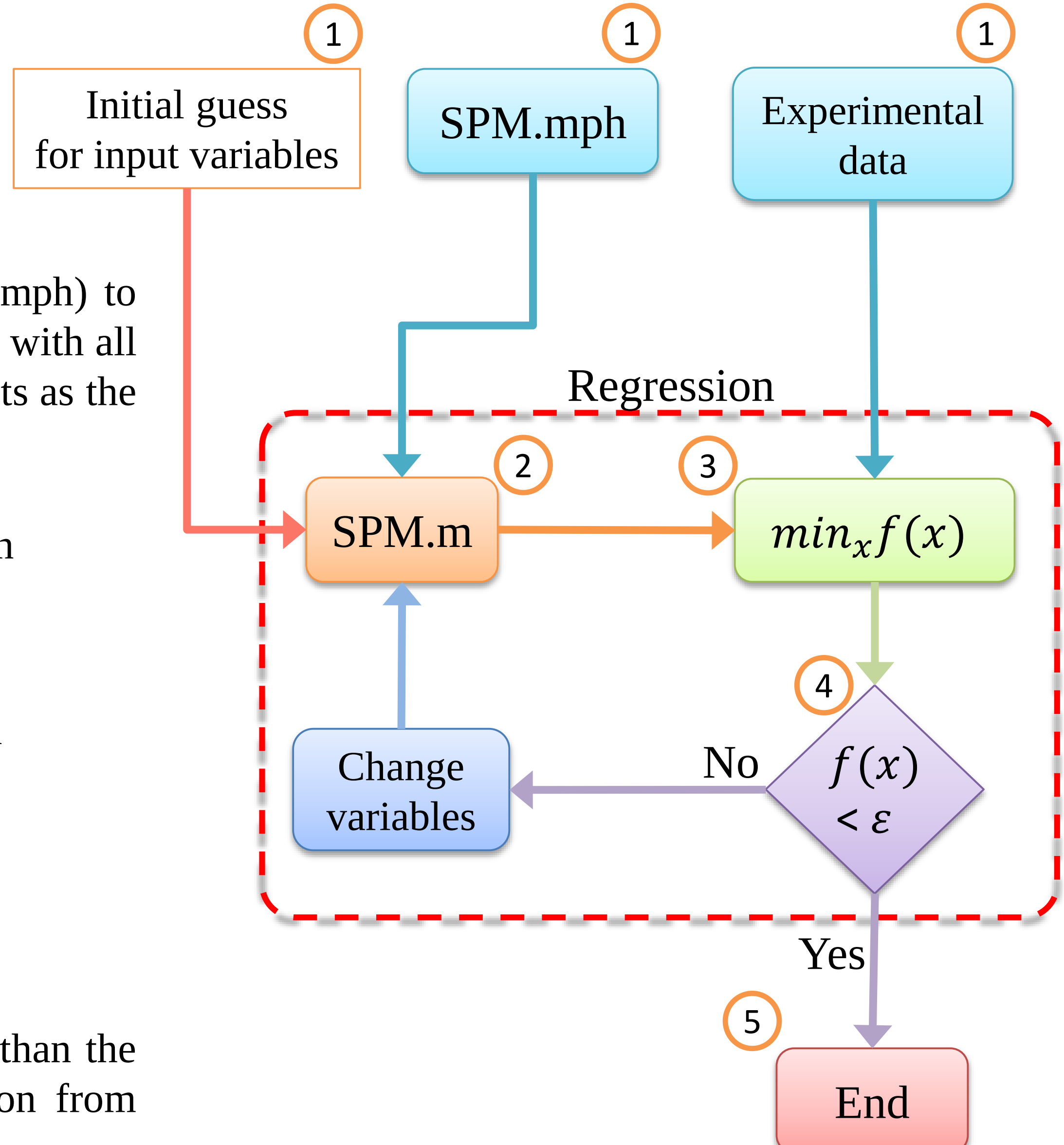
$$\min_{\theta_i} \sum_{j=1}^{n_i} \left[y_i(t_j) - y_{model,i}(t_j;\theta_i)\right]^2$$

Parameter estimation



Parameter estimation

Link to MATLAB



1. Import SPM from COMSOL (SPM.mph) to MATLAB (SPM.m) then run SPM.m with all known parameters and consider results as the experimental data

2. Assume some parameters as unknown

3. Perform regression by minimizing difference between experimental data and the results from model

4. Check the error

5. Finish regression if the error is less than the criteria. Otherwise, resume regression from step 3

COMSOL Hydro Québec UNIVERSITÉ DE SHERBROOKE

Parameter estimation

Parameters	Lower bound	Upper bound	Initial guess	Estimated	Exact	Relative Error %
$D_{sn}\ [\mathrm{m}^2/\mathrm{s}]$	2.73e-14	11.7e-14	2.73e-14	3.23e-14	3.9e-14	17.18
$D_{sp}\ [\mathrm{m}^2/\mathrm{s}]$	0.7e-13	3e-13	0.7e-13	1.2e-13	1e-13	20
ε_n	0.2	0.6	0.2	0.357	0.357	0
ε_p	0.2	0.6	0.2	0.444	0.444	0
$SOC_{0,n}$	0.5	0.7	0.5	0.5642	0.5635	0.12
$SOC_{0,p}$	0.1	0.3	0.1	0.1709	0.1706	0.059

The values of ε_n, ε_p, $SOC_{0,n}$, and $SOC_{0,p}$, have been estimated with a very good accuracy

COMSOL CONFERENCE 2015 BOSTON

Hydro Québec

UNIVERSITÉ DE SHERBROOKE

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

Single Particle Model

Parameter Estimation

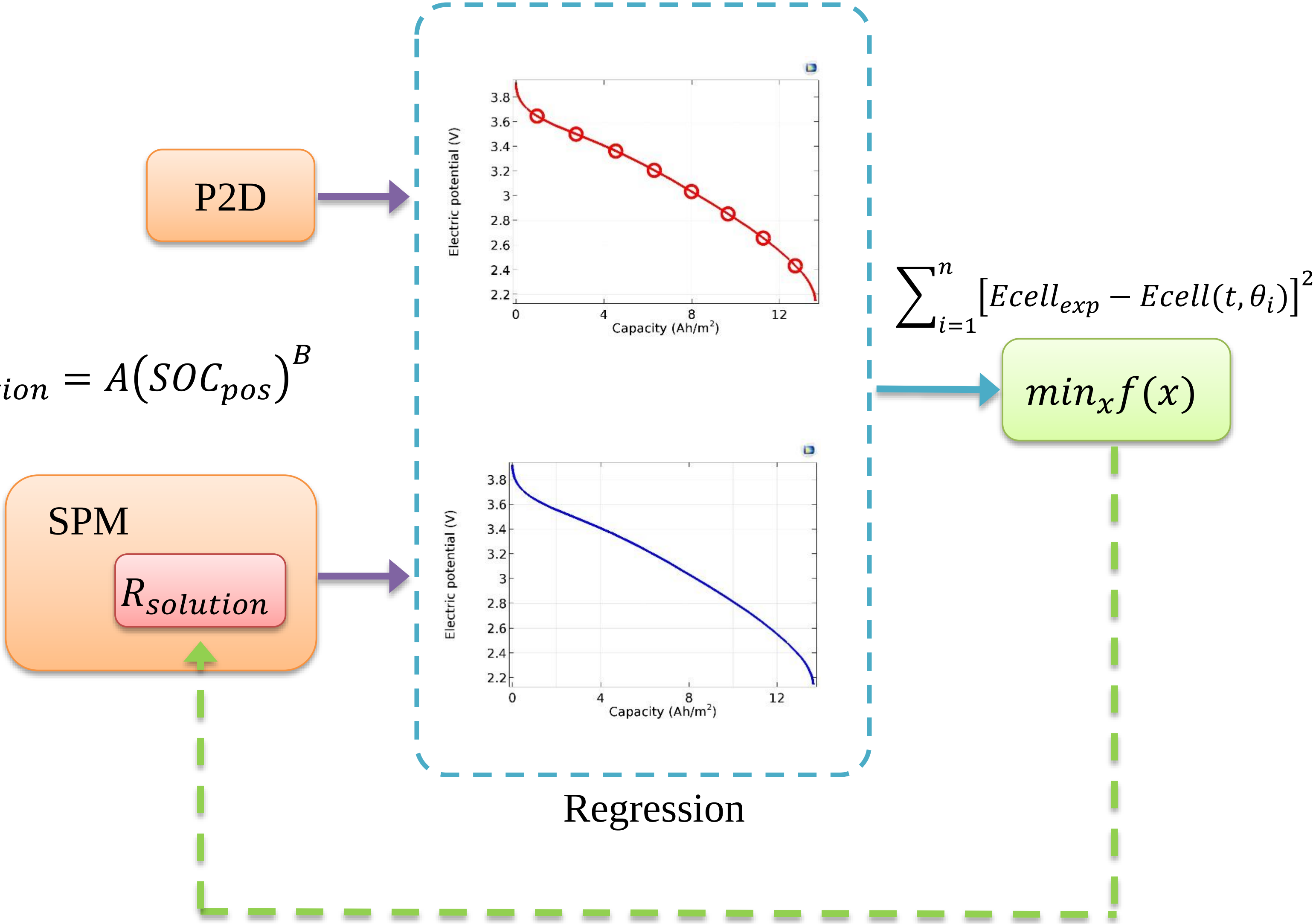
R solution

Conclusion

October 2015

R solution

$$R_{solution} = A\left(SOC_{pos}\right)^{B}$$

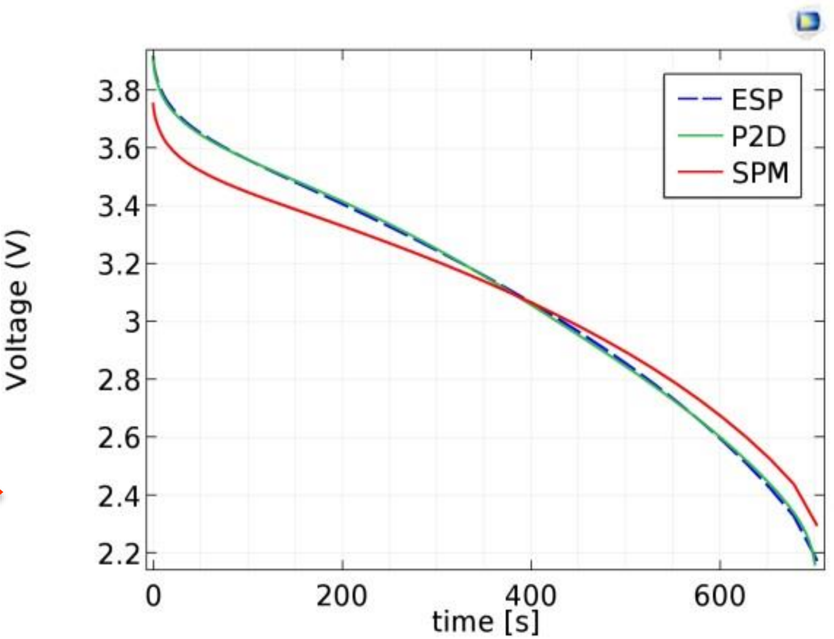


R solution

$$R_{solution} = A(SOC_{pos})^B$$

Regression was performed for various applied currents and constant coefficients A and B were estimated for each current

Applied current I	$A[\Omega.m^2]$	B
2C	4.750e-3	0.579
4C	9.387e-3	1.168
6C	1.400e-2	1.498
8C	2.458e-2	2.073
10C	3.255e-2	2.370

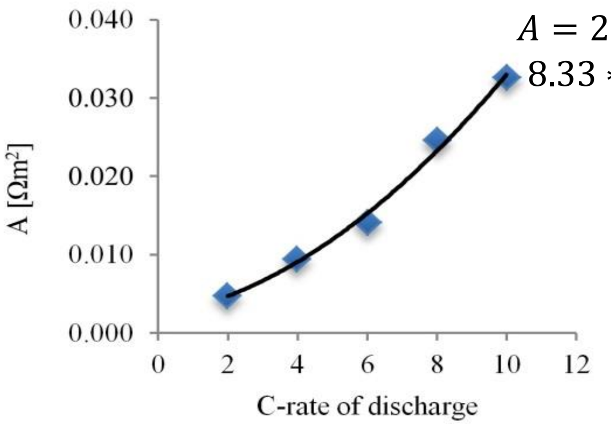


Comparison between various models for 4C discharge process

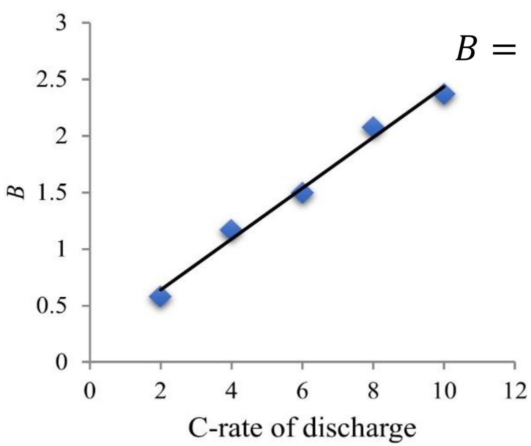
R solution

$$R_{solution} = A(SOC_{pos})^B$$

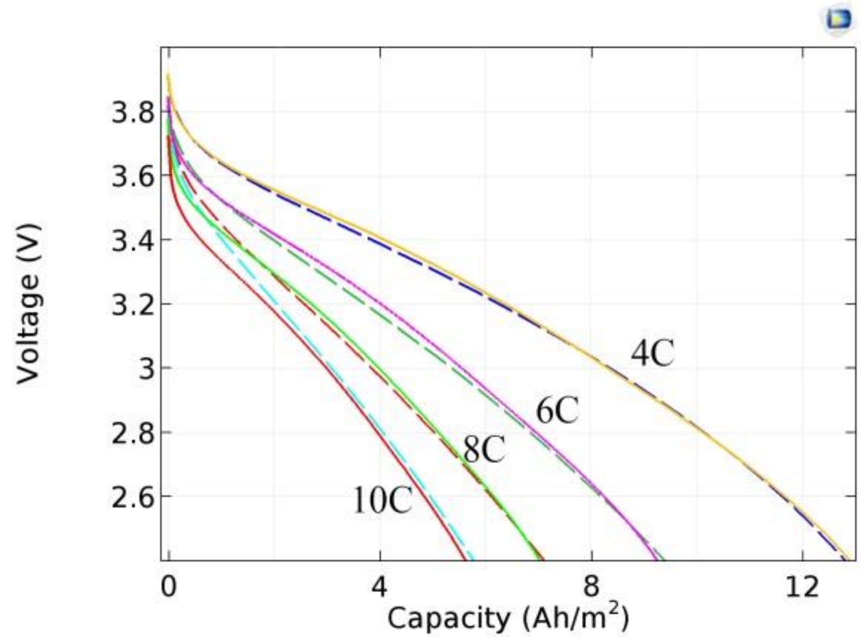
fitting two equations for A and B as a function of applied current



$$A = 2.26 * 10^{-4}c^2 + 8.33 * 10^{-4}c + 2.13 * 10^{-3}$$



$$B = 0.22c + 0.19$$



Comparison between results from ESP (dashed line) and P2D model (solid line) for higher applied currents

COMSOL CONFERENCE 2015 BOSTON

Hydro Québec

UNIVERSITÉ DE SHERBROOKE

Parameter Estimation of Single Particle Model Using COMSOL Multiphysics® and MATLAB® Optimization Toolbox

Single Particle Model

Parameter Estimation

R solution

Conclusion

October 2015

Conclusion

1. Here, "Single Particle Model” was linked to MATLAB® and some parameters of the model were estimated by the optimization toolbox in MATLAB®.

2. The parameters, which the model is more sensitive to, were calculated with a good precision (error $< 0.1\%$).

3. An empirical equation for the solution phase resistance was introduced to reduce the errors of SPM in the cases where applied current was higher.

4. Predictability of the improved SPM (called ESP) was evaluated by comparing its results with those obtained with P2D model at high applied currents (up to 10C).

5. In all cases, a good conformity was observed between the P2D and ESP.

References

1. Dubarry, M., Vuillaume, N., and Liaw, B. Y., *J. Power Sources*, **186.2**, 500-507 (2009)

2. Liaw, B. Y., Jungst, R. G., Nagasubramanian, G., Case, H. L., and Doughty, D. H., *J. Power Sources*, **140.1**, 157-161 (2005)

3. Guo, M., Sikha, G. and White, R. E., *J. Electrochem. Soc.*, **158.2**, A122-A132 (2011)

4. Dao, T. S., Vyasarayani, C. P., and McPhee, J., *J. Power Sources* **198**, 329-337 (2012)

5. Fuller, T. F., Doyle, M., and Newman, J., *J. Electrochem. Soc.*, **141.1**, 1-10 (1994)

6. Beck, J. V., and Arnold, K. J., “Parameter estimation in engineering and science”, *James Beck*, (1977)

7. Rahimian, S. K., Rayman, S., and White, R. E., *J. Power Sources* **224**, 180-194 (2013)

Acknowledgement

Hydro Québec

NSERC
CRSNG

COMSOL CONFERENCE 2015 BOSTON

Hydro Québec

UNIVERSITÉ DE SHERBROOKE

Thank you for your time and your attention!

Any