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整车 / 新能源汽车关键性仿真技术

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ANSYS电池模型最佳实践

基于ECM的电池(系统)动态性能仿真

IDAJ-China
技术部 唐连伟 陈桂杰

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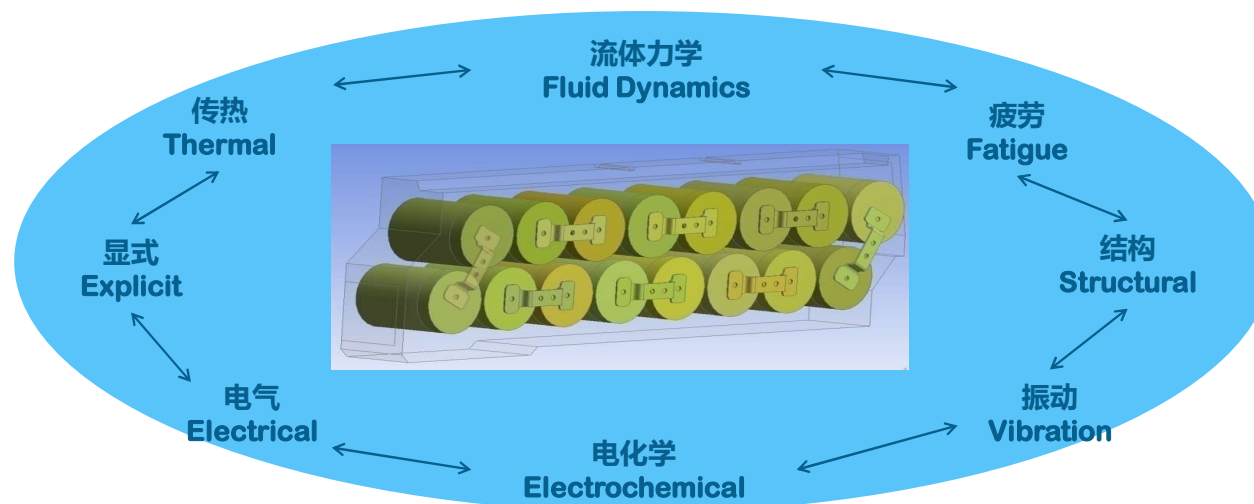
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2. ANSYS电池仿真方案介绍
3. 基于ECM的电池(系统)动态特性仿真最佳实践
4. 小结及致谢

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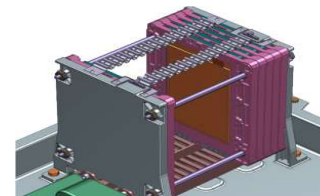
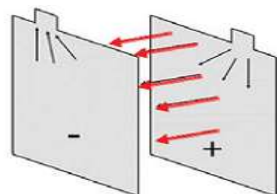
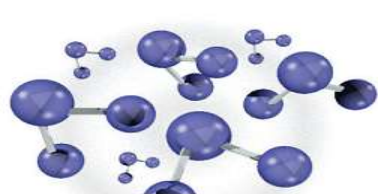
概述：电池多物理现象仿真

电池中包含着密切交互作用的多种物理现象



电池的仿真需要单一物理领域到多个物理领域结合的全面仿真方案

概述：电池多域仿真



小尺度

大尺度

分子	电极	电池	模块/包	系统集成
材料	布局 过程 寿命 SEI	充电 放电 热 安全	热管理 持久性 NVH EMI/EMC	系统集成
	Electro-chemistry	ECM CFD FEA	ECM CFD ROM FEA	ECM ROM

概述：ANSYS电池仿真方案汇总

单物理场领域

- 基于CFD的电池热管理
- 电化学模型
 - Newman Pseudo-2D (P2D) model
 - 3D electrochemistry model
- 单电池等效电路模型(ECM)
- 电池结构分析

多物理场领域

- 多尺度多维度方法 (MSMD)

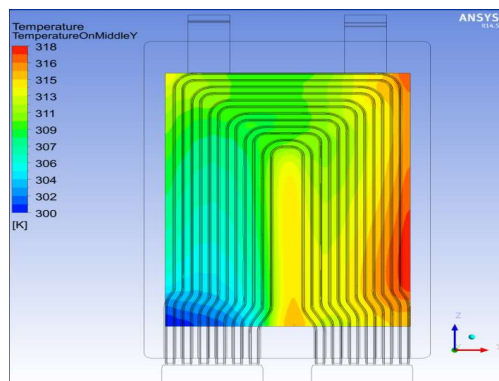
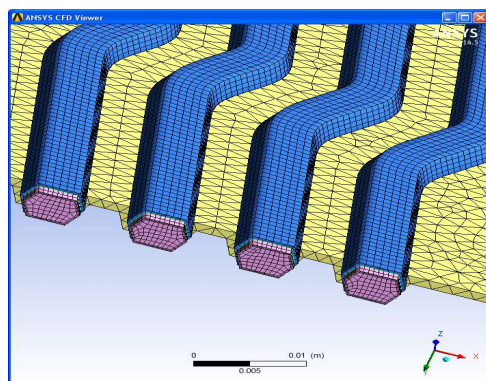
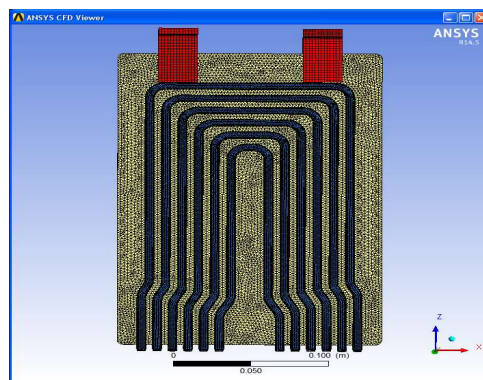
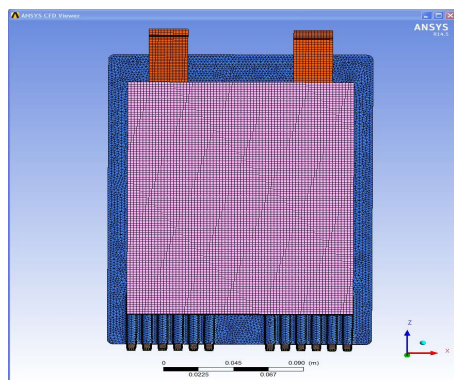
电池系统

- 使用降阶模型(ROM)的电池热管理
- 耦合ECM与ROM的电池系统仿真

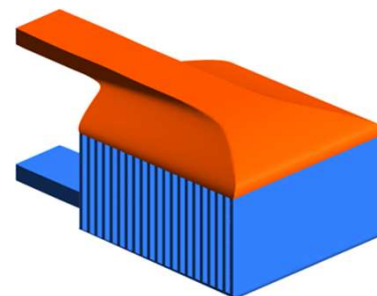
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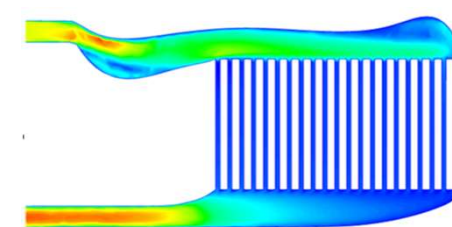
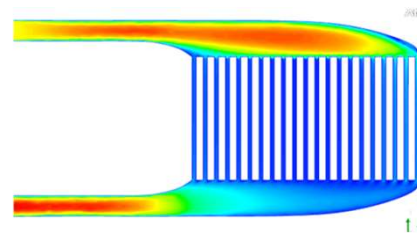
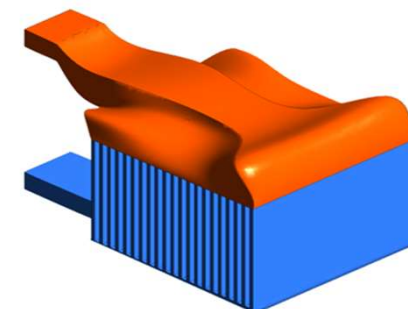
基于CFD的电池热管理：单元级/Module/Pack的CHT分析



原始设计

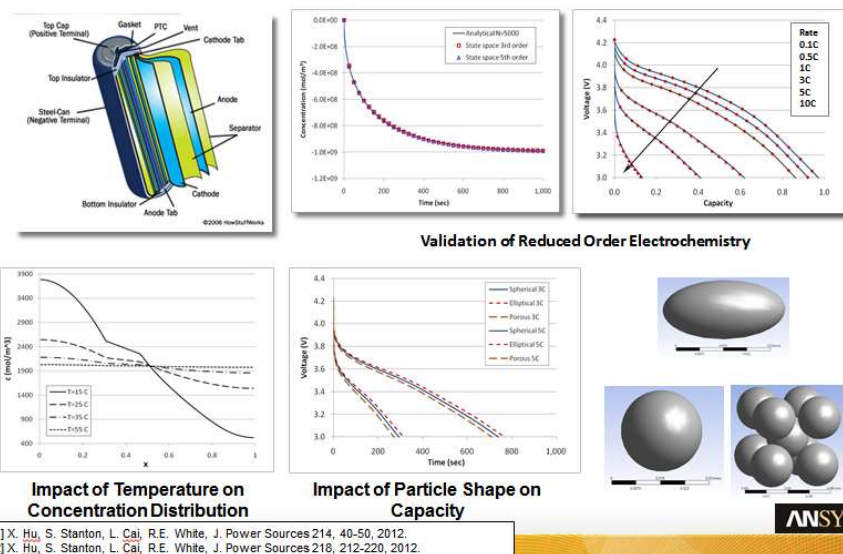


优化设计



电化学模型简介

Newman P2D Electrochemistry



[1] X. Hu, S. Stanton, L. Cai, R.E. White, J. Power Sources 214, 40-50, 2012.
[2] X. Hu, S. Stanton, L. Cai, R.E. White, J. Power Sources 218, 212-220, 2012.

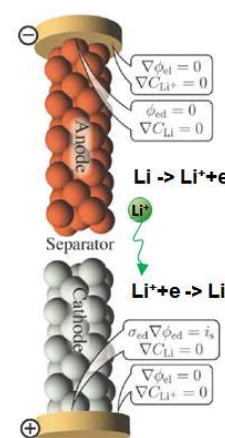
Potential and Current Distribution in Electrochemical Cells

Interpretation of the Half-Cell Voltage Measurements as a Function of Reference-Electrode Location

John Newman* and William Tiedemann*

Johnson Controls Battery Group, Incorporated, Milwaukee, Wisconsin 53201

3D Lithium-ion Electrochemistry



- Electrode(Solid Particle)**
Potential
 $\nabla \cdot (\sigma_{ed} \nabla \phi_{ed}) = 0$
Species(Li) - UDS
 $\frac{\partial C_{Li}}{\partial t} = \nabla \cdot (D_{ed} \nabla C_{Li})$
- Electrolyte**
Potential
 $\nabla \cdot (\kappa \nabla \phi_{el}) = 0$
Species (Li+)
 $\frac{\partial C_{Li^+}}{\partial t} = \nabla \cdot (D_{el} \nabla C_{Li^+})$
- Echem reaction at electrode/electrolyte interface**
 $i = i_0 \left[\exp\left(\frac{\alpha_a F}{RT} \eta\right) - \exp\left(-\frac{\alpha_c F}{RT} \eta\right) \right]$

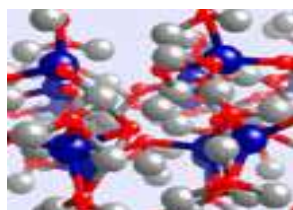
ANSYS

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多尺度多维度方法 (MSMD)

■ 应对Li⁺ 电池仿真的挑战：

材料



$10^{-9} \sim 10^{-8}$

极片



$10^{-6} \sim 10^{-4}$

单体, 包



$10^{-2} \sim 10^0$

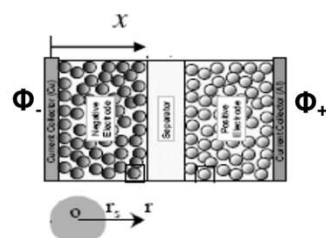
■ 多尺度多维度(Multi-Scale Multi-Dimensional) 方法

- 专注于单体电池及以上尺度级别(不用于电极结构);
- 不同的物理域使用不同的网格
- 每一个有限体积的单元都视为一个迷你电池

在每个网格上调用子模型 (如下)

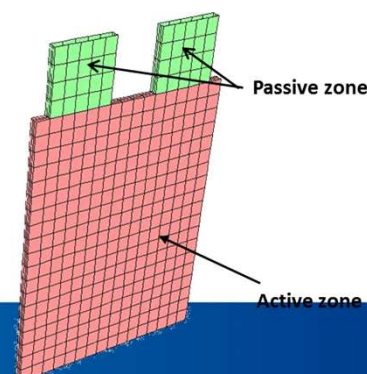
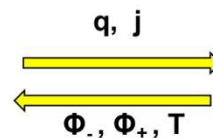
input: $\Phi_-, \Phi_+, T, C_s(X, x, r, t_0), C_e(X, x, t_0)$
output: j, q, C_s, C_e

- P2D 子模型
- NTGK子模型
- ECM子模型



Electrode scale sub-model

(NTGK for example)

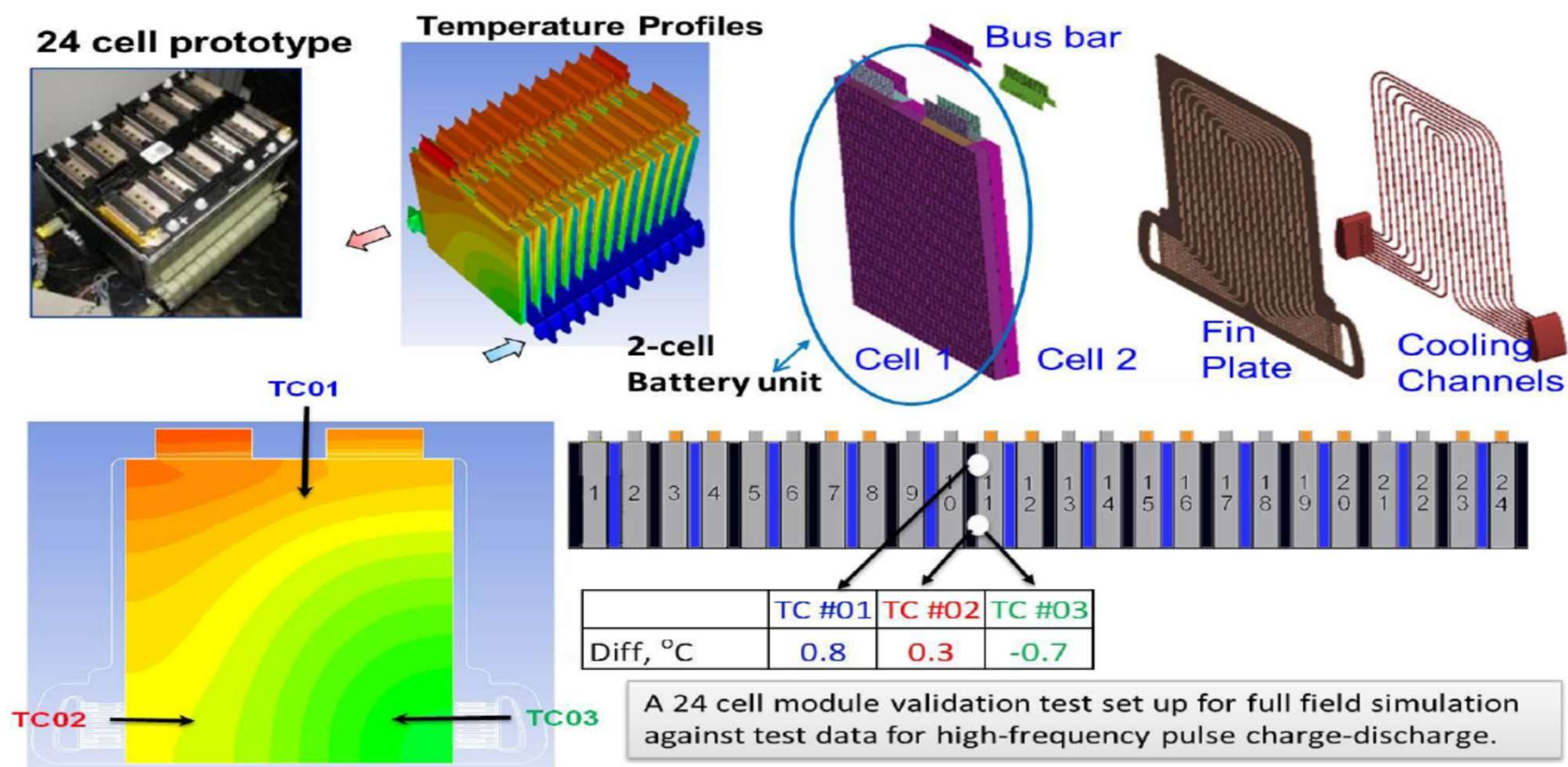


CFD网格: 不需要求解电极层

model: 各向异性电导率

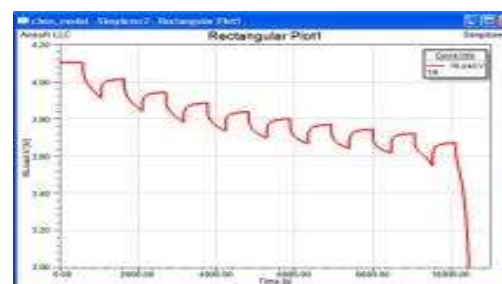
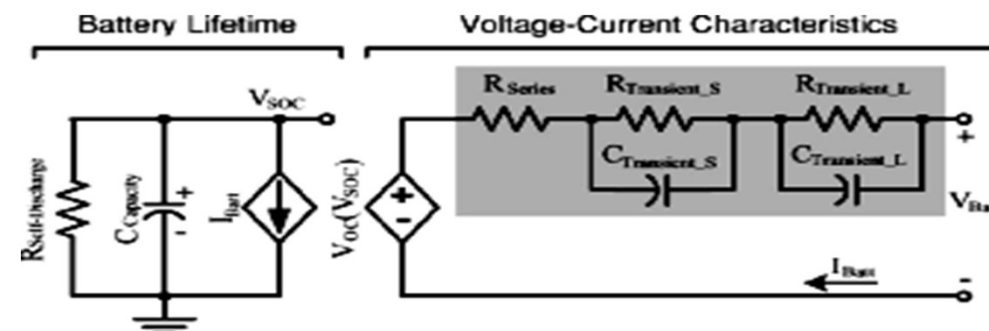
solve: Φ_-, Φ_+, T

多尺度多维度方法 (MSMD): GM电池模块仿真案例

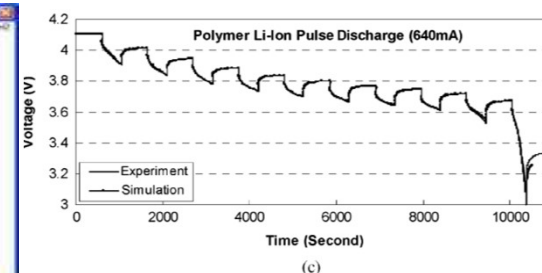


单电池等效电路模型(ECM)

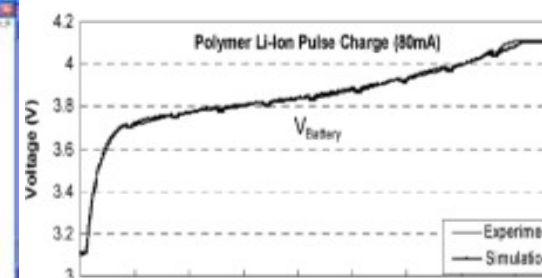
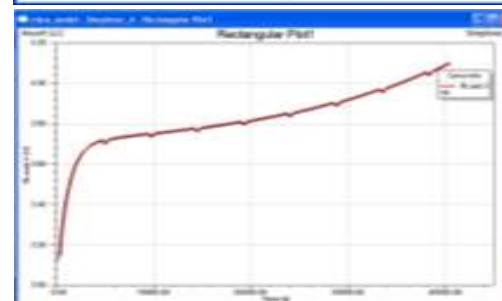
- 可使用HPPC实验数据
 - 使用Fluent的Parameter Estimation Tool拟合模型参数
 - 或Simplorer的ECM抽取工具包
- 考虑非线性开路电压
- 可以预测工作时间
 - 误差小于 0.4%
- 可以预测瞬态I-V特性 (发热特征)
 - 误差小于30-mV
- 很容易应用在电路仿真中
 - 在Simplorer® 中



仿真结果Simplorer®



文献结果

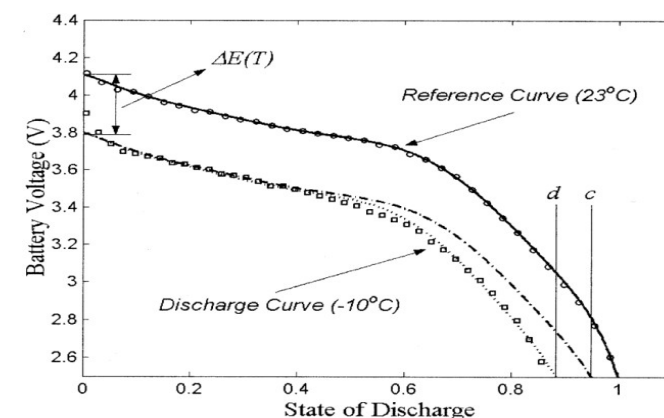


单电池等效电路模型(ECM)

温度相关的ECM

- Chen模型可以在定常温度下工作
- 温度影响非常重要，需要考虑
- Gao修订了Chen的模型，修改放电过程受温度系数(β)控制，从而实现对温度敏感

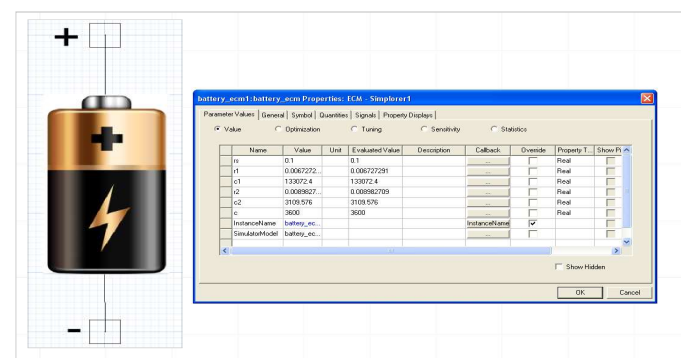
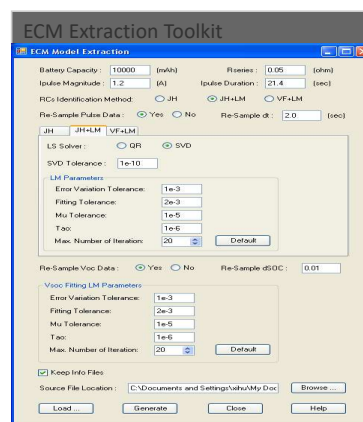
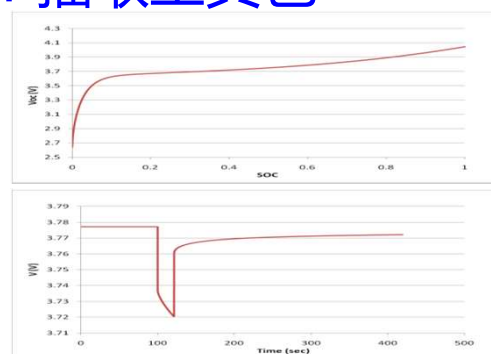
$$SOC = 1 - \frac{1}{Q} \int_0^t \beta [T(t)] \cdot i(t) dt$$



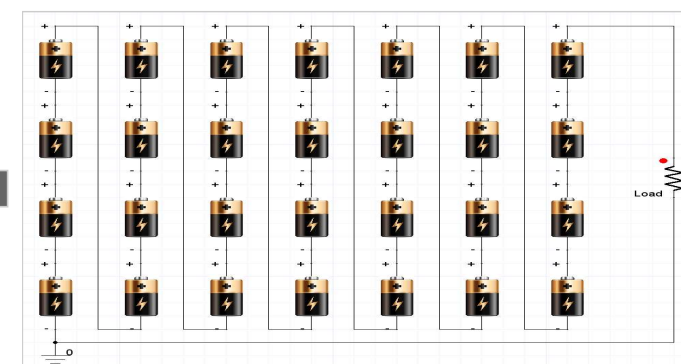
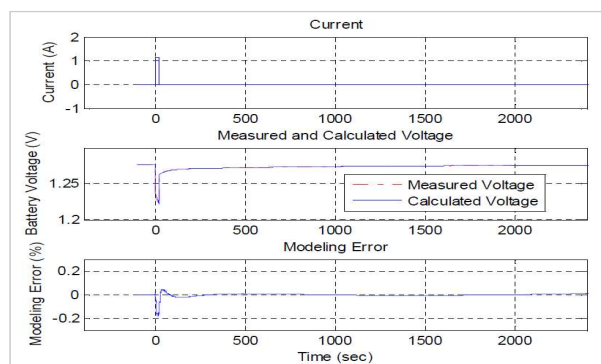
温度的影响

单电池等效电路模型(ECM)

ECM 抽取工具包



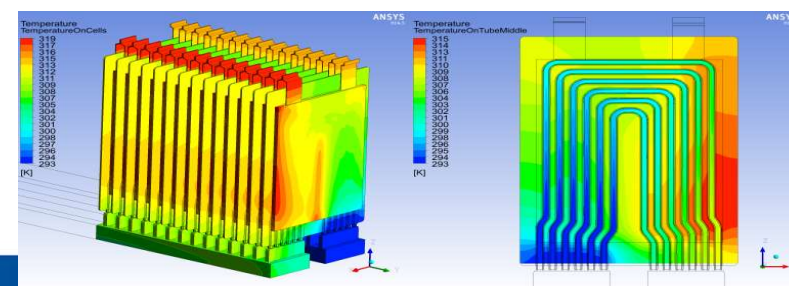
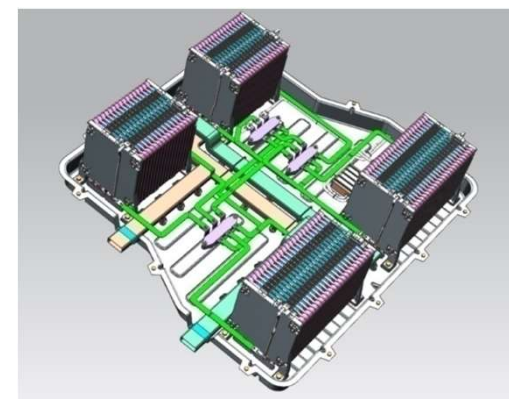
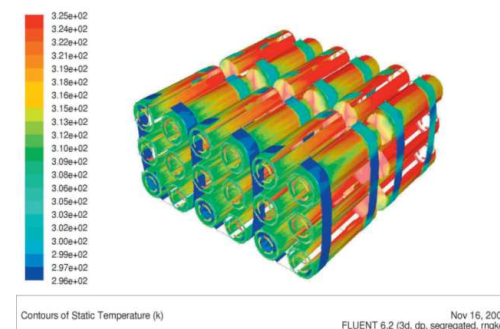
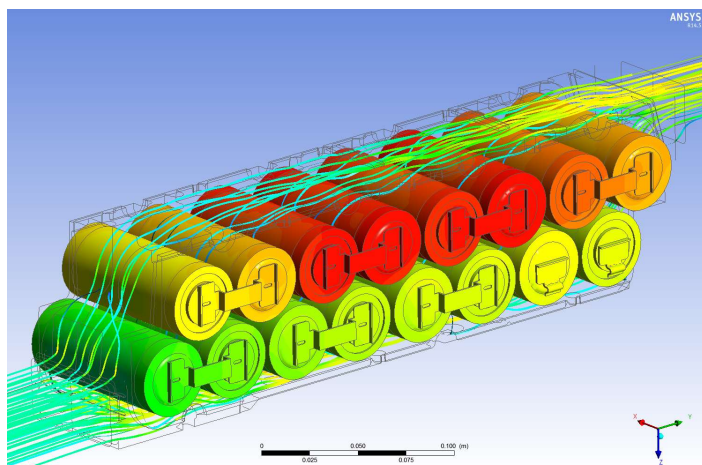
ECM 模型工作流程



使用降阶模型(ROM)的电池热管理

降阶模型(Reduced Order Model)的好处

- 作为一种通用的热分析方法，CFD是准确的，但对大规模系统级瞬态分析来说计算周期太长
- ROM可以显著降低模型规模和模拟时间，是系统级模拟的重要工具。



使用降阶模型(ROM)的电池热管理

什么是降阶模型(ROM)?

- ROMs是一种紧凑模型 (低阶),是由计算机生成的高保真(3D)模型的数值表达,用于保留模型的基本行为和主导效应。任何紧凑模型一般都可以被宽泛地称为ROM。

请注意: ROM具有设计相关性,必须针对每个设计单独生成。

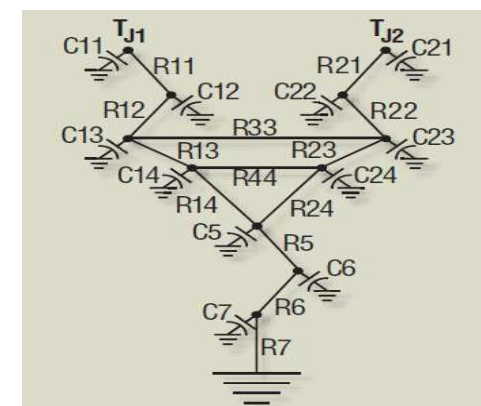
两种电池热管理模型

■ 第一种: 热网络模型

- 需要仔细计算和校准
- 精度一般
- 定义上不是ROM, 而是紧凑模型

■ 第二种: 降阶模型 (ROM)

- 可以和CFD一样准确
- 无需校准 (电容电阻值)



热网络模型

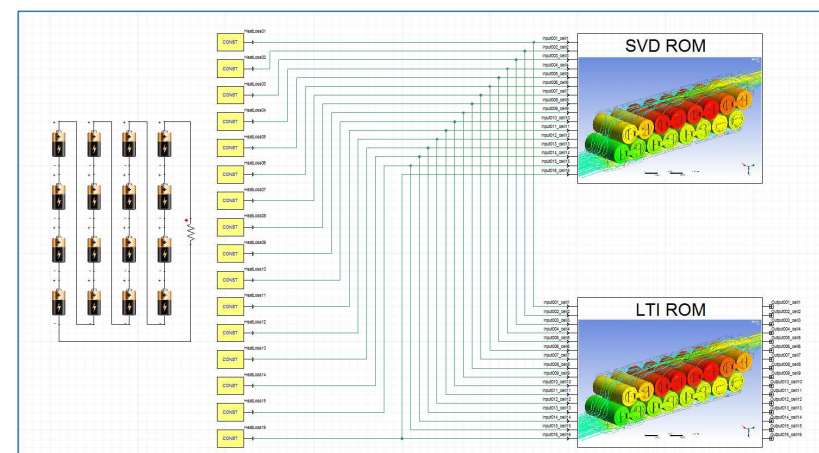
ROMs 可用于

- 大幅加速3D仿真 (ROM for 3D)
- 用于执行高效的系统模拟 (ROM for Systems)
- 支持非传统用户探索设计空间 (ROM for simulation democratization)
- 作为控制系统设计和验证的physical plant model并提高其精度(ROM for controls design, ROMs "inside" controls)

耦合ECM与ROM的电池系统仿真

ROMs/ECM 交互:

- ECM计算出电池动态I-V特性
- ECM计算热源，并将热源提供给两个ROM模型；
- LTI ROM计算各电池平均温度，并将其传入ECM中；
- SVD ROM计算各电池温度分布：
 - 温度场需要在Fluent的后处理中显示.

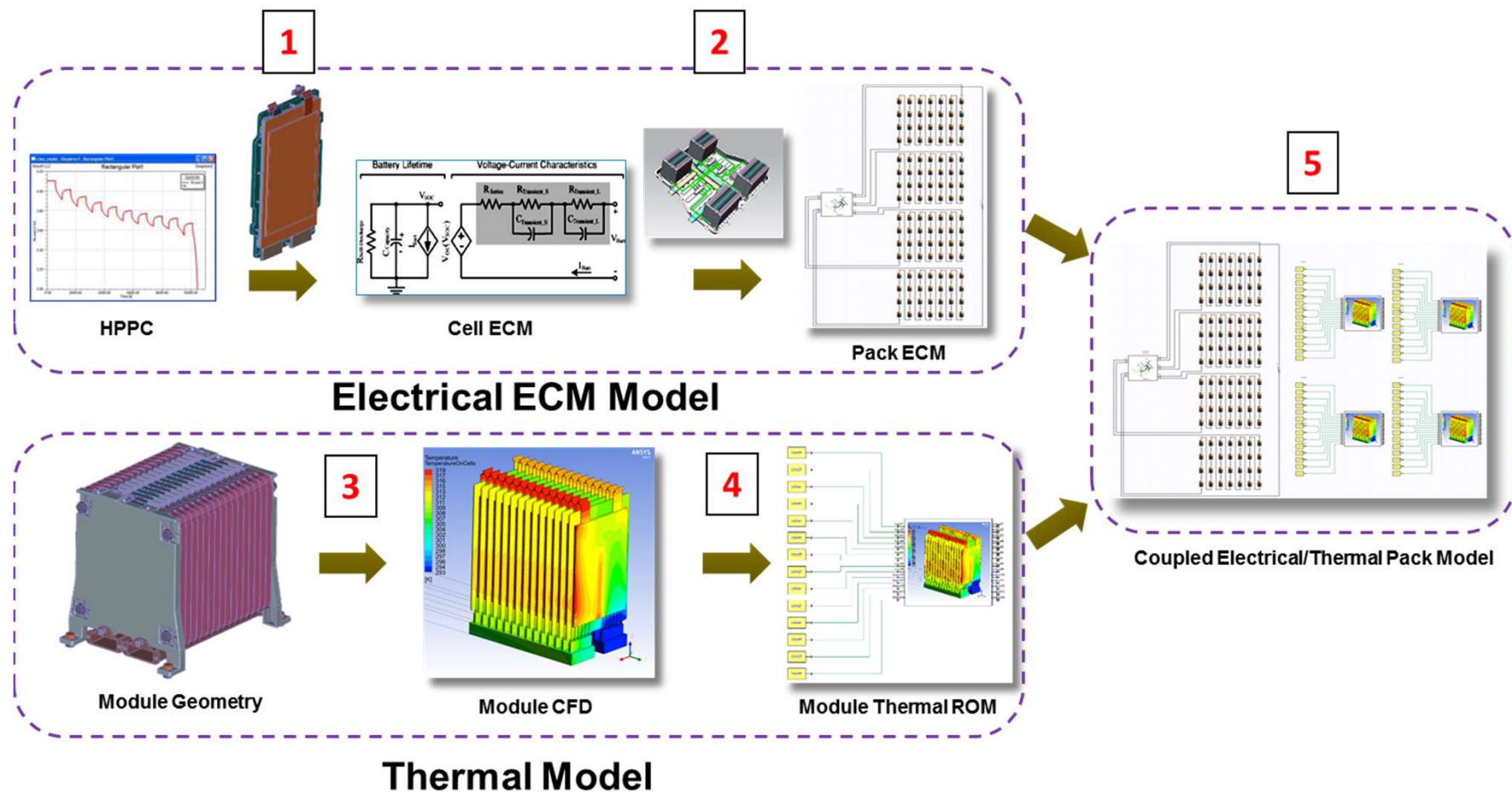


GM电池模拟案例

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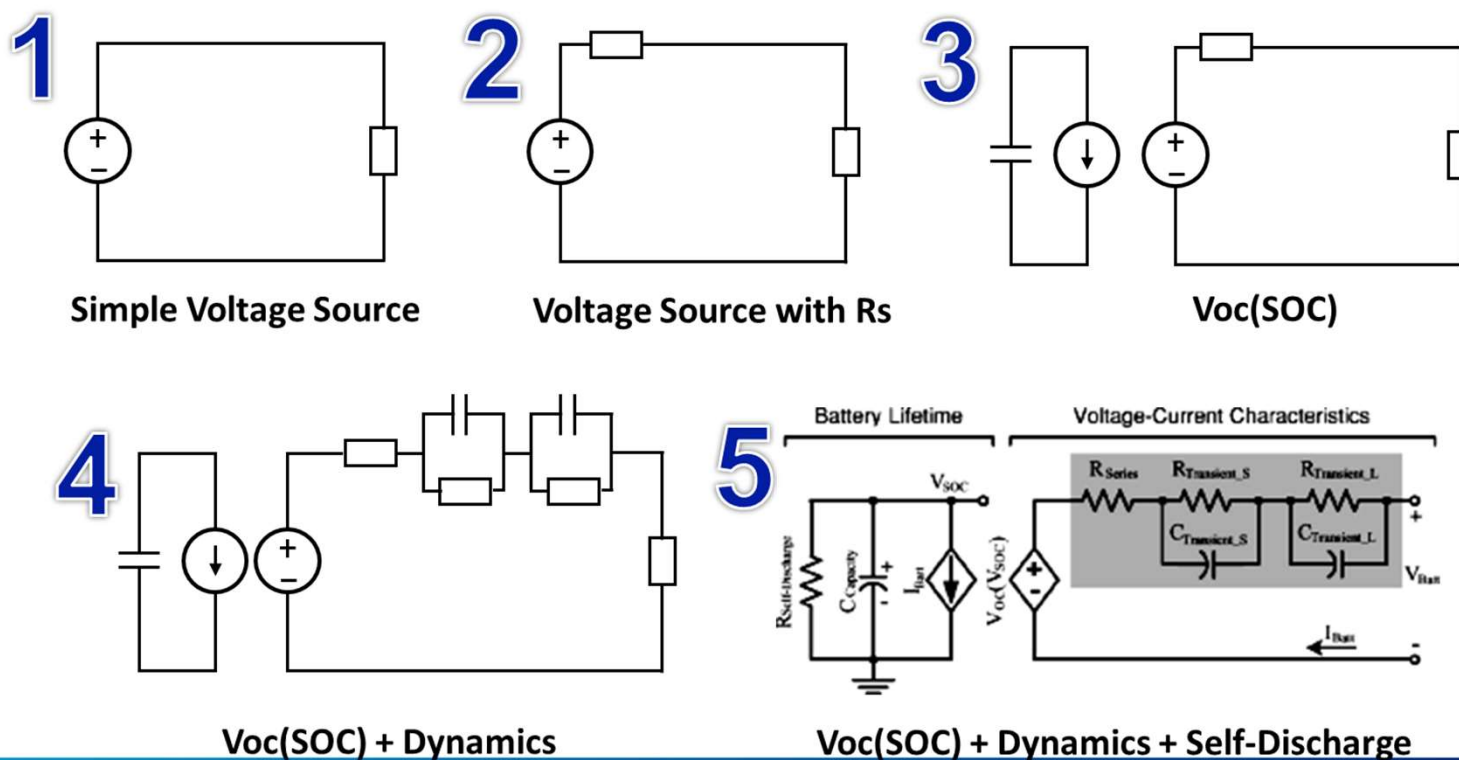
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基于ECM的电池(系统)动态特性仿真最佳实践



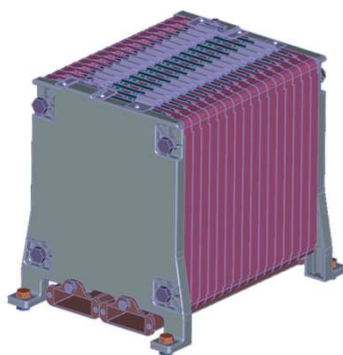
基于ECM的电池(系统)动态特性仿真最佳实践

Step 1: 单电池级ECM的搭建(原理)

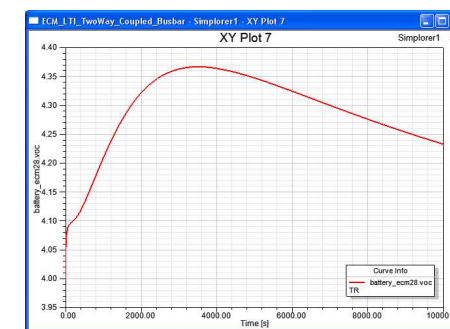
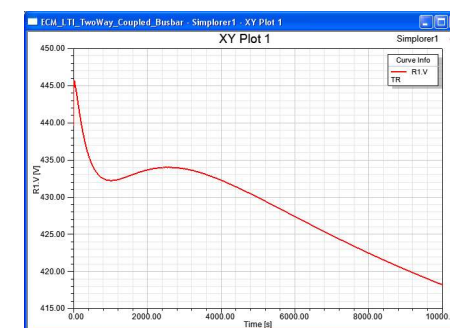
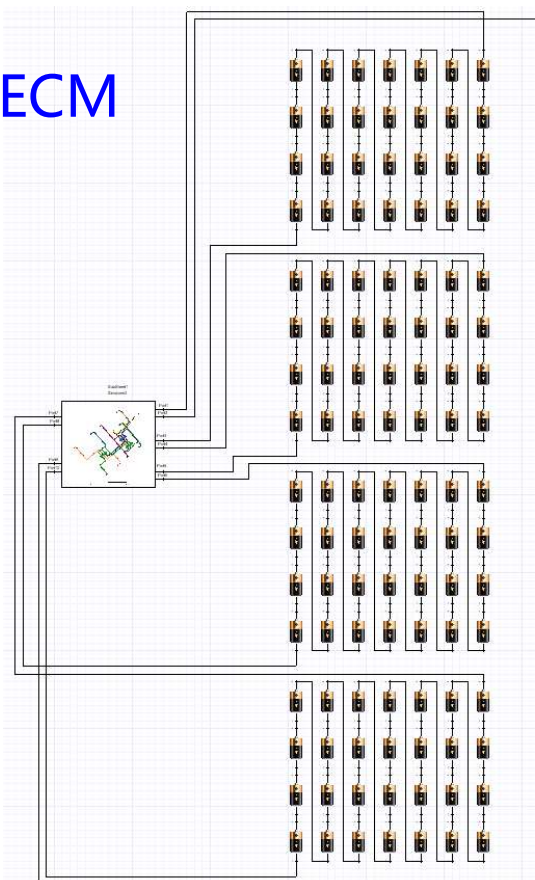


基于ECM的电池(系统)动态特性仿真最佳实践

Step 2: Module/Pack级别的电池ECM



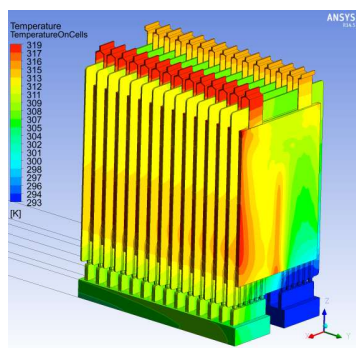
- 电池模块包含了28个电池单体
- 最终仿真的电池系统包含了4个模块



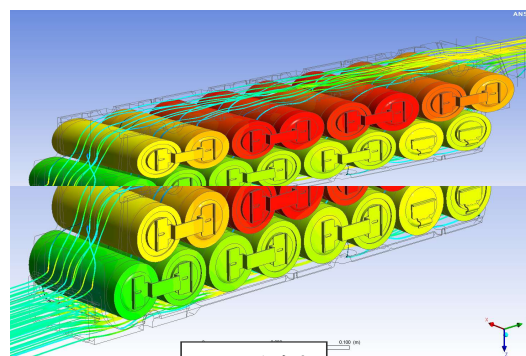
仿真结果

基于ECM的电池(系统)动态特性仿真最佳实践

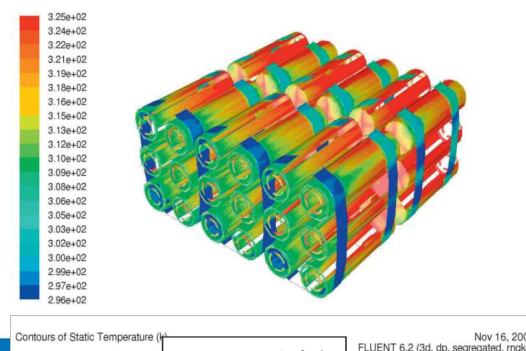
Step 3: 通过CFD进行共轭传热计算 (给定冷却方式下)



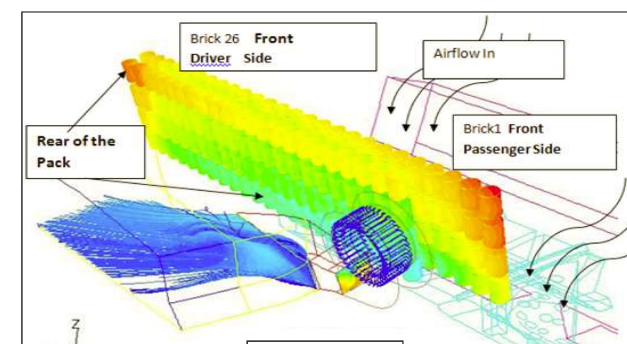
ANSYS 案例



GM 案例



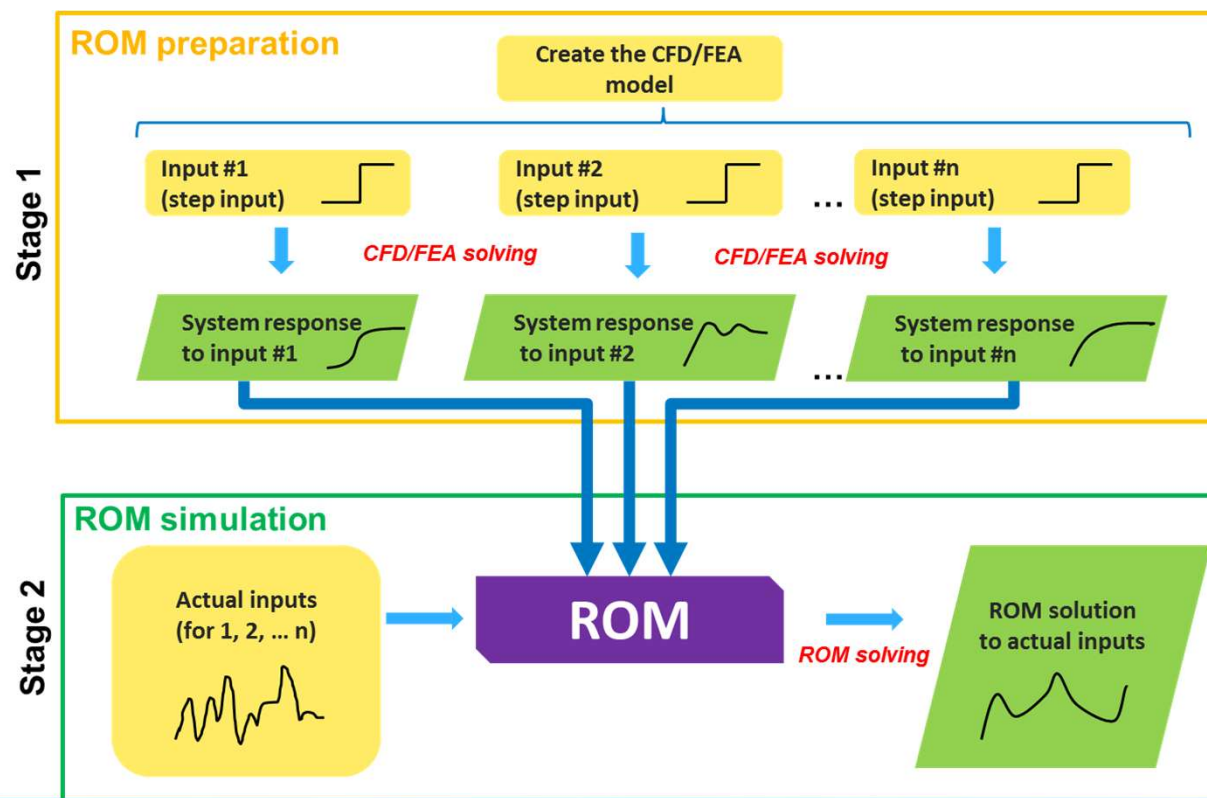
Magna 案例



Ford 案例

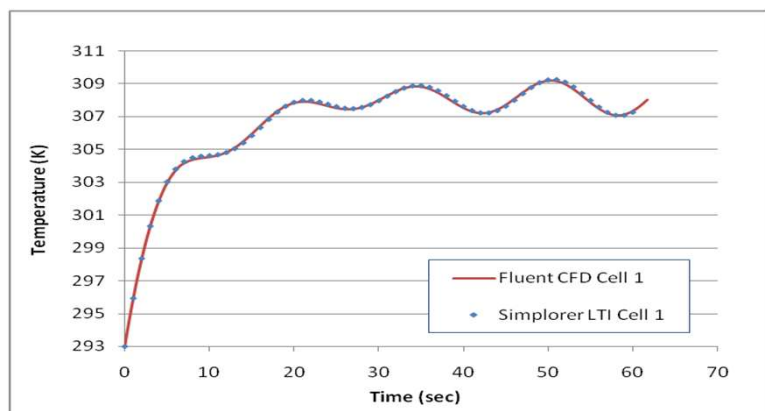
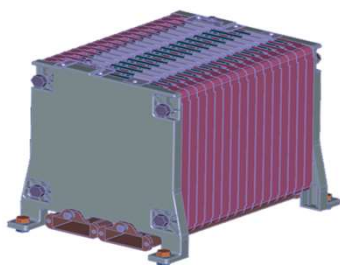
基于ECM的电池(系统)动态特性仿真最佳实践

Step 4-1: 创建降阶模型流程

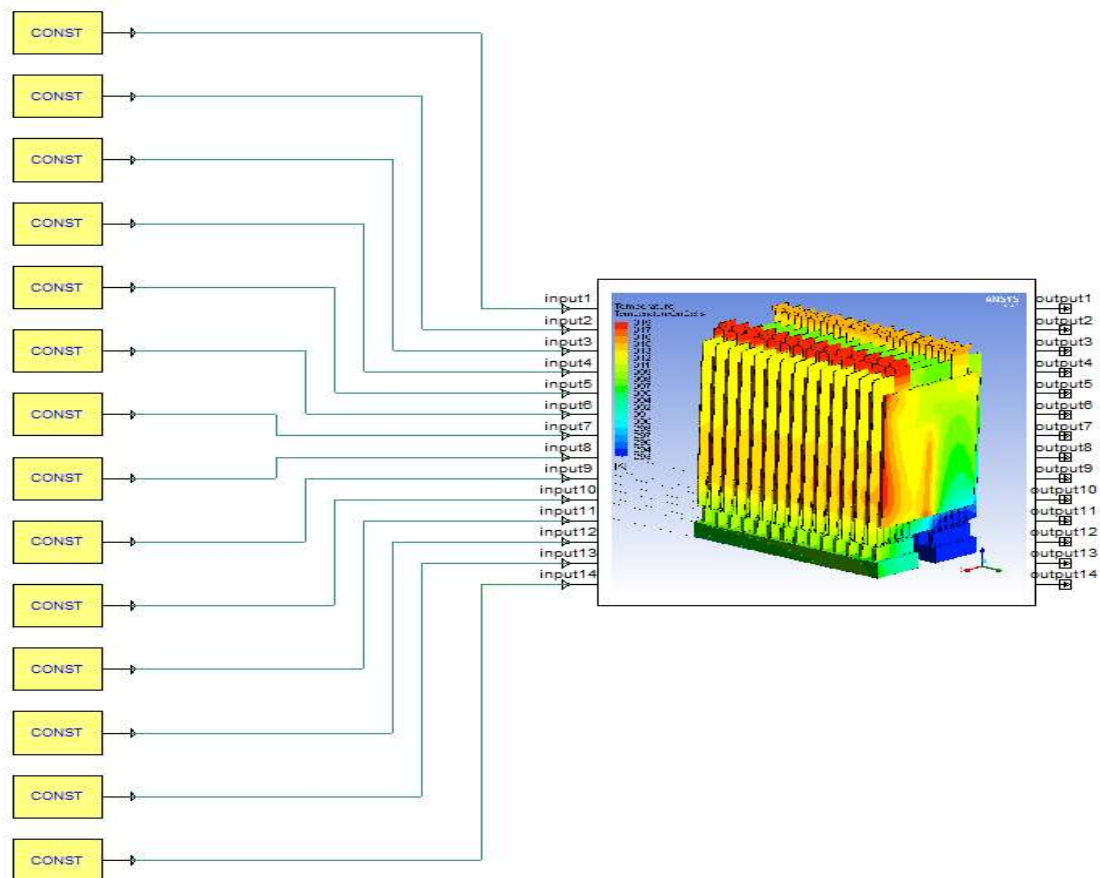


基于ECM的电池(系统)动态特性仿真最佳实践

Step 4-2: 降阶模型结果分析

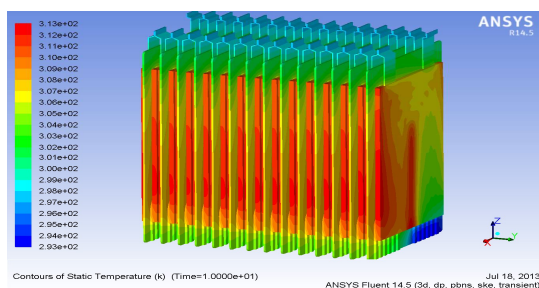


ROM vs CFD

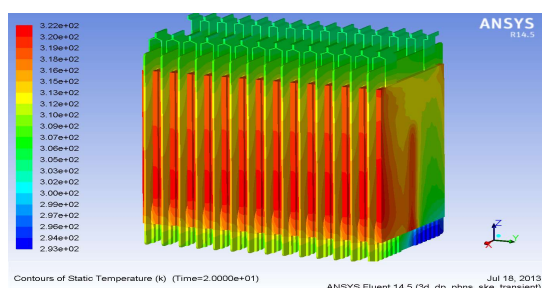


基于ECM的电池(系统)动态特性仿真最佳实践

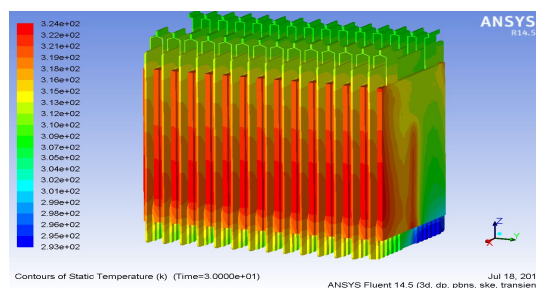
Step 4-2: 降阶模型结果分析 (续)



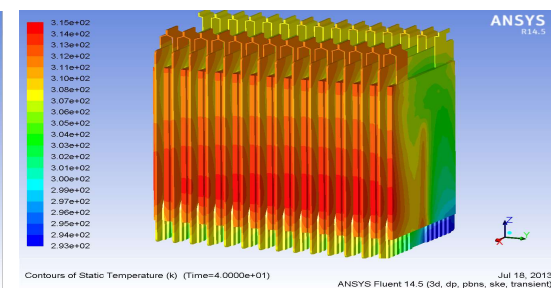
CFD (10 sec)



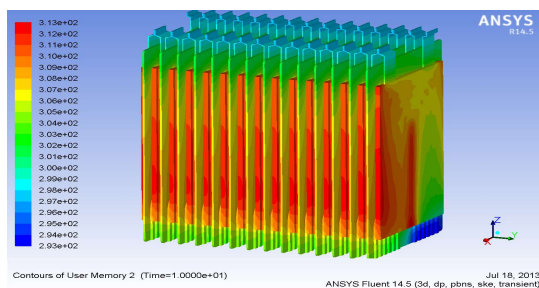
CFD (20 sec)



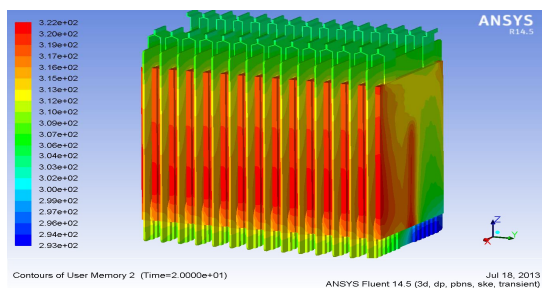
CFD (30 sec)



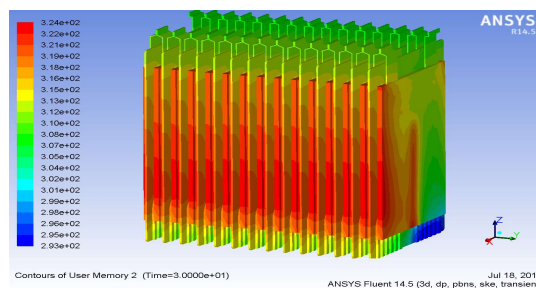
CFD (40 sec)



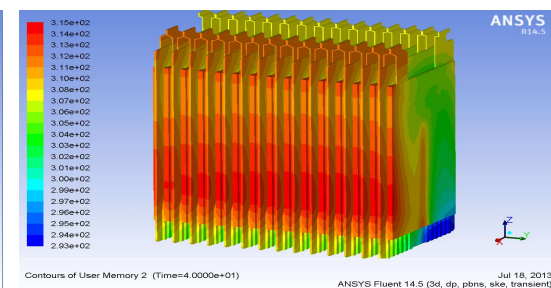
SVD ROM
(10 sec)



SVD ROM
(20 sec)



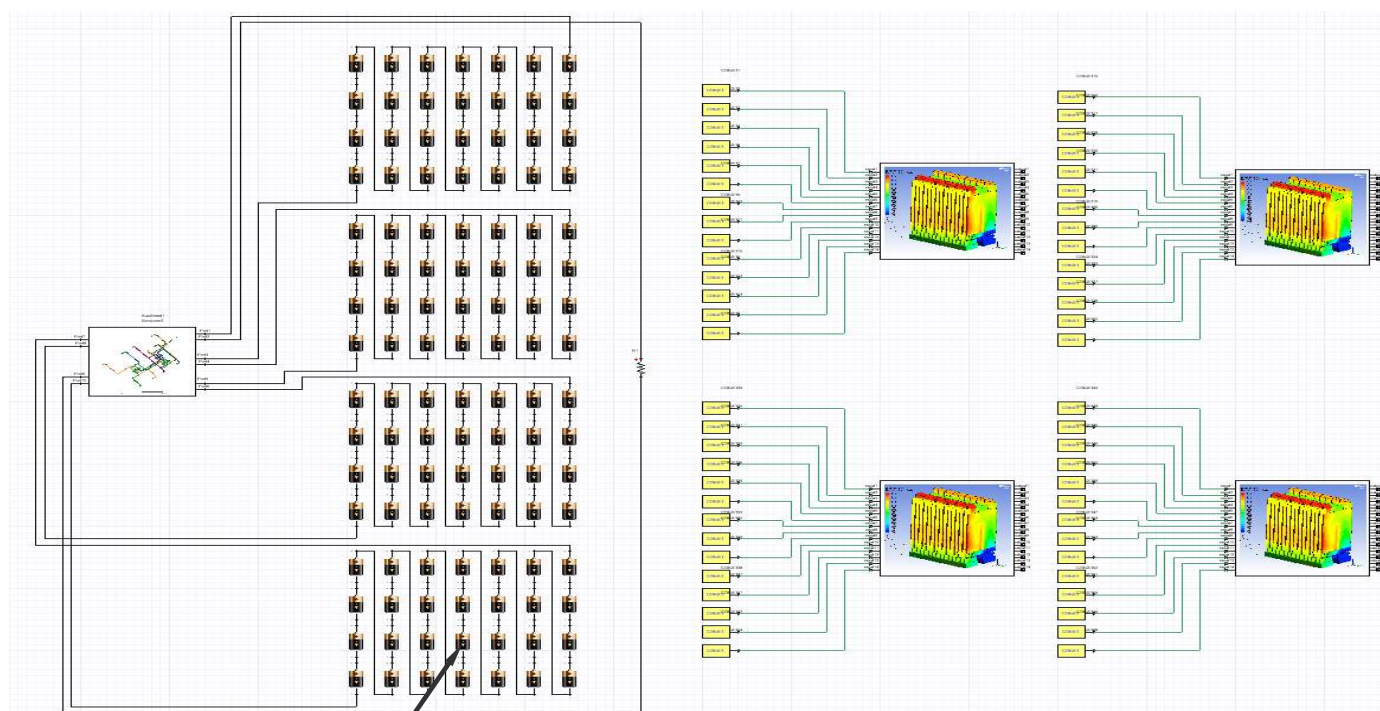
SVD ROM
(30 sec)



SVD ROM
(40 sec)

基于ECM的电池(系统)动态特性仿真最佳实践

Step 5: ECM和ROMs耦合分析

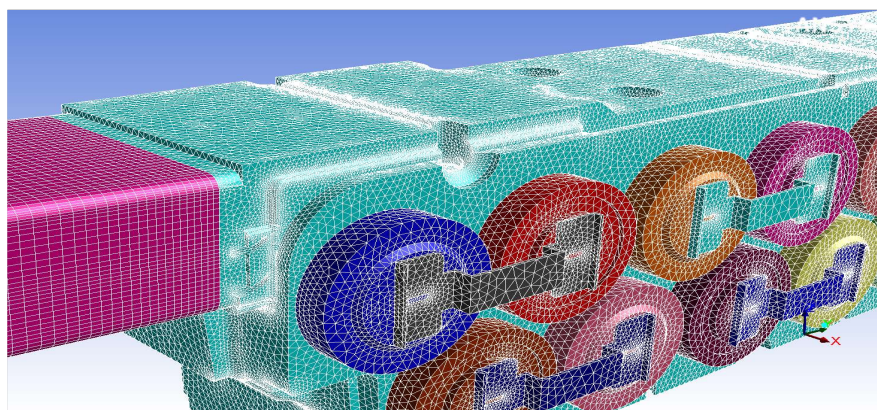
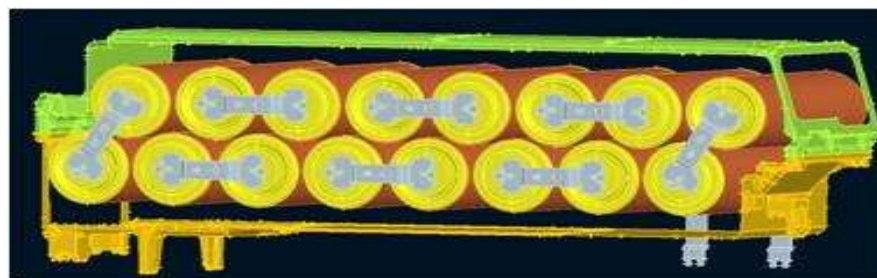


$$V_{oc} = -1.031 \cdot \exp(-35 \cdot (\text{abs}(\text{IBatt.V/Vinit}))) + 3.685 + 0.2156 \cdot (\text{abs}(\text{IBatt.V/Vinit})) - 0.1178 \cdot (\text{abs}(\text{IBatt.V/Vinit}))^2 + 0.3201 \cdot (\text{abs}(\text{IBatt.V/Vinit}))^3 + 0.3/30.0 \cdot (U1.Temp_block_1-273)$$

基于ECM的电池(系统)动态特性仿真最佳实践

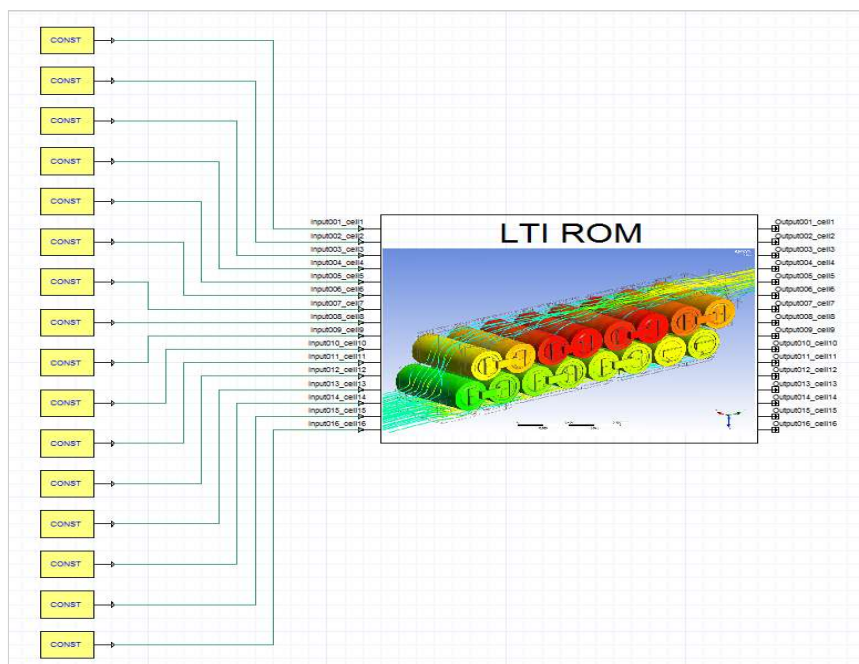
成功案例- GM电池

- 模块由16个电池单体组成.
- CFD模型
 - 混合网格, 网格数量3 百万.

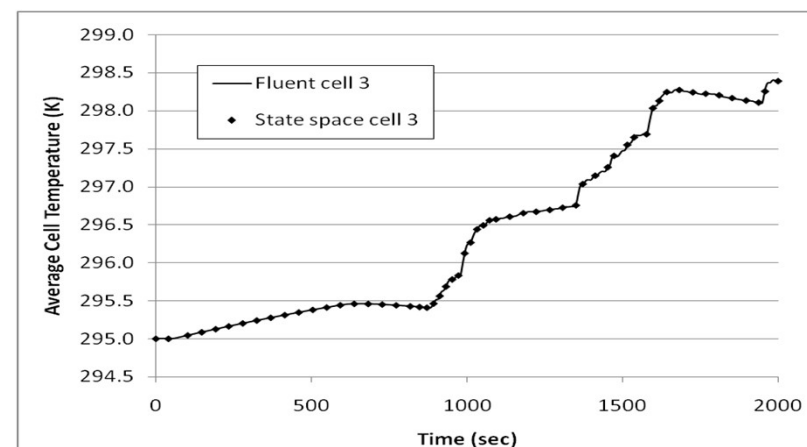
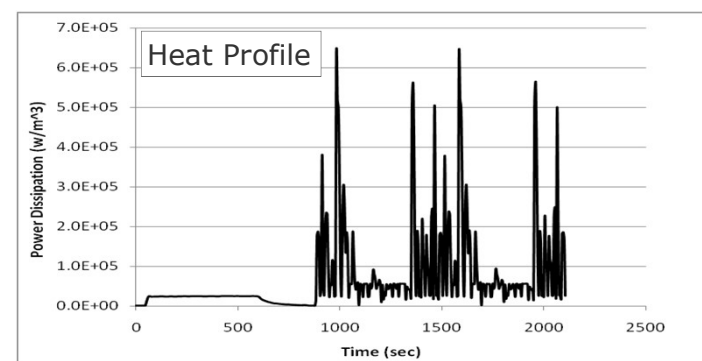


基于ECM的电池(系统)动态特性仿真最佳实践

成功案例- ROM模型



LTI ROM 给出和CFD相同的结果. LTI ROM运行小于20s, 而CFD在单CPU上运行2 小时.

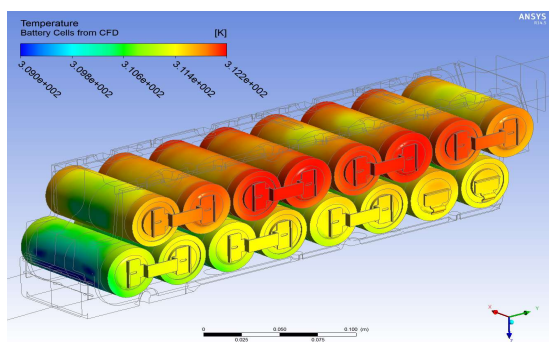


X. Hu, S. Lin, S. Stanton, W. Lian, "A Foster Network Thermal Model for HEV/EV Battery Modeling," IEEE TRANSACTIONS ON INDUSTRY APPLICATIONS, VOL. 47, NO. 4, JULY/AUGUST 2011

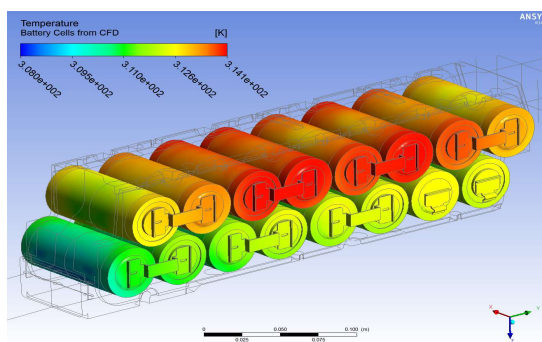
X. Hu, S. Lin, S. Stanton, W. Lian, "A State Space Thermal Model for HEV/EV Battery Modeling", SAE 2011-01-1364

基于ECM的电池(系统)动态特性仿真最佳实践

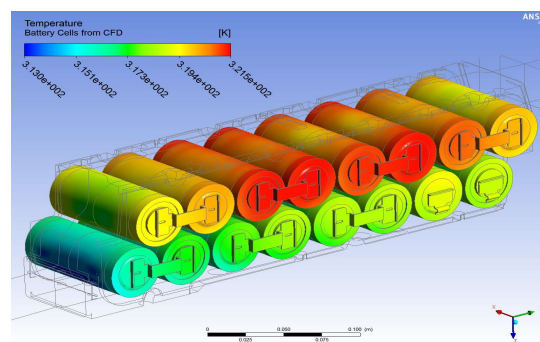
成功案例- ROM结果验证



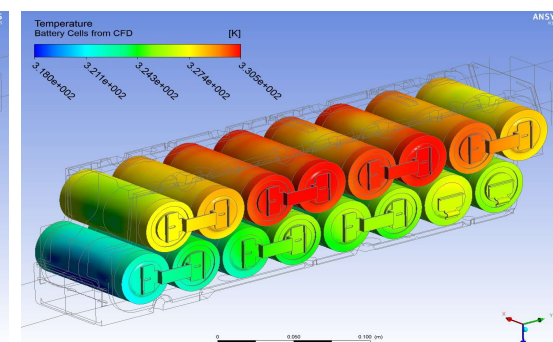
CFD (200 sec)



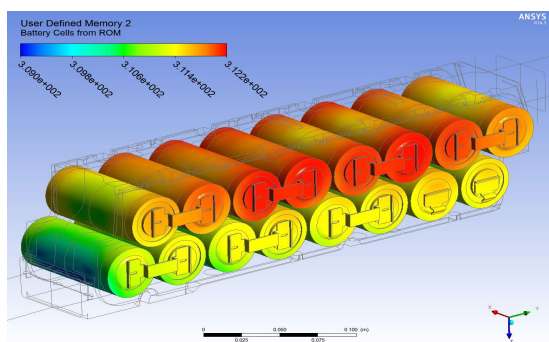
CFD (400 sec)



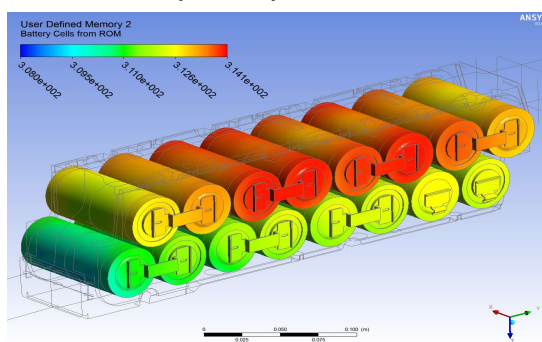
CFD (600 sec)



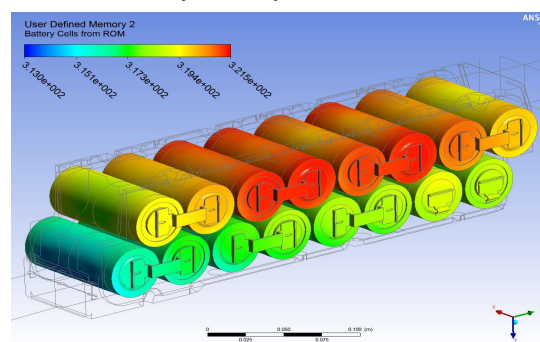
CFD (800 sec)



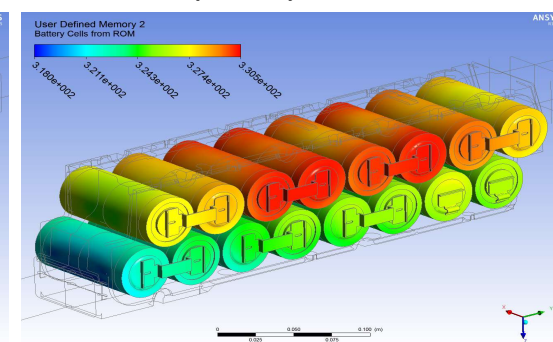
SVD ROM



SVD ROM



SVD ROM



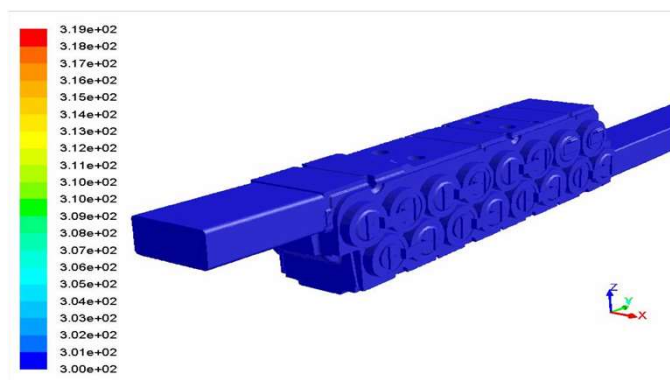
SVD ROM

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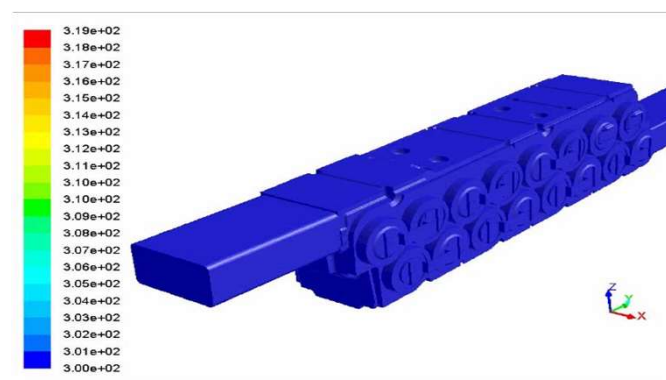
X. Hu, S. Asgari, I. Yavuz, S. Stanton, C-C Hsu, Z. Shi, B. Wang, H-K Chu, "A Transient Reduced Order Model for Battery Thermal Management Based on Singular Value Decomposition," ECCE 2014.

基于ECM的电池(系统)动态特性仿真最佳实践

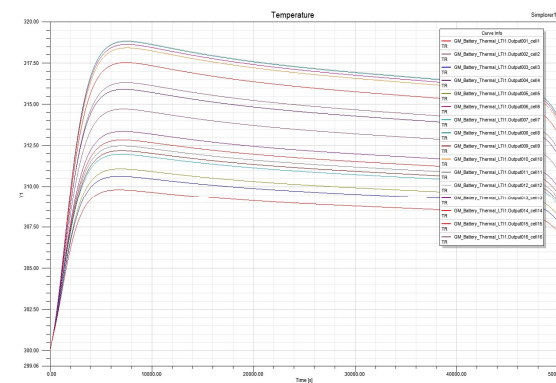
成功案例- 计算结果



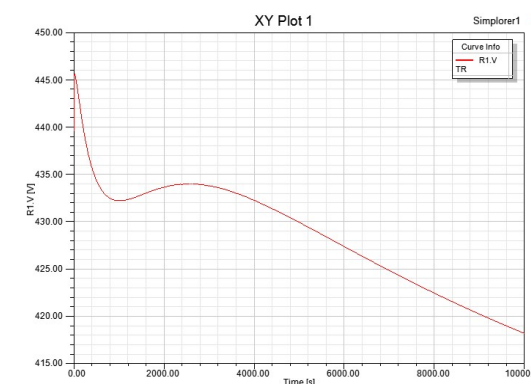
CFD计算的温度结果.
仿真时间7 小时, 使用6个CPU.



SVD ROM计算的温度结果.
仿真时间0.5 小时, 使用1个CPU.



平均 Cell 温度



电池电压随时间变化曲线

目录

1. 综述
2. ANSYS电池仿真方案介绍
3. 基于ECM的电池(系统)动态特性仿真最佳实践
4. 小结及致谢

小结及致谢

小结

- 基于等效电路模型（ECM）的电池动态性能分析方法是一种快速、准确且高效的综合解决方案，充分体现了ANSYS产品在新能源车领域强大的仿真能力，IDAJ在汽车行业深耕多年，将与ANSYS携手为您提供高水平的专业仿真软件和一流的技术服务，期待与您的进一步合作。

致谢

- 感谢ANSYS中国井文明、马世虎，ANSYS北美胡晓博士提供案例资料。



感谢倾听
期待与您的进一步合作 😊



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获得第一手巡展报告下载资讯

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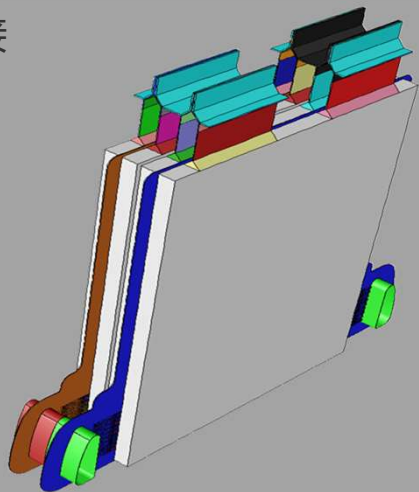
- web: <https://www.idaj.cn/>
- e-mail: support@idaj.cn
- Tel: 021-50588290; 010-65881497

附录1：特别专题

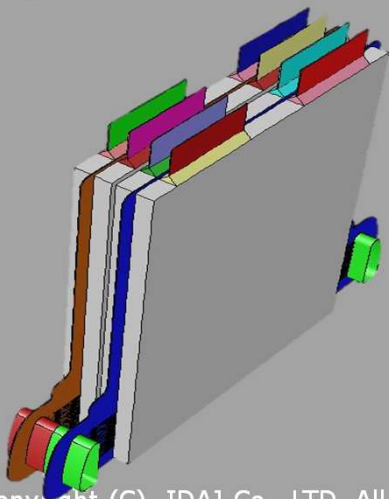
- 虚拟连接 (Virtual connection)
- 电负载输入 (Electric load profile)
- 参数估计工具 (Parameter estimation tool)
- 热滥用模型 (Thermal abuse models)
 - 内部短路模型 (Internal short circuit model)
 - 热滥用模型 (Thermal abuse models)
- Fluent的降阶模型 (ROM)
- 独立的Echem 模型^β (Standalone Echem Model^β)

虚拟连接

真实连接



虚拟连接



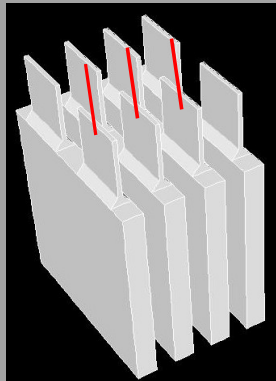
为什么需要虚拟连接?

- 连接通过真实几何/网格实现。电流会自动从负极流到正极。母排上的焦耳热同时获得求解
- 但母排通常非常薄，这会对网格的产生造成一定程度的困难。
 - 虚拟连接可以解决上述问题
- 数值上，虚拟连接也要比真实连接更稳定

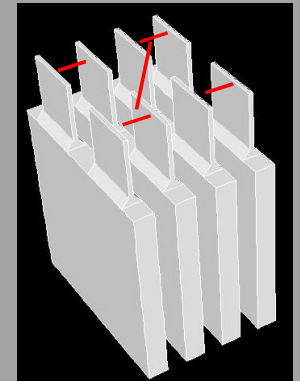
- 文件格式: 串联一级中的并联电池数量 (mP), 串联级数 (nS), 后面跟着每个电池负极片和正极片的名称, 顺序为 1P1S ... 1PnS 到 mP1S ... mPnS

虚拟连接文件格式

```
mp      1
nS      4
tab_N_1  tab_P_1
tab_N_2  tab_P_2
tab_N_3  tab_P_3
tab_N_4  tab_P_4
```



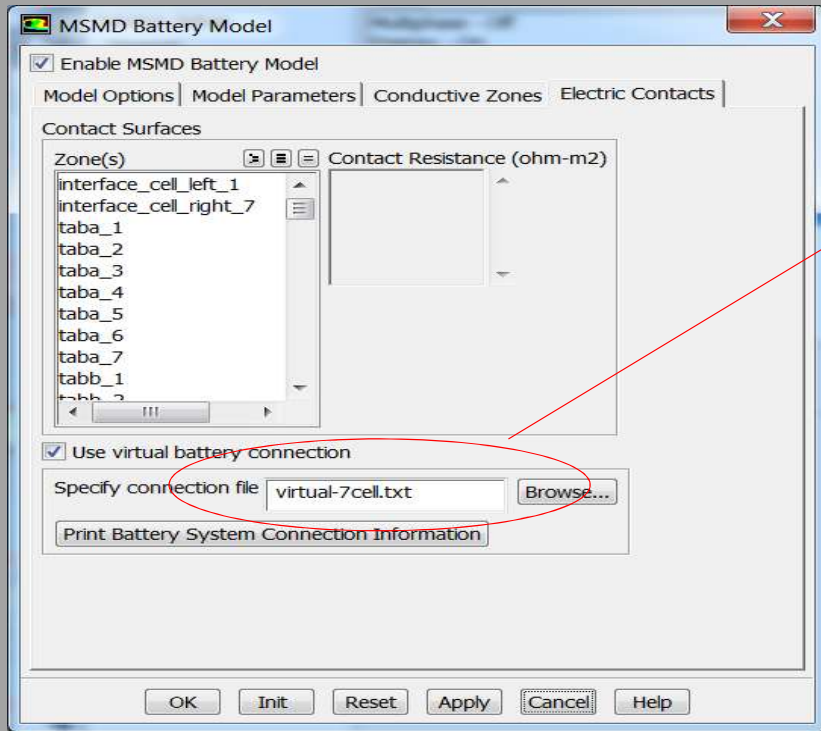
```
mp      2
nS      2
tab_N_1  tab_P_1
tab_N_2  tab_P_2
tab_N_3  tab_P_3
tab_N_4  tab_P_4
```



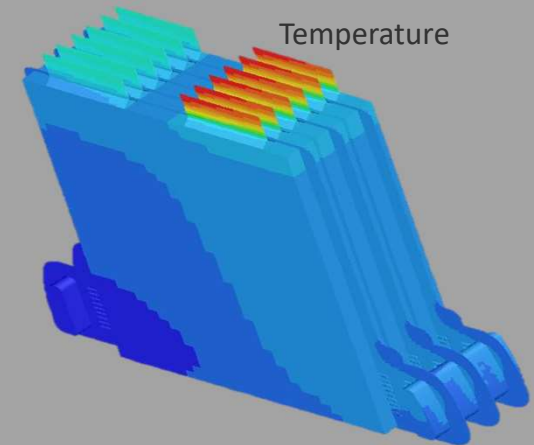
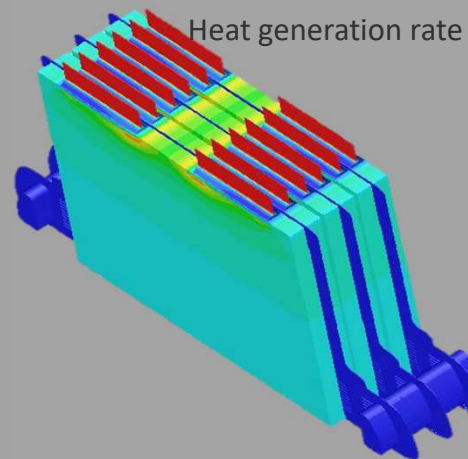
- 通过电池标签和mP和nS值的顺序定义电池连接。
 - 求解器会找出哪个导电区属于哪个电池.
 - 求解器将通过虚拟连接处理每个单独电池的边界条件.

案例 - GM's quarter model (液冷, 2P3S)

- 就像真实连接一样, 用户提供最少的信息。求解器尝试做最多的工作
- !!
- 连接信息在一个简单的文本文件中定义

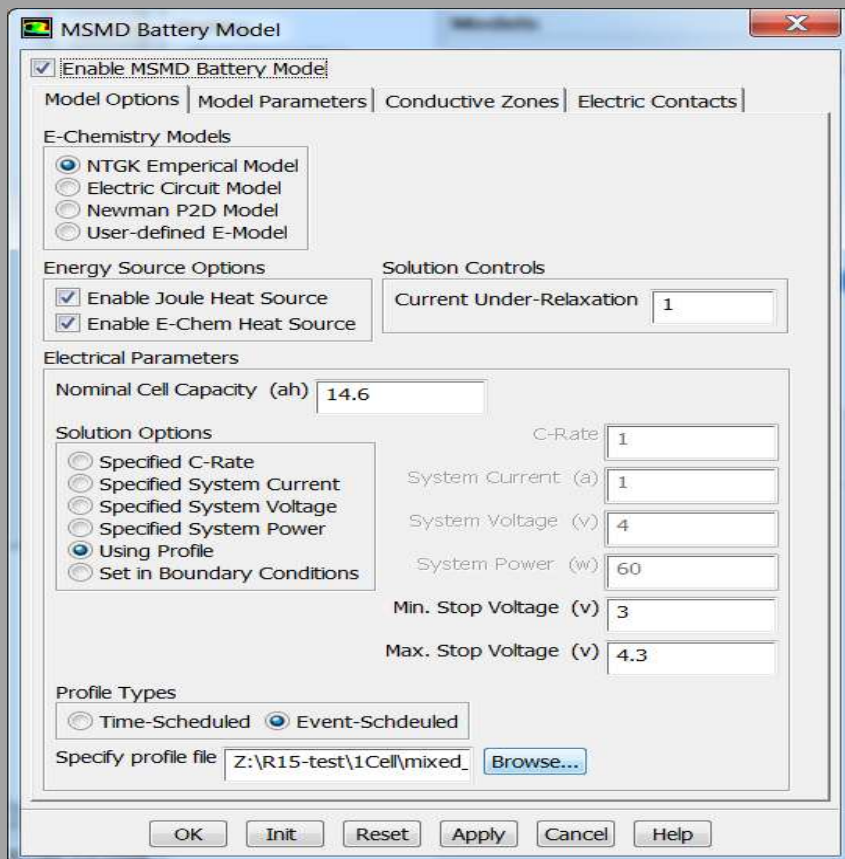


```
virtual-connection-2P3S.txt
mp      2
nS      3
tab_negative_a_1  tab_positive_a_1
tab_negative_b_1  tab_positive_b_1
tab_negative_a_2  tab_positive_a_2
tab_negative_b_2  tab_positive_b_2
tab_negative_a_3  tab_positive_a_3
tab_negative_b_3  tab_positive_b_3
```



■电负载输入

Electric Load Profiles

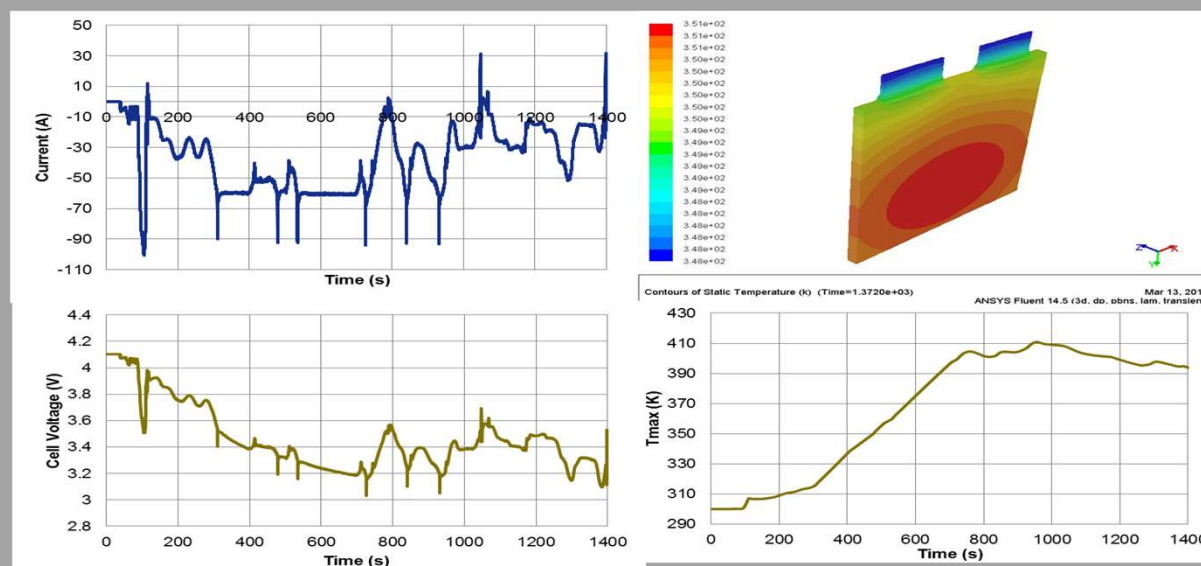


- **FLUENT中可以执行两种格式的profile文件:**
 - 基于时间的Profile
 - 基于事件的Profile
- **两种方法均支持在模拟过程中改变负载类型和数值**

案例

USO6循环试验

time-scheduled-profile.dat				
0	0			3
19	0			3
20	0			3
21	36.076500			3
22	35.5065			3
23	57.531			3
24	70.2525			3
25	79.3665			3
26	87.7215			3
27	23.9235			3
28	34.9365			3
29	104.43			3
30	49.3665			3
31	39.873			3
32	17.2785			3



基于事件的profile案例

event-scheduled-profile.dat				
1	15	1	500	0
1	0	1	1000	0
3	60	4	3.5	0
1	-15	5	4.1	0
2	4.1	3	-5.0	1



参数估计工具

参数估计工具

NTGK，ECM和热滥用模型中的模型参数是电池专用的。用户需要在模拟之前对来自测试数据的那些参数进行曲线拟合。

所需的测试数据

- NTGK:以不同的C率放电曲线
- ECM:不同SOC水平下脉冲电流下的电压响应曲线（HPPC测试数据）
- 热滥用模型: Oven test data (temperature ~ time)

该工具在FLUENT的文本用户界面(TUI)中可用

define/model/battery-model/parameter-estimation-tool

NTGK模型的拟合工具

```
/define/models/battery-model> parameter-estimation-tool
Parameter Estimation for Model:
  1: NTGK Model
  2: ECM Model
  3: Thermal Abuse Model
Model option: [3] 1
Number of discharging curves: [2]

-- Make sure every input file has this format --
Crate      1.0
time_1      voltage_1
time_2      voltage_2
...         ...

-----

file name for curve 1 [] ntgk_1C.txt
file name for curve 2 [] ntgk_2C.txt
Battery capacity (Ah) [14.6]
Battery active zone volume (m^3) [1]
Specific area (1/m) [1]
Number of DOD-levels [30]
```

U, Y 拟合成5阶多项式，多项式系数自动输入到面板中！

Table of U and Y as a function of DOD

DOD	U	Y	Dev_U	Dev_Y	R^2
0.002778	4.117775	1144.649157	0.000025	0.000001	0.999999
0.035010	4.093107	915.083533	0.000039	0.000001	0.999998
0.067241	4.070459	767.265281	0.000023	0.000000	1.000000
0.099473	4.049471	681.071473	0.000012	0.000000	1.000000
0.131705					1.000000
0.163937					1.000000
0.196169					1.000000
0.228400					1.000000
0.260632					1.000000
0.292864					1.000000
0.325096					1.000000
0.357328					0.999999
0.389559					1.000000
0.421791					1.000000
0.454023					1.000000
0.486255					1.000000
0.518487					1.000000
0.550718					1.000000
0.582950					1.000000
0.615182					1.000000
0.647414					1.000000
0.679646					1.000000
0.711877					1.000000

Curve-fitting results using 4-th order polynomial:
U= + 4.120002e
Y= + 1.003439e

Curve-fitting results using 4-th order polynomial:

U= + 4.119995e+00×DOD⁰ - 8.038110e-01×DOD¹ + 1.074002e+00×DOD² - 1.175381e+00×DOD³
Y= + 1.045233e+03×DOD⁰ - 3.879759e+03×DOD¹ + 1.143114e+04×DOD² - 1.322104e+04×DOD³

Curve-fitting results using 5-th order polynomial:

U= + 4.119983e+00×DOD⁰ - 8.032986e-01×DOD¹ + 1.069836e+00×DOD² - 1.162907e+00×DOD³
Y= + 1.169159e+03×DOD⁰ - 8.940600e+03×DOD¹ + 5.258548e+04×DOD² - 1.364417e+05×DOD³

MSMD Battery Model

☒ Enable MSMD Battery Model

Model Options | Model Parameters | Conductive Zones | Electric Contacts

NTGK Model Polarization Parameters

Initial DoD: 0 Reference Capacity (ah): 14.6

U Coefficients

a0: 4.119983 a1: -0.8033 a2: 1.069836 a3: -1.16291

a4: -0.01638 a5: 0.006851

Y Coefficients

b0: 1169.159 b1: -8940.6 b2: 52585.48 b3: -136442

b4: 158771.7 b5: -67677.9

Temperature Corrections

C1: 0 C2: 0

ECM模型的拟合工具

```
/define/models/battery-model> parameter-estimation-tool
Parameter Estimation for Model:
  1: NTGK Model
  2: ECM Model
  3: Thermal Abuse Model
Model option: [3] 2
Number of different SOC-level curves: [1] 9
```

```
-- Make sure every input file has this format --
SOC      0.6
I        3.153
time_1   voltage_1
time_2   voltage_2
...
```

```
-----
where SOC: soc level
I: current
file name for curve 1 [] ecm-soc01.txt
file name for curve 2 [] ecm-soc02.txt
file name for curve 3 [] ecm-soc03.txt
file name for curve 4 [] ecm-soc04.txt
file name for curve 5 [] ecm-soc05.txt
file name for curve 6 [] ecm-soc05.txt
```

Uoc, Rs, R1, C1, R2,

Uoc	Rs
10e+00	2.296226e-02
10e+00	2.277196e-02
10e+00	2.251824e-02
10e+00	2.226451e-02
10e+00	2.220108e-02
10e+00	2.220108e-02
10e+00	2.197907e-02
10e+00	2.191564e-02
10e+00	2.169363e-02

MSMD Battery Model

☒ Enable MSMD Battery Model

Model Options | Model Parameters | Conductive Zones | Electric Contacts

Electric Circuit Model Parameter

Initial State of Charge: 1 | Reference Capacity (ah): 0.85

☒ Using polynomials
☐ Using different coefficients for charging and discharging

Discharging parameters

Rs Coefficients

rs0	0.022836	rs1	0.0042393	rs2	-0.03816
rs3	0.0951994	rs4	-0.102394	rs5	0.0399531

R1 Coefficients

r10	0.0977778	r11	-0.149711	r12	0.4472866
r13	-2.13994	r14	3.647721	r15	-1.957207

error

-02 (D)
-02 (D)
-02 (D)
-02 (D)
-02 (D)
-02 (D)
-02 (D)
-02 (D)

Curve-fitting results using 4-th order polynomial:

UOC = + 3.216624e+00 *SOC^0 - 1.609146e-01 *SOC^1 + 8.490771e-01 *SOC^2 - 9.194593e-01 *SOC^3 + 2.762556e-01 *SOC^4
RS = + 2.308944e-02 *SOC^0 - 4.286351e-04 *SOC^1 - 9.700839e-03 *SOC^2 + 1.966657e-02 *SOC^3 - 1.199468e-02 *SOC^4
R1 = + 8.536319e-02 *SOC^0 + 7.895776e-02 *SOC^1 - 9.468551e-01 *SOC^2 + 1.560227e+00 *SOC^3 - 7.807255e-01 *SOC^4
C1 = + 5.948013e+02 *SOC^0 + 8.311781e+01 *SOC^1 + 4.331012e+01 *SOC^2 + 4.480362e+03 *SOC^3 - 3.447726e+03 *SOC^4
R2 = + 1.238981e-02 *SOC^0 - 3.713808e-04 *SOC^1 - 1.350004e-02 *SOC^2 + 1.115110e-02 *SOC^3 - 2.675919e-02 *SOC^4
C2 = + 1.199374e+02 *SOC^0 - 7.873988e+01 *SOC^1 + 4.100710e+02 *SOC^2 - 5.820765e+02 *SOC^3 + 2.648964e+02 *SOC^4

Curve-fitting results using 5-th order polynomial:

UOC = + 3.176970e+00 *SOC^0 + 5.694929e-01 *SOC^1 - 3.604045e+00 *SOC^2 + 1.089949e+01 *SOC^3 - 1.386894e+01 *SOC^4 + 5.124187e+00 *SOC^5
RS = + 2.283602e-02 *SOC^0 + 4.239268e-03 *SOC^1 - 3.815994e-02 *SOC^2 + 9.519936e-02 *SOC^3 - 1.023941e-02 *SOC^4 + 1.957207e-02 *SOC^5
R1 = + 9.777778e-02 *SOC^0 - 1.497114e-01 *SOC^1 + 4.472866e-01 *SOC^2 - 2.139940e+00 *SOC^3 + 3.647721e+00 *SOC^4 - 1.957207e+00 *SOC^5
C1 = + 4.525364e+02 *SOC^0 + 2.703549e+03 *SOC^1 - 1.593284e+04 *SOC^2 + 4.688238e+04 *SOC^3 - 5.419546e+04 *SOC^4 + 5.124187e+04 *SOC^5
R2 = + 1.200167e-02 *SOC^0 + 6.777861e-03 *SOC^1 - 5.708728e-02 *SOC^2 + 1.268352e-01 *SOC^3 - 1.411294e-01 *SOC^4 + 1.957207e-01 *SOC^5
C2 = + 1.335598e+02 *SOC^0 - 3.296563e+02 *SOC^1 + 1.939849e+03 *SOC^2 - 4.642233e+03 *SOC^3 + 5.124187e+03 *SOC^4 - 5.124187e+03 *SOC^5

```
/define/models/battery-model>
```

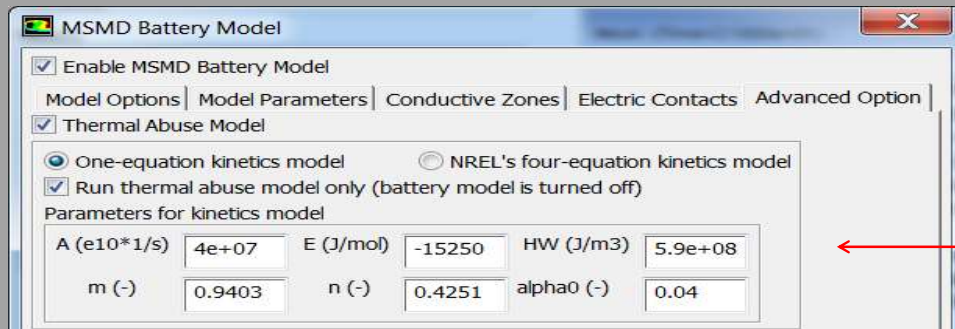
所有6个模型参数都拟合为5阶多项式，多项式系数自动输入到面板中！

热滥用模型的拟合工具

数据可以被拟合为以下两种函数形式:

$$\frac{d\alpha}{dt} = A \exp\left[-\frac{E}{RT}\right] \alpha^m (1-\alpha)^n$$
$$\frac{d\alpha}{dt} = A \exp\left[-\frac{E}{RT}\right] \alpha^m$$

拟合结果自动传到电池的GUI面板上



```
/define/models/battery-model> parameter-estimation-tool
Parameter Estimation for Model:
  1: NTGK Model
  2: ECM Model
  3: Thermal Abuse Model
Model option: [3] 3
```

The fitting is based on the following equation

$$Uol \times rho \times Cp \times dT/dt = Uol \times H \times A \times \exp(-E/RT) \times \alpha^m \times (1-\alpha)^n - Area \times h \times (T-T0) - Area \times \sigma \times \epsilon \times (T^4 - T_{inf}^4)$$

where: Uol battery volume
Area external area
Rho density
Cp specific heat
h heat transfer coefficient
sigma stefan-boltzmann constant
epsilon surface emissivity
H heat of reaction
A pre-exponential factor
E activation energy
alpha reaction progress variable
m,n reaction order

User provides battery's ARC testing data, i.e., temperature~time, and this tool will find kinetics parameters for the one-equation thermal abuse model: H, A, E, m and n.

Note:

n can be set to 0 if user does not want to include (1-alpha)^n term.

```
File name for temperature testing data: [] Cell_T.txt
Density*Cp (J/m3) [2368000]
Battery external area (m^2) [0]
Battery volume (m^3) [0.0001722]
Battery's initial temperature (K) [300]
Ambient temperature for convection (K) [300]
External heat transfer coefficient (W/m^2K) [0]
Enclosure temperature for radiation (K) [300]
Battery's surface emissivity [0]
Fix n=0 or not? [no]
```

Parameter Estimation Results:

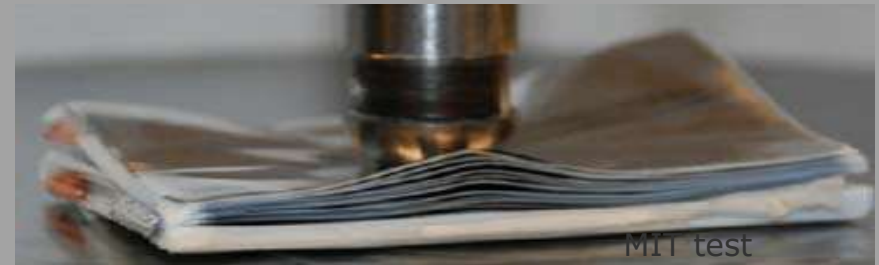
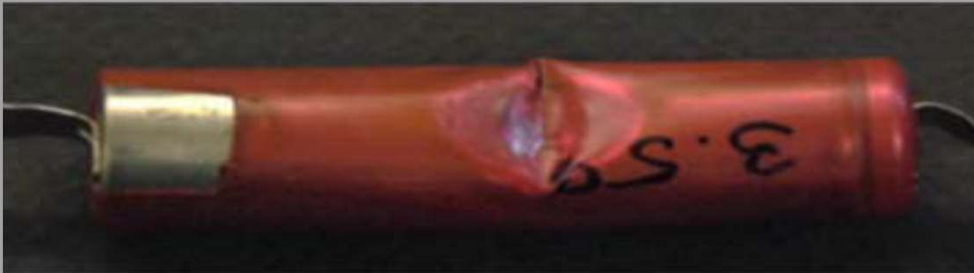
HW=5.858699e+08 A=3.972702e-03 E=-1.524988e+04 m= 0.9403 n= 0.4251

```
/define/models/battery-model>
```

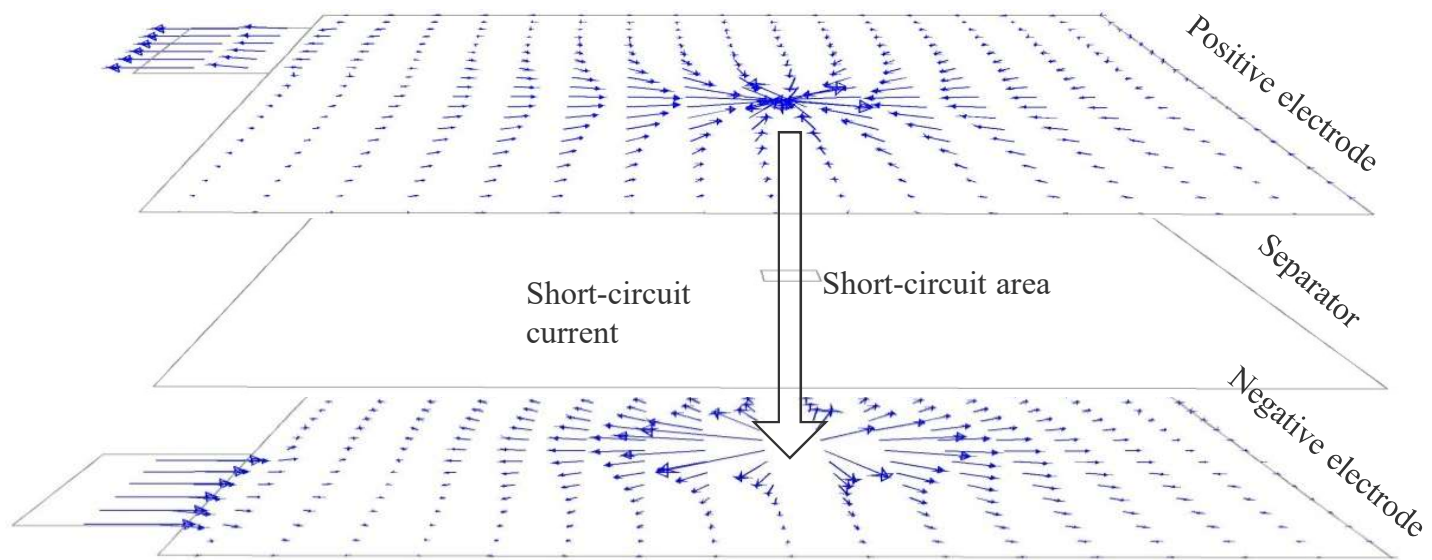
热滥用模型

内部短路

- 内部短路
- 由于电池局部损坏（隔膜破损），产生穿刺或其他事件，导致正极和负极直接接触。



- 内部短路是电池运行的重要故障模式。 这涉及到电池的安全问题。



$$j'_{\text{short}} = \frac{\phi_+ - \phi_-}{r_c}$$

$$q'_{\text{short}} = \frac{(\phi_+ - \phi_-)^2}{r_c}$$

$$I_{\text{ECh}} = I_{\text{short}} + I_{\text{tab}}$$

内部短路处理

- 在存在内部短路的情况下，可以如下修改控制方程：

$$\frac{\partial \rho C_p T}{\partial t} - \nabla \cdot (k \nabla T) = \sigma_+ |\nabla \phi_+|^2 + \sigma_- |\nabla \phi_-|^2 + \dot{q}_{\text{ECh}} + \dot{q}_{\text{short}}$$

$$\nabla \cdot (\sigma_+ \nabla \phi_+) = -(j_{\text{ECh}} - j_{\text{short}})$$

$$\nabla \cdot (\sigma_- \nabla \phi_-) = j_{\text{ECh}} - j_{\text{short}}$$

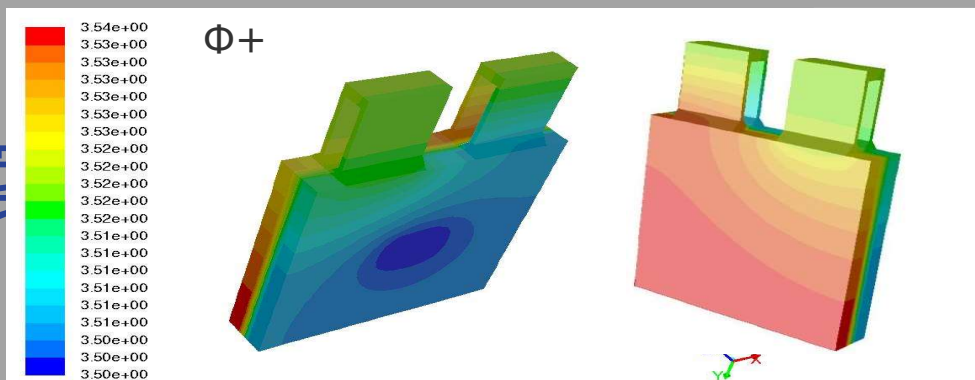
其中

$$j_{\text{short}} = a j'_{\text{short}} = \frac{a(\phi_+ - \phi_-)}{r_c} \quad \dot{q}_{\text{short}} = a \dot{q}'_{\text{short}} = \frac{a(\phi_+ - \phi_-)^2}{r_c}$$

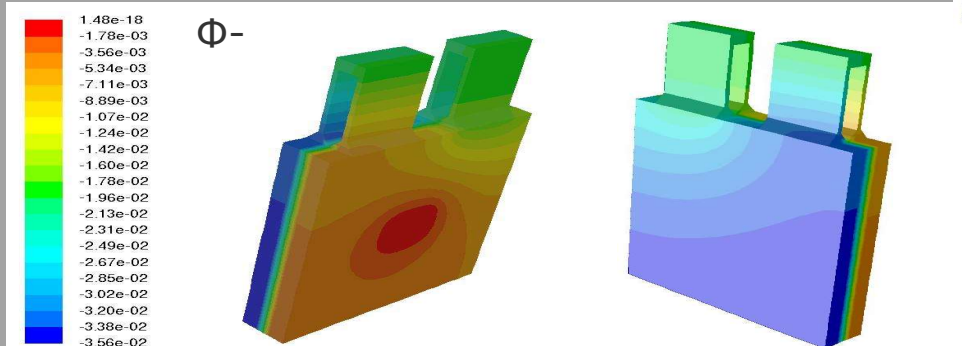
- 短路处理在MSMD框架中完成

注释

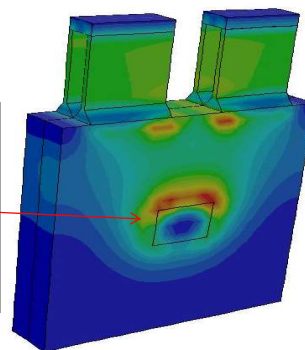
- **All the battery model features are compatible with the electric short treatment** 所有电池型号功能都**兼容**电短路处理
 - 它可以与任何电化学子模型耦合
 - 它可以与热滥用模型耦合
 - 它可以用于电池包仿真
 - 外部短路和内部短路可能同时发生
 - 在正常电池电负载边界条件下会发生电短路
 - 例如，如果电池在恒定电流下工作并发生短路，则由电化学反应产生的总电流=总电极系统电流+总短路电流。 .



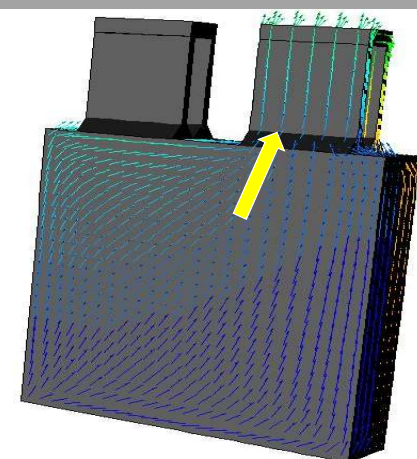
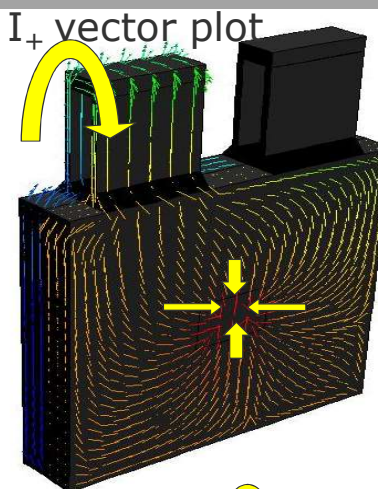
Short circuit occurs only in the square zone of the first battery



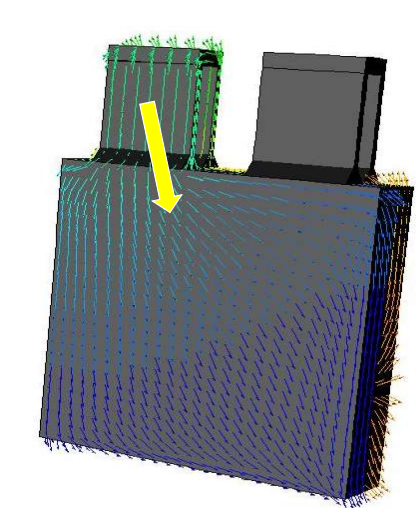
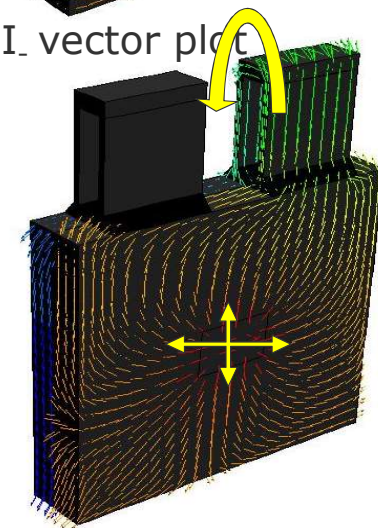
Joule heating rate



I_+ vector plot



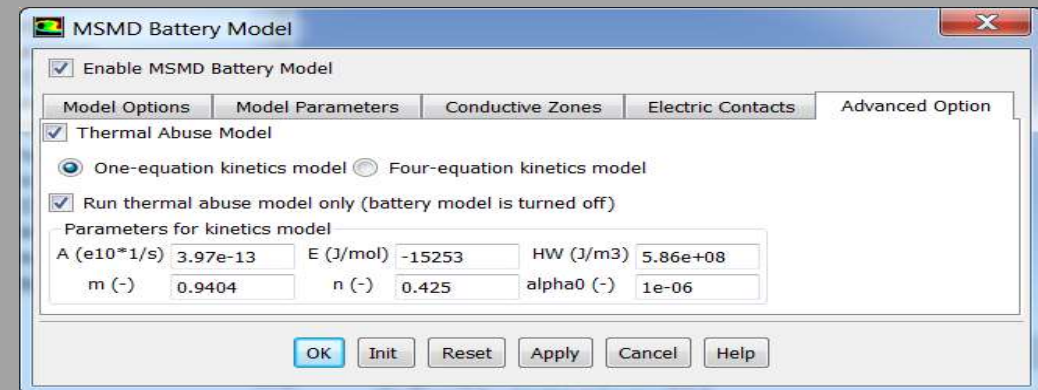
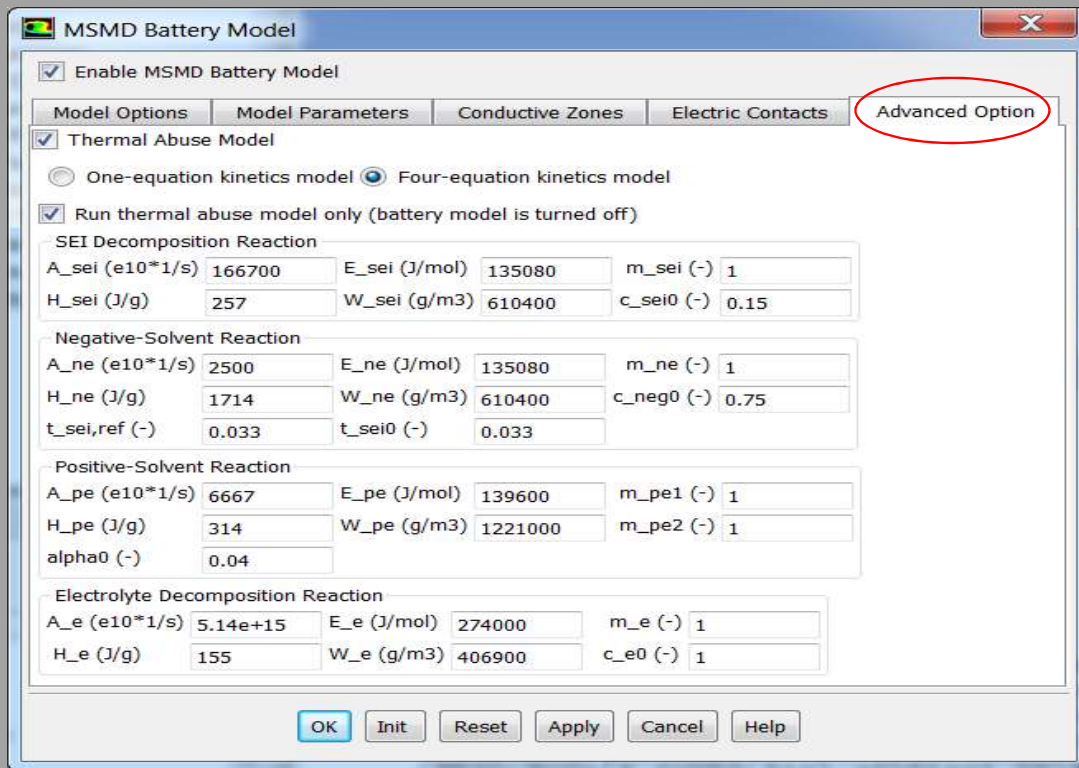
I_- vector plot



热滥用模型

- 在高温下，电池内可能会发生放热分解反应。 Lump kinetics团块动力学模型用于模拟这些分解反应。 .
- Fluent 中提供了两种热滥用模型
 - 一方程模型
 - NREL 四方程模型
- 一个参数估计工具已被放入FLUENT中，以从电池的测试数据中获得单方程模型参数（如前所述）

热滥用模型的GUI设计



- 热滥用模型可以单独运行 (不需要运行电化学模型).
- 单方程模型中的动力学参数可以通过运行FLUENT提供的参数估计工具来获得.

使用拟合工具的过程

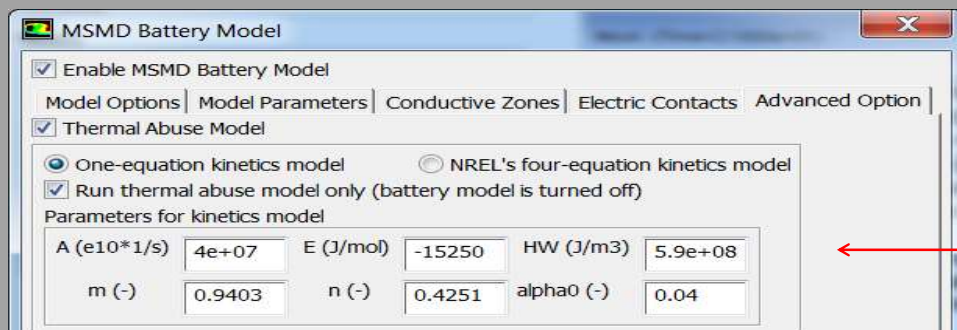
拟合工具在TUI下

define/model/battery/parameter-estimation-tool

数据可以拟合以下两种函数形式:

$$\frac{d\alpha}{dt} = A \exp\left[-\frac{E}{RT}\right] \alpha^m (1-\alpha)^n$$
$$\frac{d\alpha}{dt} = A \exp\left[-\frac{E}{RT}\right] \alpha^m$$

拟合结果自动传到电池的GUI面板上



```
/define/models/battery-model> parameter-estimation-tool
Parameter Estimation for Model:
  1: NTGK Model
  2: ECM Model
  3: Thermal Abuse Model
Model option: [3] 3

-----
The fitting is based on the following equation

Uol*rho*Cp*dT/dt = Uol*H*A*exp(-E/RT)*alpha^m*(1-alpha)^n
- Area*h(T-T0) - Area*sigma*epsilon*(T^4-T_inf^4)

where: Uol      battery volume
       Area     external area
       Rho      density
       Cp       specific heat
       h        heat transfer coefficient
       sigma    stefan-boltzmann constant
       epsilon  surface emissivity
       H        heat of reaction
       A        pre-exponential factor
       E        activation energy
       alpha    reaction progress variable
       m,n      reaction order

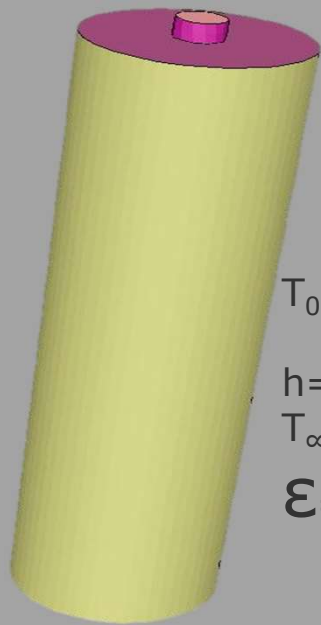
User provides battery's ARC testing data, i.e., temperature~time,
and this tool will find kinetics parameters for the one-equation
thermal abuse model: H, A, E, m and n.
Note:
  n can be set to 0 if user does not want to include (1-alpha)^n term.
-----
File name for temperature testing data: [] Cell_T.txt
Density*Cp (J/m3) [2368000]
Battery external area (m^2) [0]
Battery volume (m^3) [0.0001722]
Battery's initial temperature (K) [300]
Ambient temperature for convection (K) [300]
External heat transfer coefficient (W/m^2K) [0]
Enclosure temperature for radiation (K) [300]
Battery's surface emissivity [0]
Fix n=0 or not? [no]

Parameter Estimation Results:
HW=5.858699e+08 A=3.972702e-03 E=-1.524988e+04 m= 0.9403 n= 0.4251

/define/models/battery-model>
```

案例：NREL 四方程模型

18650 cell

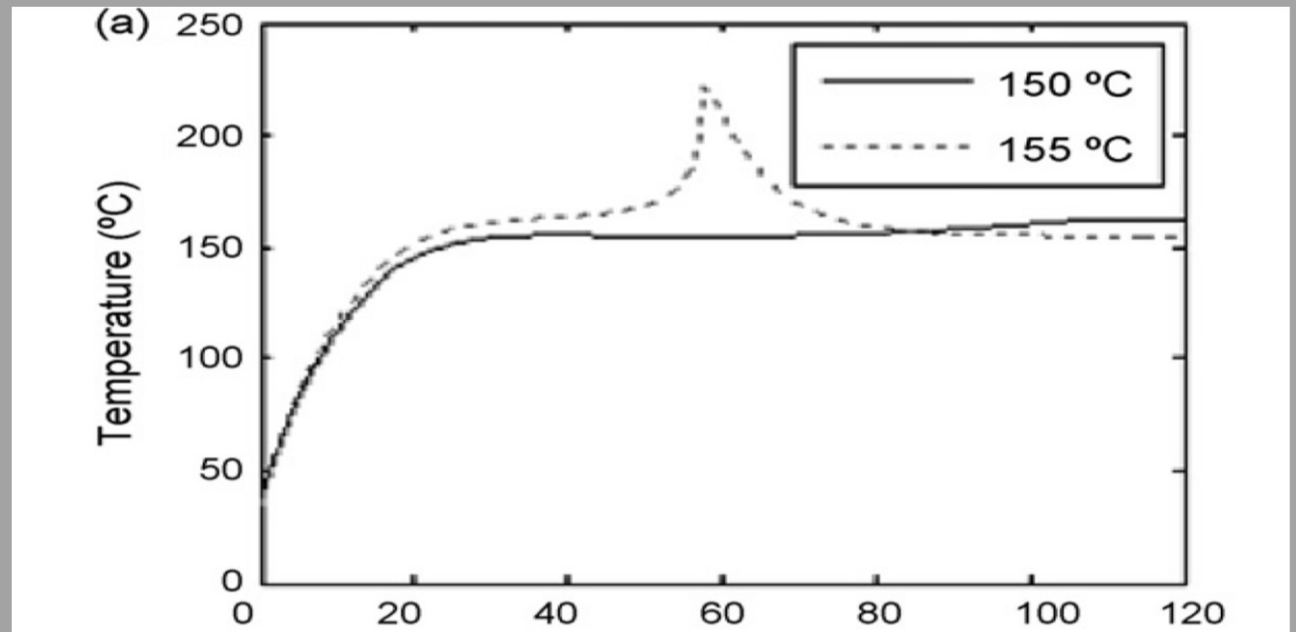


$$T_0 = 35^\circ\text{C}$$

$$h = 7.17 \text{ W/m}^2\text{K}$$

$$T_\infty = T_{\text{rad}} = 150^\circ\text{C}$$

$$\epsilon = 0.8$$



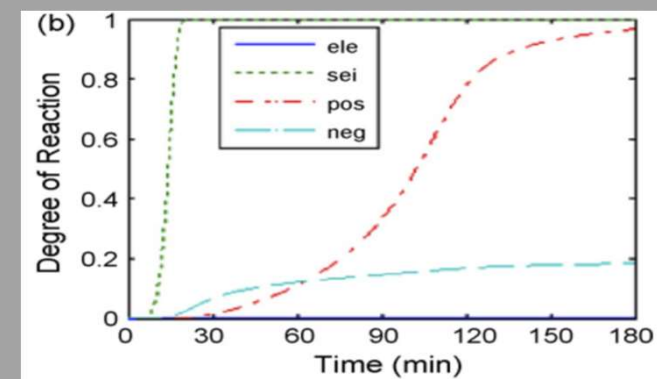
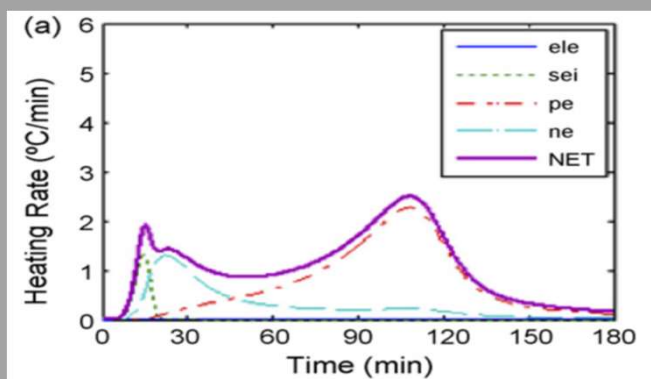
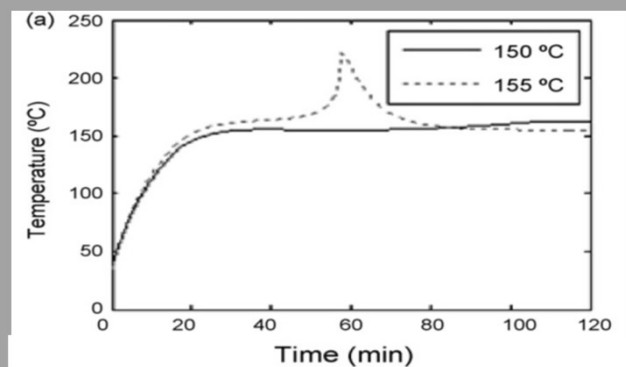
测试案例来源于NREL论文：

Gi-Heon Kim, Ahmad Pesaran, Robert Spotnitz, "A Three-dimensional thermal abuse model for lithium-ion cells", J. of Power Resources, 170. 2007

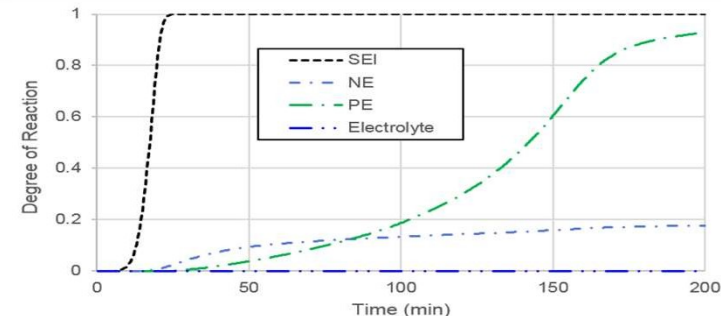
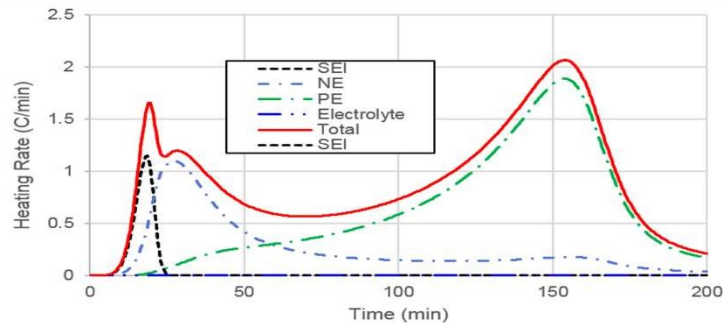
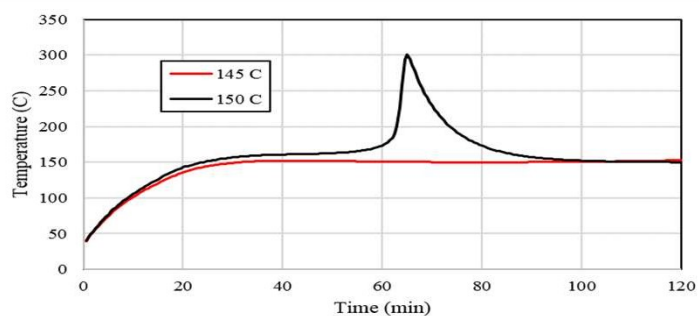
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NREL验证案例

NREL论文结果



Fluent 运行结果



结果非常相似，细微的差异可能是由不同的热边界条件引起的。

降阶模型(ROM)

在MSMD框架中，在瞬态求解器中重复求解两个势能方程。

$$\nabla \cdot (\sigma_+ \nabla \phi_+) - j = 0$$

$$\nabla \cdot (\sigma_- \nabla \phi_-) + j = 0$$

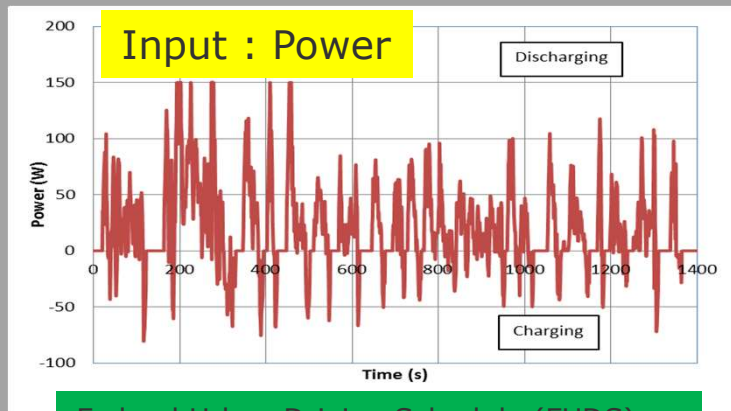
在统一的电化学反应条件下（这通常是电池模拟中的良好假设），有一种简单的方法可以获得两个势场，而不是直接求解它们。

- 电导率不依赖于温度
- 转移电流密度在电池的有效区域内是均匀的
- 没有内部短路

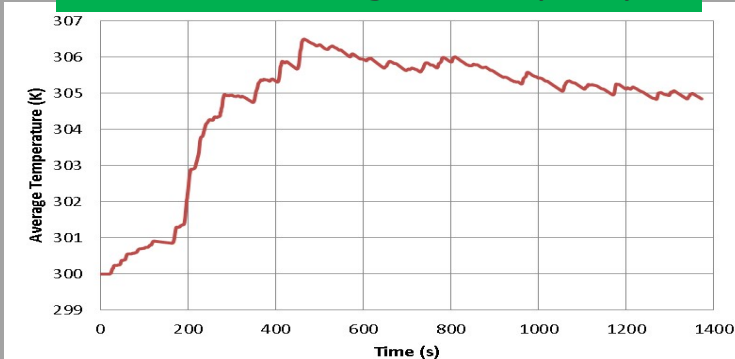
完整的电化学 - 热耦合仿真的成本降低到纯热模拟。

Why ROM?

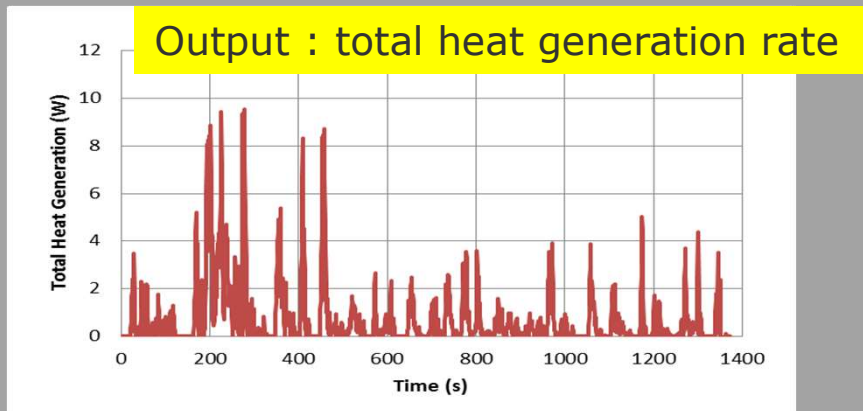
在具有实际行驶循环的电池仿真中，优先使用小时间步进行电仿真，而对于其他流场变量使用大时间步



Federal Urban Driving Schedule (FUDS)



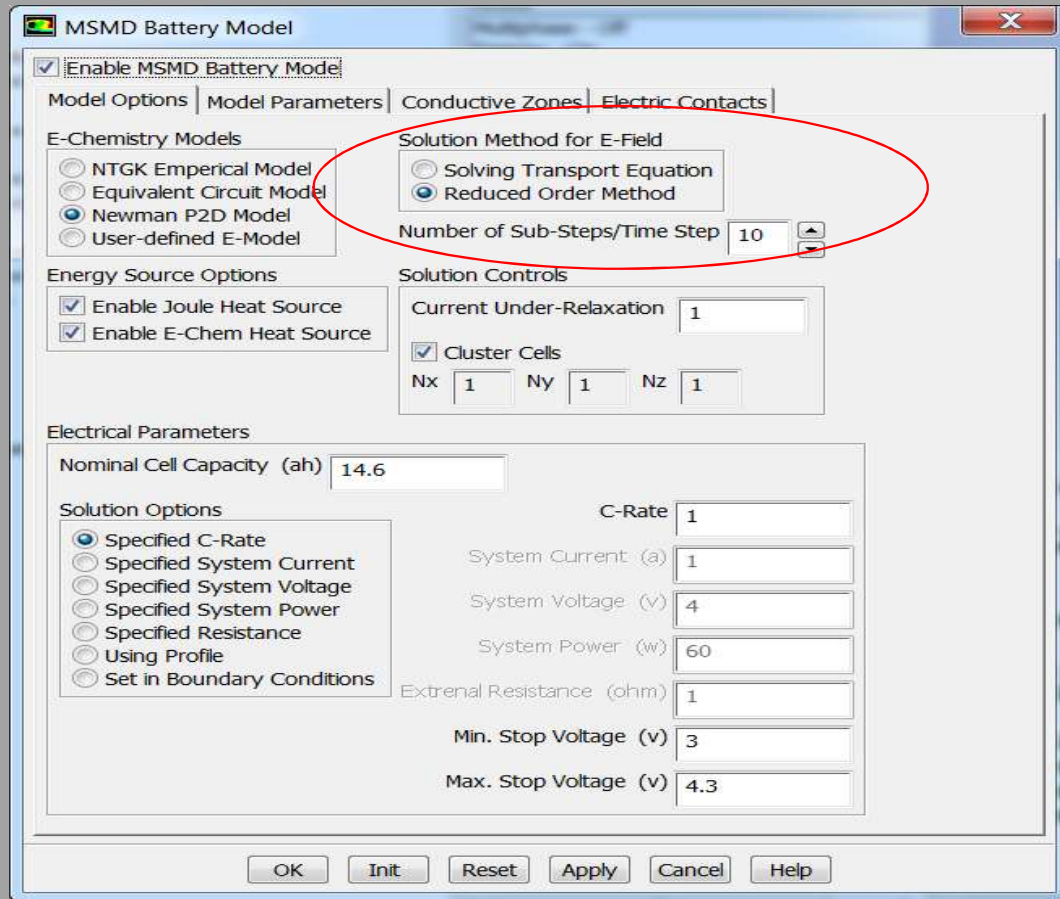
Output: battery's average temperature



电场变化剧烈，而温度场变化相对平稳。

- 我们可以使用一小段时间步计算电场，大时间步计算热场
- 在热量计算中使用电场计算的时间平均热量生成

FLUENT GUI 设计



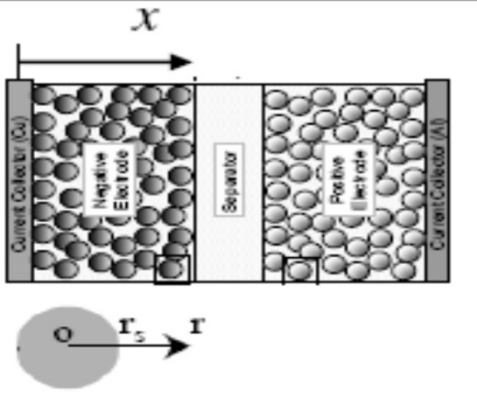
注意:

- 在使用“Reduced Order Method”之前, 用户必须首先使用“Solving Transport Equation”方法计算几个时间步骤以获取参考场。

附录2：MSMD子模型

- Newman P2D 子模型
- NTGK 子模型
- ECM子模型

Newman P2D 子模型



Domains

- negative electrode
- separator
- positive electrode
- spherical particles

$$\nabla \cdot (\sigma \nabla \phi_s) - j^{Li} = 0 \quad \nabla \cdot (k \nabla \phi_e) + \nabla \cdot (k_D \nabla \ln c_e) + j^{Li} = 0 \quad j^{Li} = \xi_a i_0 \left\{ \exp \left(\frac{\alpha_a F}{RT} \eta \right) - \exp \left(- \frac{\alpha_c F}{RT} \eta \right) \right\}$$

$$\frac{\partial (\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_e \nabla c_e) + \frac{1-t^+}{F} j^{Li} \quad \frac{\partial c_s}{\partial t} = \frac{D_s}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_s}{\partial r} \right)$$

- 每个CFD网格中求解一系列偏微分方程
 - 方程总数: $(n_{Cs}+2) * n_{NE} + 2n_{SP} + (N_{Cs}+2) n_{PE}$
 - 内存需求: $N_{cell} * \{ (n_{Cs}+1) * n_{NE} + n_{SP} + (N_{Cs}+1) n_{PE} \}$
- 单元集群可用于降低子模型计算成本

L. Cai and R.E. White, "Reduction of Model Order Based on Proper Orthogonal Decomposition for Lithium-Ion Battery Simulations" J. of Electrochemical. Soc. 156(3) A154-A161 (2009).

NTGK 子模型

$$\nabla \cdot (\sigma_+ \nabla \phi_+) = -j$$

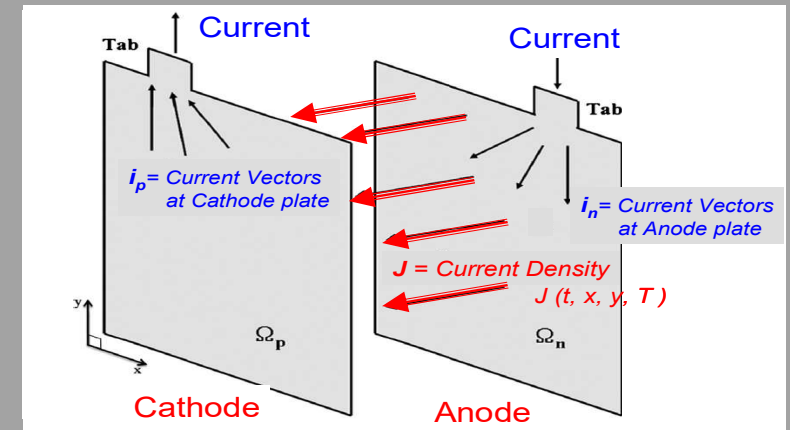
$$\nabla \cdot (\sigma_- \nabla \phi_-) = +j$$

$$j = Y(\phi_+ - \phi_- - U)$$

$$DoD = \left(\int_0^t j \, dt \right) / Q_T$$

$$Y = \left(\sum_{n=0}^5 b_n (DoD)^n \right) e^{C_1 \left(\frac{1}{T_{ref}} - \frac{1}{T} \right)}$$

$$U = \left(\sum_{n=0}^5 a_n (DoD)^n \right) - C_2 (T - T_{ref})$$



- 使用给定电池的不同C-rate放电曲线，用 Parameter estimation tool来拟合参数

NTGK Model Evolution

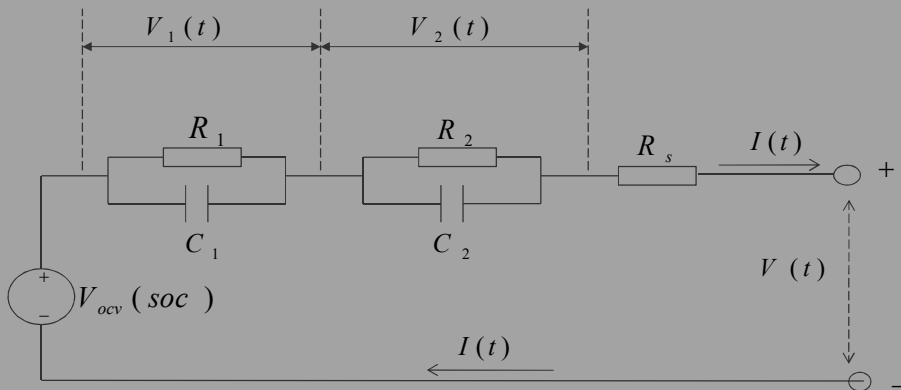
- Newman & Tiedemann: 1D
- Gu: 1D
- Kim et al: 2D
- ANSYS: 3D

U.S. Kim et al, "Modeling the Dependence of the Discharge behavior of a Lithium-Ion Battery on the Environmental Temperature" J. Electrochem. Soc., 158(5), A611-A618 (2001)

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等效电路模型(ECM)子模型

Chen & Rincon-Mora (2006)



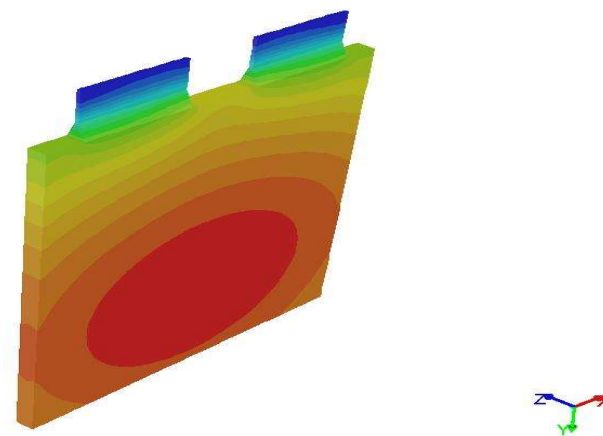
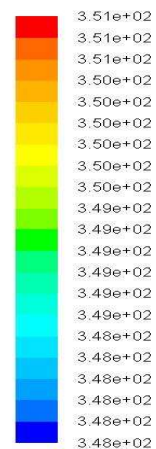
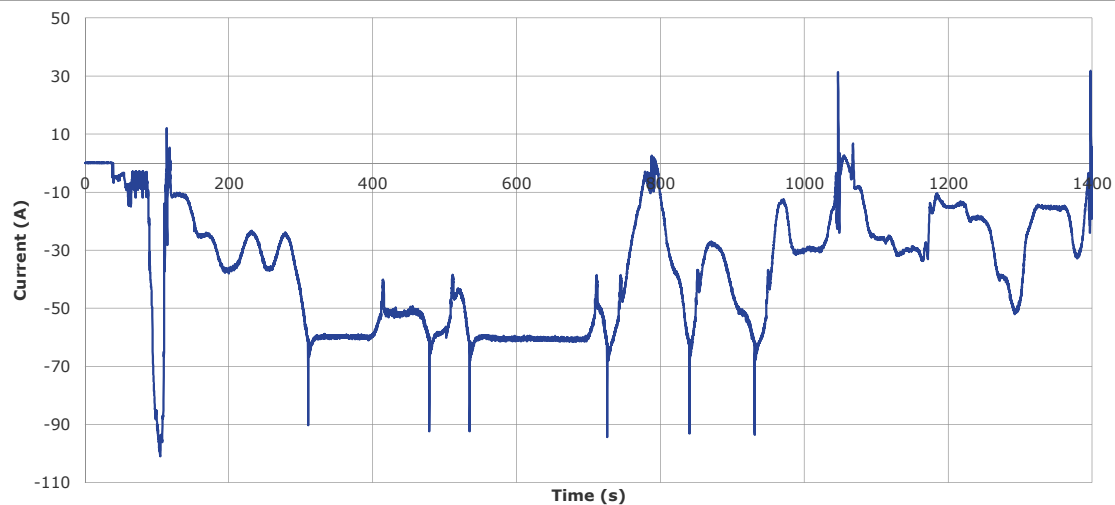
Model Equations

$$\begin{cases} V(t) = V_{ocv}(soc) + V_1 + V_2 - R_s(soc)I(t) \\ \frac{dV_1}{dt} = -\frac{1}{R_1(soc)C_1(soc)}V_1 - \frac{1}{C_1(soc)}I(t) \\ \frac{dV_2}{dt} = -\frac{1}{R_2(soc)C_2(soc)}V_2 - \frac{1}{C_2(soc)}I(t) \\ soc = soc_0 - \frac{\int_0^t I(t) dt}{3600 Q_{Ah}} \end{cases}$$

- 对于每个CFD单元, 4种微分和代数方程 (DAEs) 都是用自适应时间步长方法求解的
- 使用HPPC 实验数据, 用Parameter estimation tool拟合模型参数

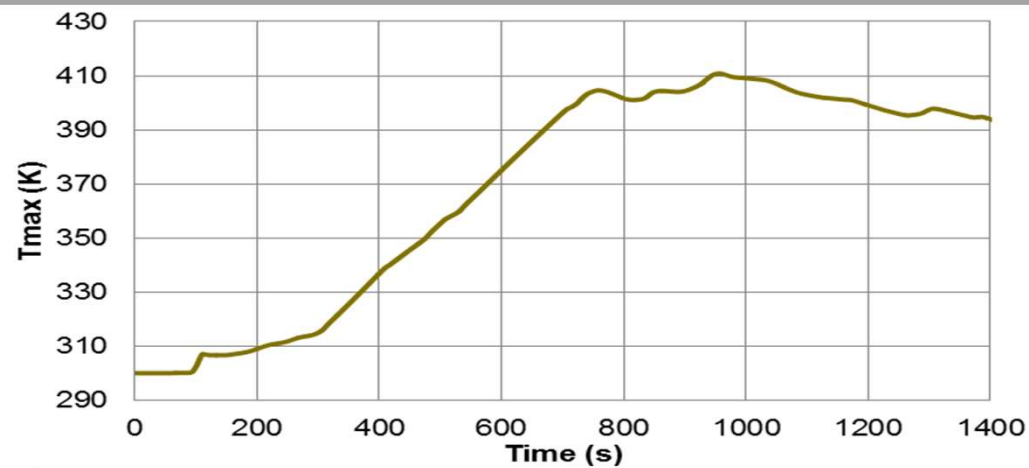
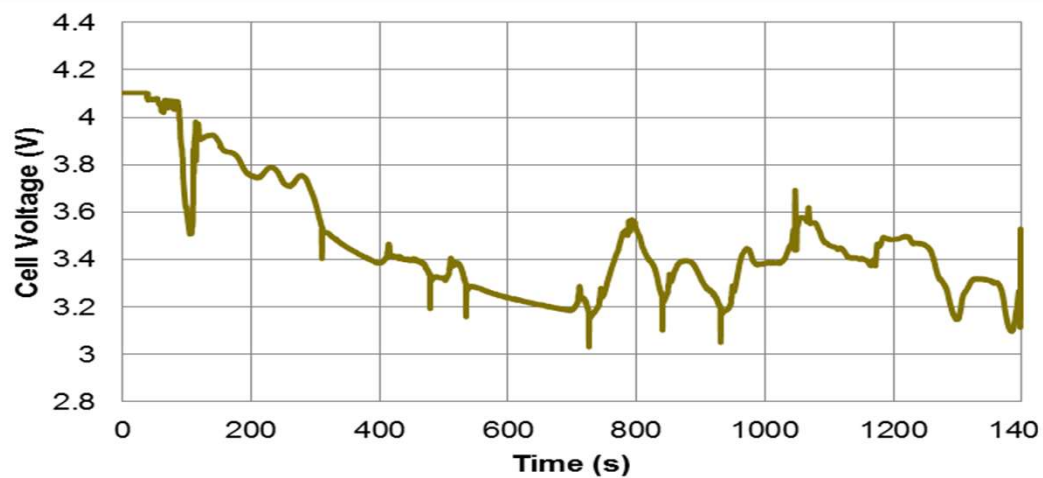
M. Chen and G. A. Rincon-Mora, "Accurate Electrical Battery Model Capable of Predicting Runtime and I-V Performance" IEEE Trans. On Energy Conversion, Vol. 21. No.2, June 2006

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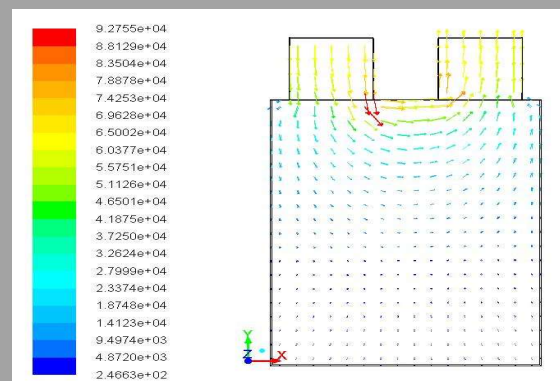
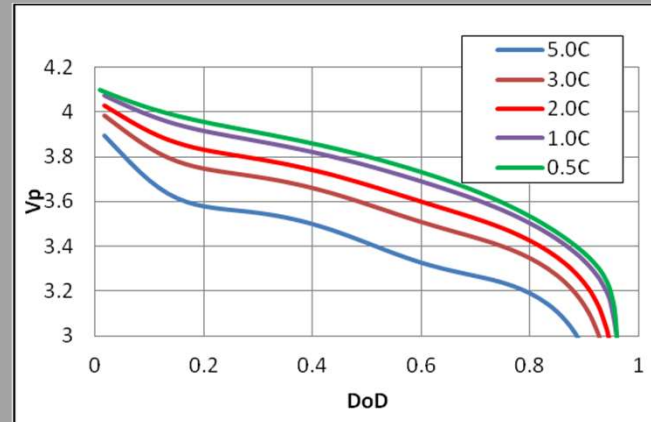
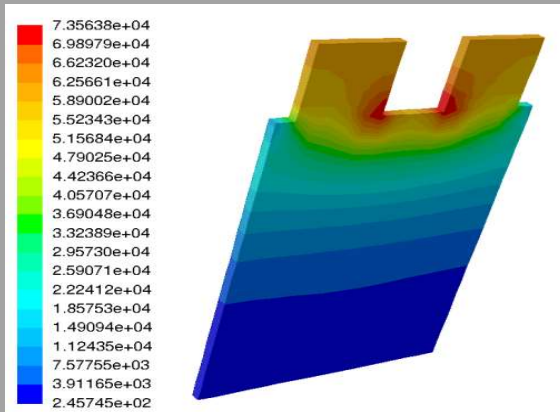


Contours of Static Temperature (K) (Time=1.3720e+03)

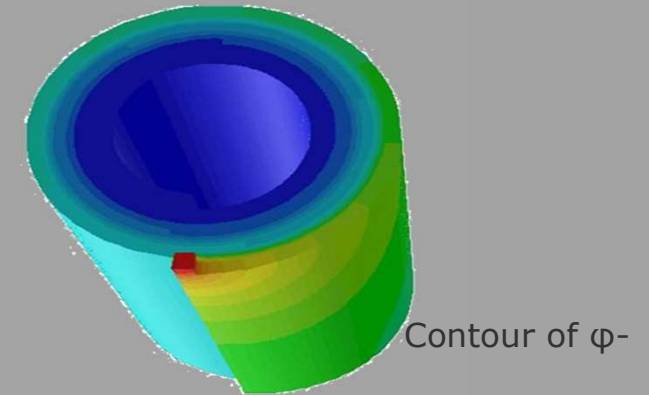
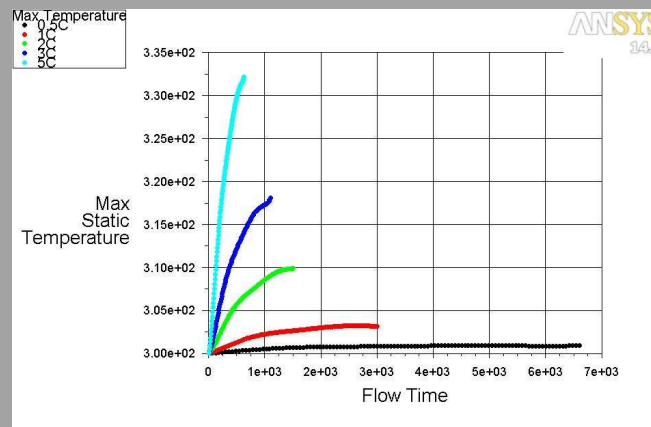
Mar 13, 2013
ANSYS Fluent 14.5 (3d, dp, pbns, lam, transient)



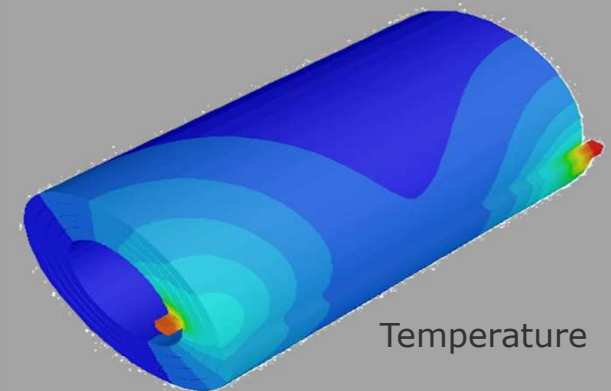
基于NTGK 子模型的计算结果



方形电池



Contour of ϕ -



Temperature

圆柱形电池with discrete tabs