# New Techniques for Thermo-electrochemical Analysis of Lithium-ion Batteries for Space Applications

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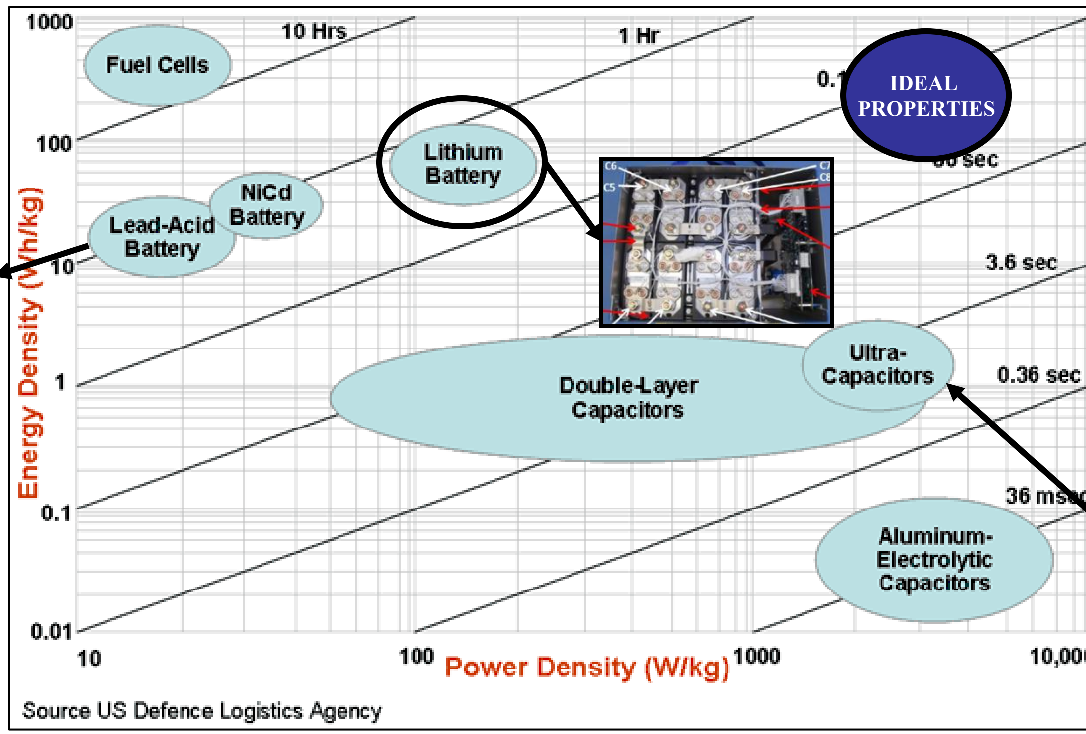
# Presentation Overview

- Introduction to the Topic
- Lithium-ion Battery (LIB) Charge/Discharge Heat Transfer Mechanisms
- Thermal Desktop Model Development
- Results:
  - Case 1
  - **Case 2 Excluded*
  - Case 3
- Conclusion and Future Work
- References
- Disclaimer Statement

# Section 1:
# Introduction to the Topic

# Introduction to the Topic

- The need for renewable energy, more efficient energy consumption, and the incorporation of advanced energy storage technologies escalates each year with the increasing consumption of non-renewable resources and decreasing availability of said resources
- The need to survive in space environments where fuel sources are not readily available also leads to a high dependence on advanced energy storage capabilities
- Advanced energy storage devices are compared on a Ragone plot (batteries tend to have higher energy density and lower power density while capacitors tend to have high power density and low energy density)
- LIBs are quickly moving towards the “ideal” location on the Ragone plot, are becoming more popular in the space industry, and thus are the focus of my research (though popular in use, LIBs face numerous thermal issues)


Ragone plot image above belongs to the US Defense Logistics Agency

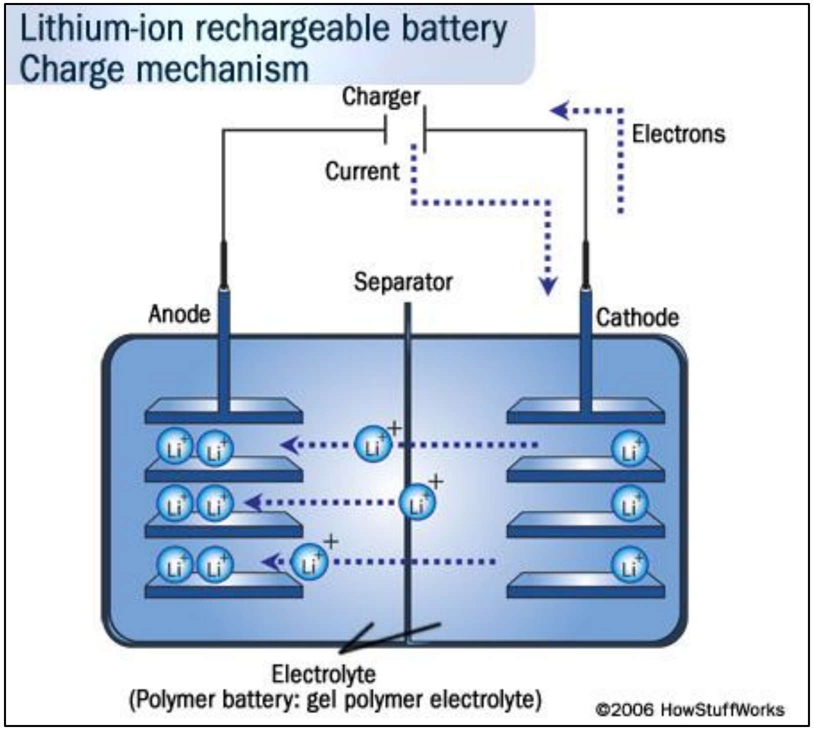
# Introduction to the Topic

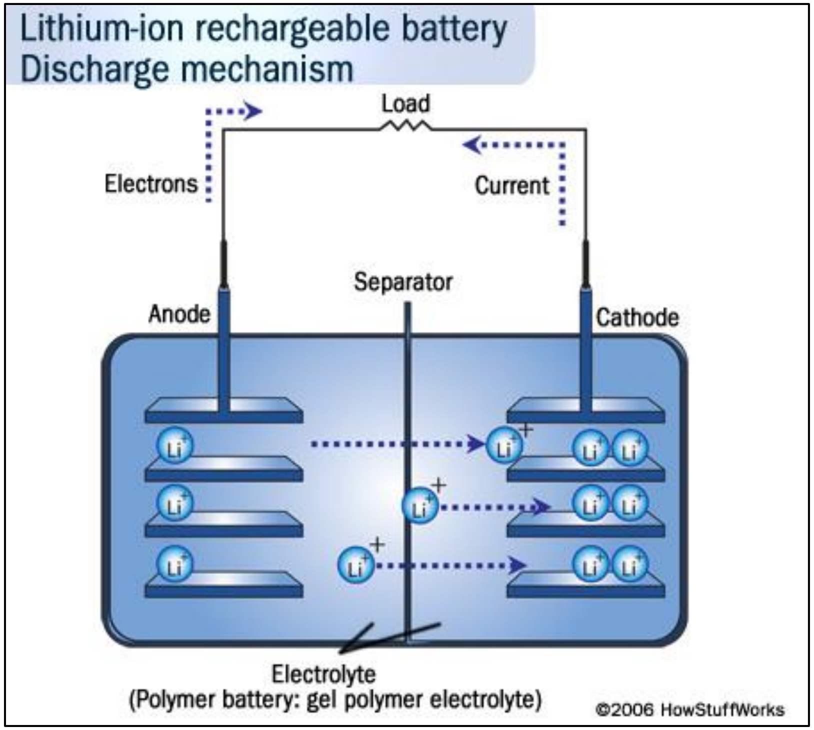
- LIBs are increasing in popularity for space applications because of their superior performance in:
  - Energy density and power density
  - Ionic conductivity
  - Operating and storage temperature ranges
  - Life cycles and shelf life
- LIBs are generally challenged by thermal runaway situations, thermal safety concerns (e.g. Boeing 787 incident in January 2013), and operating/storage temperatures that are exceeded by orbital-space environments
- The selection of LIBs for space applications invokes the need to predict thermal performance in orbital environments; batteries thermal performance is a function of environment **and** local heating rates
- Note that the thermal analysis of LIBs is not new:
  - Sophisticated numerical methods began in 1985
  - Presently it is well known that the optimal way to perform this type of analysis is through a coupled (or multi-physics) methodology which combines the effects of:
    - Heating through electrochemical reactions
    - Heating through environmental factors
  - This type of analysis is easily conducted for simple thermal environments in multi-physics software like COMSOL; however, implementing orbital environments requires more specialized software (Thermal Desktop (TD), NX Space Systems Thermal, TSS, TRASYS, etc…)
- Research seeks to develop a coupled thermo-electrochemical model in thermal orbital analysis software of a Lithium-ion battery whose local heat generation rate is a function of the environment (orbital or sink based), local temperature, and depth of discharge

# Section 2:
# LIB Charge/Discharge Heat Transfer Mechanisms

# LIB Charge/Discharge Heat Transfer Mechanisms

- LIBs store and provide energy through a series of charge/discharge processes that occur through the simultaneous electrochemical reactions between the electrodes and the flow of electrons through a completed circuit
- Typical LIB components: anode, cathode, electrolytic material, separator, and current collectors

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# LIB Charge/Discharge Heat Transfer Mechanisms

- As with any object, the three modes of heat transfer apply: convection, conduction, radiation
- Local heat generation rate:
  - In 1985 Bernardi et. al. developed a basic equation to represent the local heat generated in the cells of a LIB as a result of electrochemical processes
  - Equation captures heat due to Ohmic losses, charge-transfer at the interface, and mass transfer limitations:

$$q = -IV - \sum_k I_k T^2 \frac{d\frac{U_{k,avg}}{T}}{dT} + \sum_j \frac{d}{dt}\left(\int_{v_i}^{-} \sum_i c_{ij} RT^2 \frac{\partial}{\partial T} ln\left(\frac{y_{ij}}{y_{ij}^{avg}}\right) dv_j\right) + \sum_{jjm} \sum_i \left[\left(\Delta H_{ij\to m}^{*} - RT^2 \frac{d}{dT} \ln\left(\frac{\gamma_{i,m}^{avg}}{\gamma_{i,j}^{avg}}\right)\right) \frac{dn_{i,j}}{dt}\right] \quad (1)$$

$$Q_{Total} = I\left(E_{OC} - E - T\frac{\partial E_{OC}}{\partial T}\right) \quad (2)$$

  - I is the total current (constant value)
  - $E_{OC}$ is the open circuit potential (variable value)
  - E is the working voltage (variable value)
  - T is the local temperature (variable value)

**Images retrieved from electronics.howstuffworks.com**

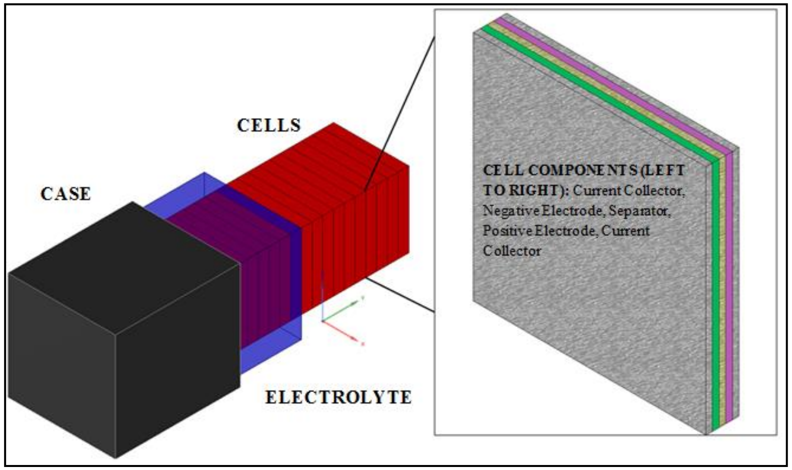
# Section 3:

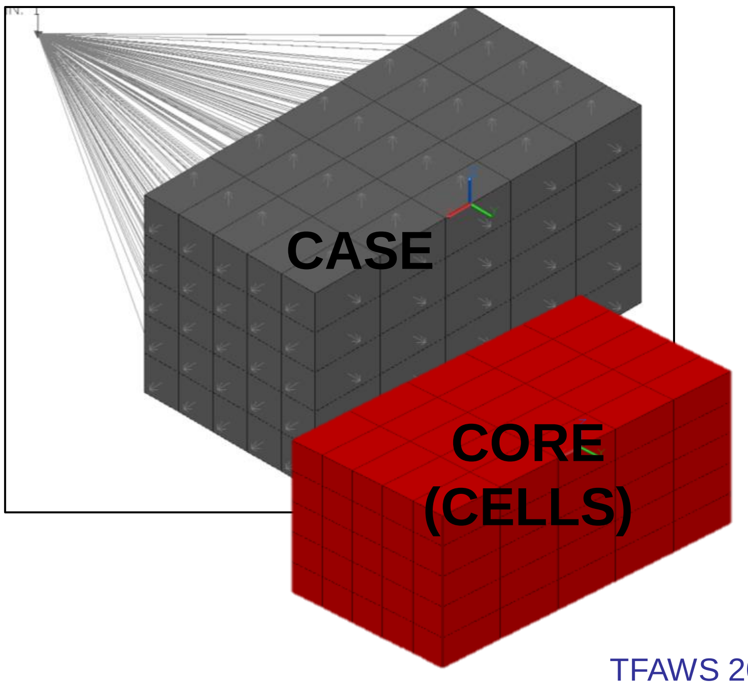
# Thermal Desktop Model Development

# Thermal Desktop Model Development

- Before conducting an orbital analysis, development of a simple non-orbital (sink temperature based) TD model of a LIB with Bernardi's equation for local heating was needed
- Chose a convection/radiation and numerically based assessment of a 185 Ah LIB conducted by Chen et. al. (primary source) who also utilized Bernardi's equation for local heating generated through electrochemical processes
  - Several copies are available for those who are interested
- In short, we recreated a previously conducted numerical analysis in TD to determine if TD had the ability to be coupled with thermo-electrochemical math models (i.e. Bernardi's equation)
- Three Cases Analyzed:
  - Case 1: Exact Replication of Chen's Study
  - Case 2: Constant Power Case (No Arrays/Change w/ Time)
  - Case 3: Attempted Improvement to Chen's Study

# Thermal Desktop Model Development



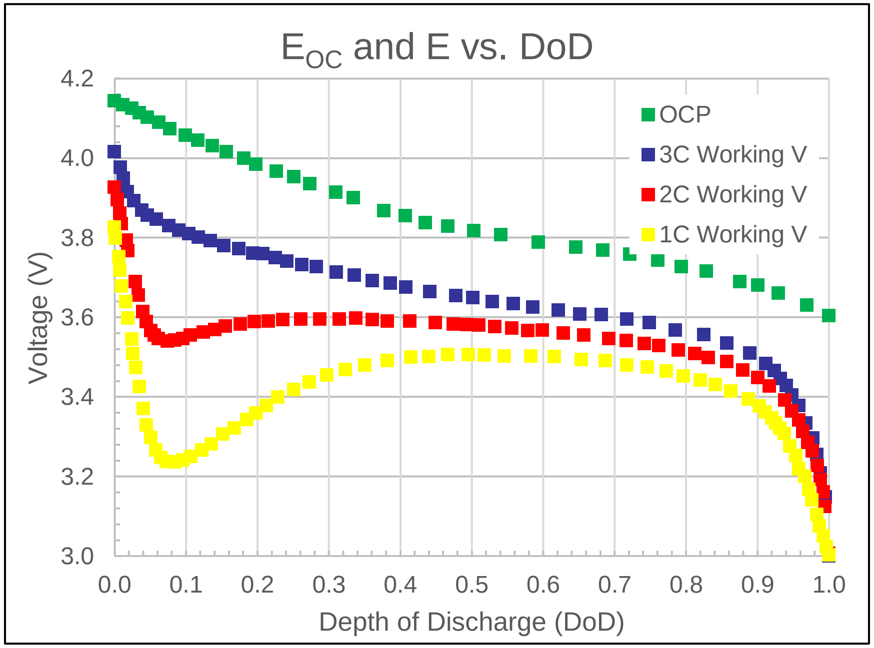




- Thermal Definition:
  - Geometries and material properties provided in table
  - Convection represented through a 300 K boundary node connected to the exterior encasement surfaces with a natural convection conductor (4.3-10 W/m$^2$K depending on location and DoD)
  - External surfaces set to radiate to a 300 K sink temperature
  - Assumed 200 W/m$^2$/K contact between the core, the electrolytic layer, and the encasement

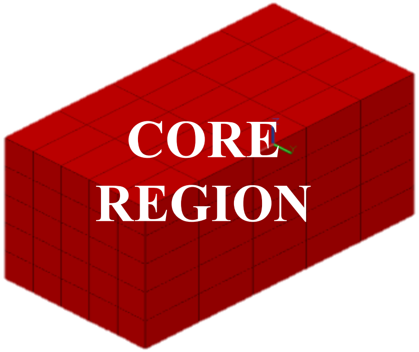
| Variable | Density (kg/m3) | Heat Capacity (J/kg/K) | Thermal Conductivity (W/m/K) |
|---|---|---|---|
| Aluminum (Encasement) | 2770 | 875 | 170 |
| Liquid Electrolyte (Contact Layer) | 1130 | 2055 | 0.60 |
| Core Region (Cells) | 3264 | 1194 | 1.04, 24.8, 24.8 |
| **Variable** | **Magnitude** | | **Unit** |
| Size of Core Region | 19.08 x 10.00 x 10.00 | | cm*cm*cm |
| Thickness of Encasement | 0.07 | | cm |
| Thickness of the Contact Layer | 0.05 | | cm |
| Ambient Temperature | 300 | | K |
| Theoretical Capacity | 185 | | Ah |
| Change in $E_{OC}$ vs. Time | 0.00022 | | V/K |
| Encasement Emissivity | 0.25 | | N/A |

# Thermal Desktop Model Development

- Local heating applied to the 125 "core" region nodes (load divided volumetrically)
- Applying Bernardi's equation:
  - Current was based on a 185 Ah battery and which discharge case was under consideration
    - 1C = 60 Minutes Discharge Time @ I = 185 A
    - 2C = 30 Minutes Discharge Time @ I = 370 A
    - 3C = 20 Minutes Discharge Time @ I = 555 A
  - Open Circuit Potential and Working Voltages for 1, 2, and 3 C discharge profiles provided in the image below
  - Developed arrays of the voltage vs. DoD location for each discharge case
  - Developed TD logic to update the local heating on the "core" region after every iteration in the solution process
  - *Case 3 implemented logic to update the local T value of Bernardi's equation after each iteration*




$$Q_{Total} = I\left(E_{OC} - E - T\frac{\partial E_{OC}}{\partial T}\right) \qquad (2)$$



# Thermal Desktop Model Development

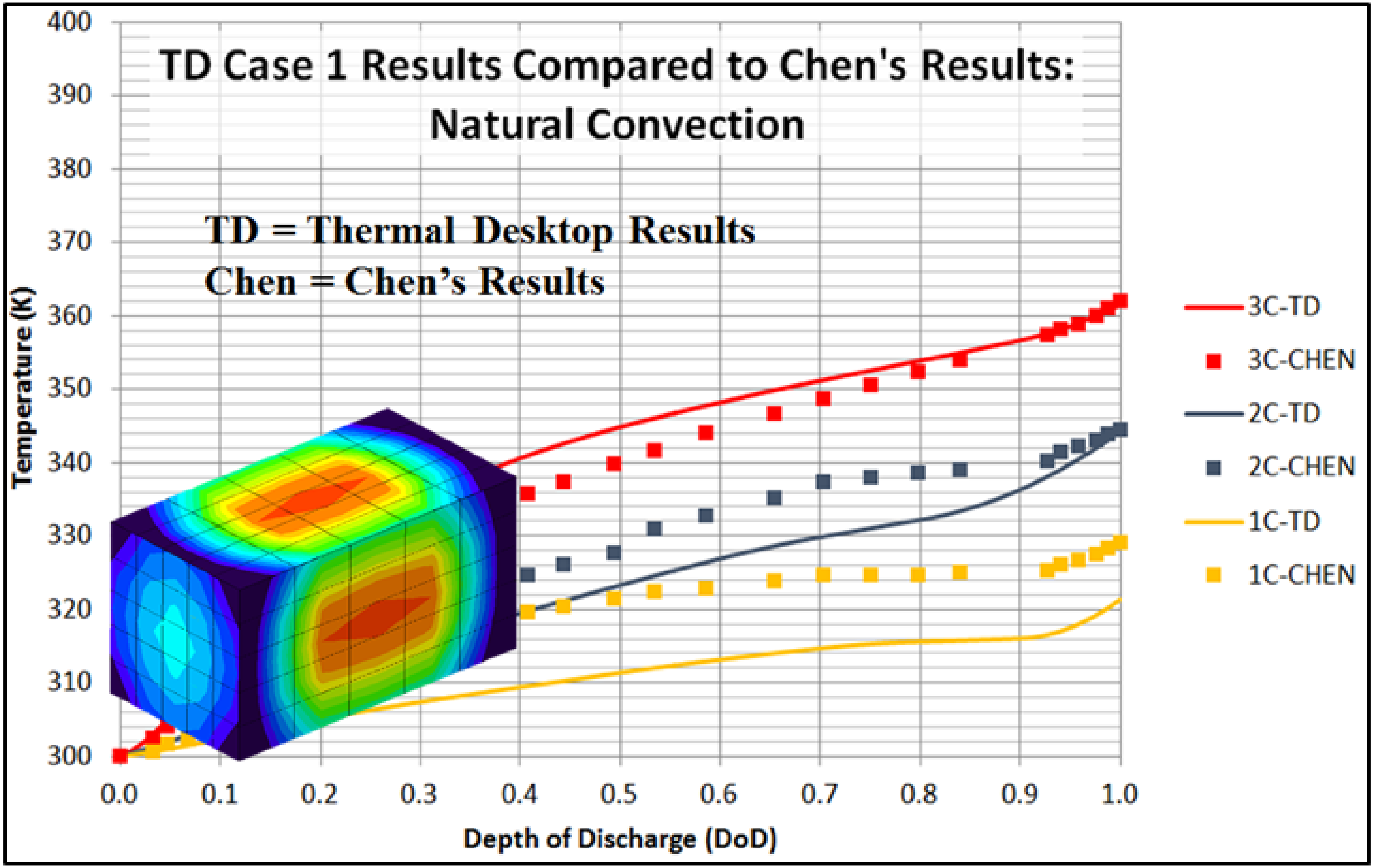
## Test Case Matrix

| Case ID | Case Type | Discharge Rate (C) | Total Discharge Time (s) | Current (A) | Convection (W $m^{-2}$ $K^{-1}$) |
|---|---|---|---|---|---|
| C1-3C-NAT | Case 1 | 3 | 1200 | 555 | Natural |
| C1-2C-NAT | Case 1 | 2 | 1800 | 370 | Natural |
| C1-1C-NAT | Case 1 | 1 | 3600 | 185 | Natural |
| C1-3C-20 | Case 1 | 3 | 1200 | 555 | 20 (Forced) |
| C1-3C-50 | Case 1 | 3 | 1200 | 555 | 50 (Forced) |
| C1-3C-100 | Case 1 | 3 | 1200 | 555 | 100 (Forced) |
| C1-3C-200 | Case 1 | 3 | 1200 | 555 | 200 (Forced) |
| C1-3C-300 | Case 1 | 3 | 1200 | 555 | 300 (Forced) |
| C2-3C-NAT | Case 2 | 3 | 1200 | 555 | Natural |
| C2-2C-NAT | Case 2 | 2 | 1800 | 370 | Natural |
| C2-1C-NAT | Case 2 | 1 | 3600 | 185 | Natural |
| C3-3C-NAT | Case 3 | 3 | 1200 | 555 | Natural |
| C3-2C-NAT | Case 3 | 2 | 1800 | 370 | Natural |
| C3-1C-NAT | Case 3 | 1 | 3600 | 185 | Natural |
| C3-3C-20 | Case 3 | 3 | 1200 | 555 | 20 (Forced) |
| C3-3C-50 | Case 3 | 3 | 1200 | 555 | 50 (Forced) |
| C3-3C-100 | Case 3 | 3 | 1200 | 555 | 100 (Forced) |
| C3-3C-200 | Case 3 | 3 | 1200 | 555 | 200 (Forced) |
| C3-3C-300 | Case 3 | 3 | 1200 | 555 | 300 (Forced) |

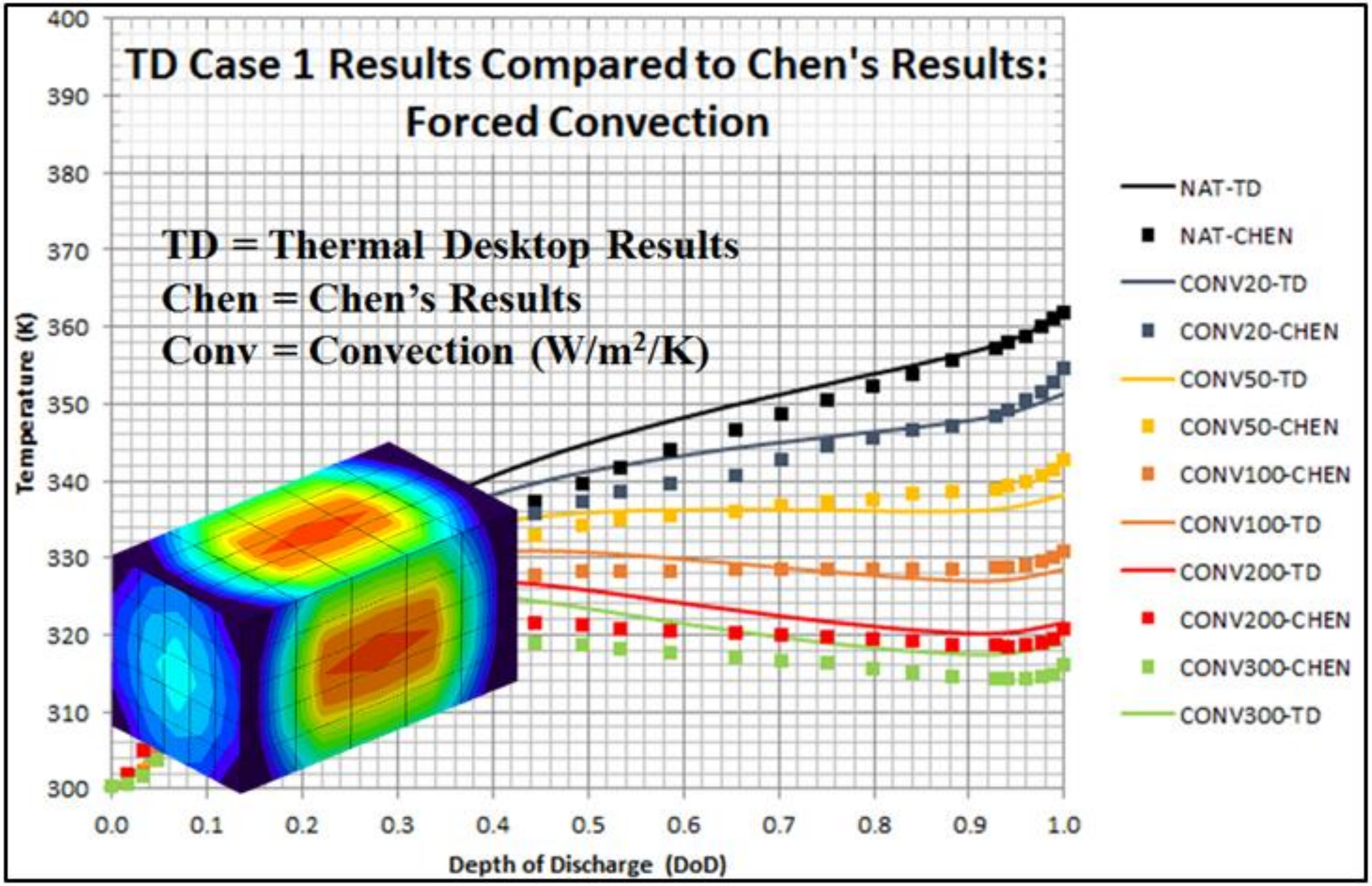
- Case 1: Exact Replication of Chen's Study
  - $E_{OC}$ and E update in the Q equation (Bernardi's) after each iteration
  - I, T, and $\frac{\partial E_{OC}}{\partial T}$ held constant
- Case 2: No-Logic, Constant/Averaged Local Heating Applied
  - Constant local heating applied based on average of entire DoD
- Case 3: Attempted Improvement to Chen's Numerical Thermal Model
  - EOC, E, <u>and T</u> update in Q equation (Bernardi's) after each iteration
  - Updated thermophysical properties to include an electrolytic layer between the electrodes

# Section 4:
# Thermal Desktop Results

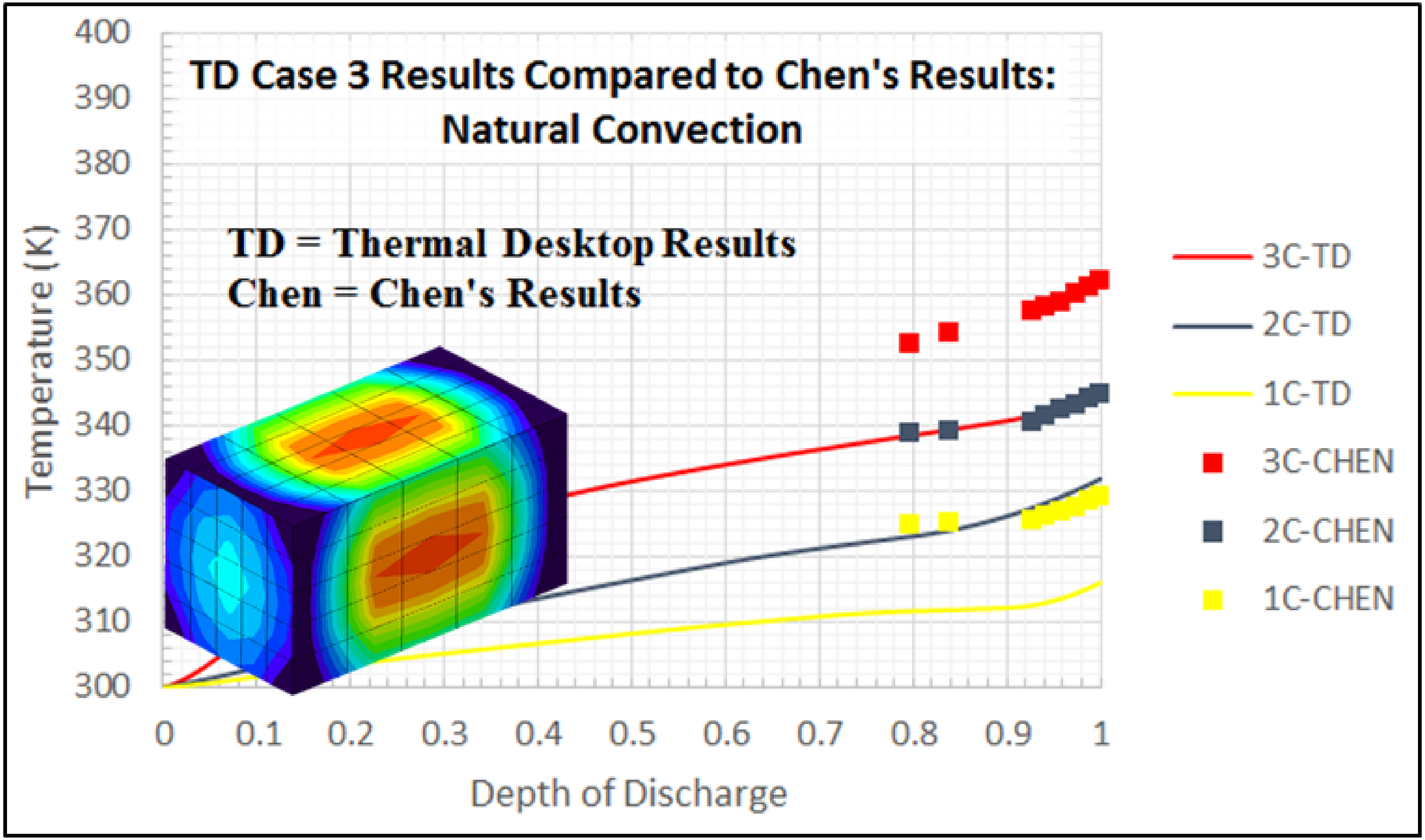
# Case 1 Natural Convection Results



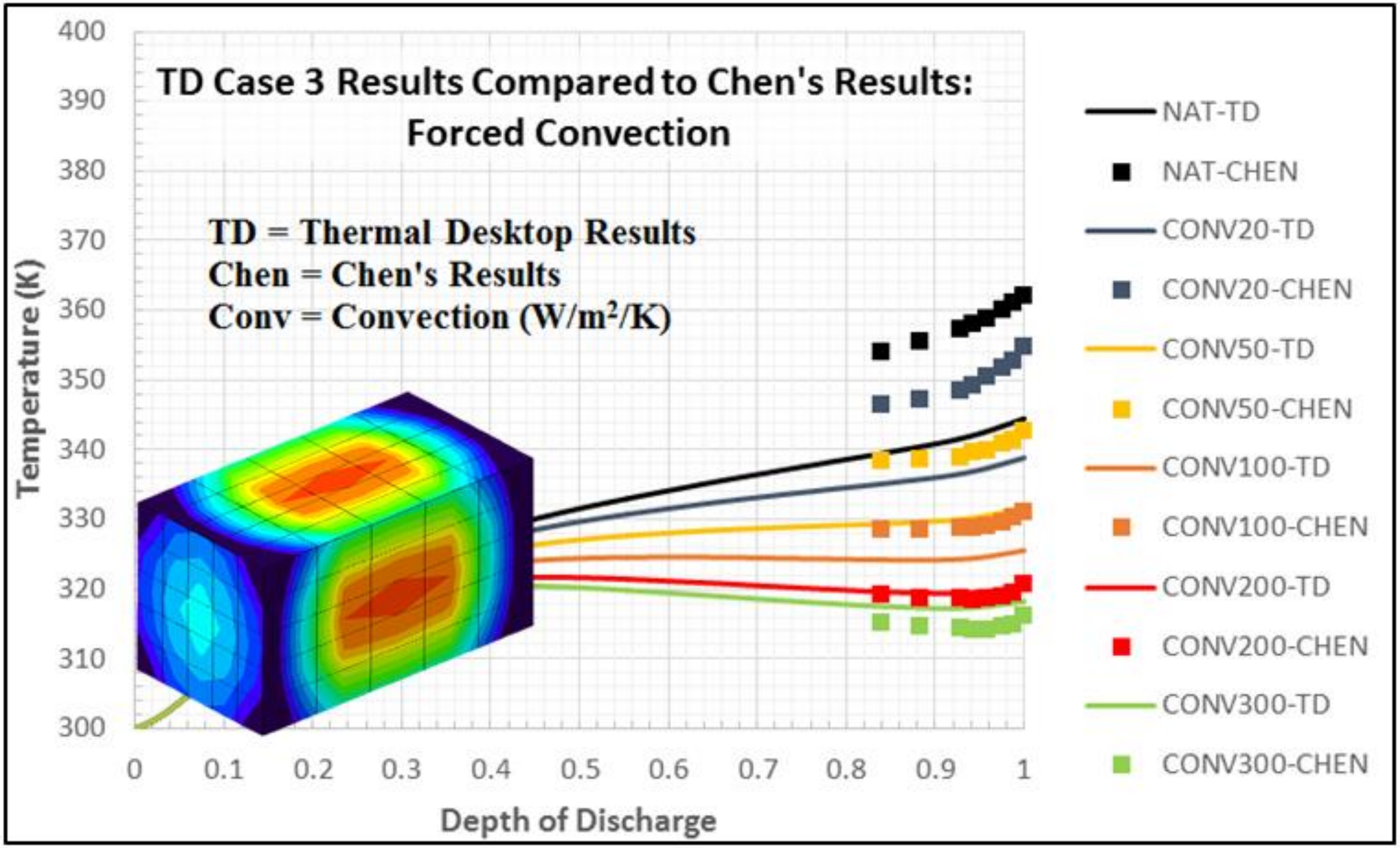
# Case 1 Forced Convection Results



# Case 3 Natural Convection Results



# Case 3 Forced Convection Results



# Section 5:
# Conclusion and Future Work

# Conclusion and Future Work

- The overall goal of this study was achieved:
  - Replicated the numerical assessment performed by Chen et. al. (2005)
  - Displayed the ability of Thermal Desktop to be coupled with thermo-electrochemical analysis techniques such that the local heat generated on the cells is a function of the model itself using logic blocks and arrays
- Differences in the TD temperature vs. depth of discharge profiles and Chen's was most likely due to differences in two primary areas:
  - Contact regions and conductance values
  - Differences in density and specific heat values
- The model results are highly dependent on the accuracy of the material properties with respect to the multiple layers of an individual cell
- Future work:
  - **Fall 2013:** Develop and contact a highly controlled test where all factors are known – replicate test in Thermal desktop – compare to provide final validation of these new techniques
  - **Spring 2014:** Implement these techniques into an orbital model to investigate the effects of this analysis technique combined with orbital analysis techniques
  - **Present to Spring 2014:** Develop a detailed COMSOL model of the Fall 2013 battery and attempt combination with NX Space Systems Thermal
  - **Summer 2014 to Fall 2014:** Explore the following items with the most effective model:
    - Predict beta angles and solar conditions which could invoke a thermal run-away condition
    - Implement thermal considerations into the design of the battery rather than waiting until the battery is complete
    - Parametric studies exploring the impact of materials variations
    - Develop combinations of charge/discharge cycles to minimize the need for passive/active thermal control

# Section 6:
# References

# References


[1] Ardebili, Dr. H. "Materials for Energy Storage." Course Notes and Presentations. Spring 2013.

[2] Bandhauer, T. "Electrochemical-Thermal Modeling and Microscale Phase Change for Passive Internal Thermal Management of Lithium Ion Batteries." Dissertation. Georgia Institute of Technology. December 2011.

[3] Bernardi, D., Pawlikowski, E., and Newman, J. "A General Energy Balance for Battery Systems." J. Electrochemical Society, 132, 5 (1985).

[4] Chen, S. C., Wan, C. C., and Wang, Y.Y. "Thermal Analysis of Lithium-Ion Batteries." Tsing-Hua University. Elsevier 19 May 2004.

[5] C&R Technology. Thermal Desktop and SINDA v5.5. April 2013.

[6] Cutchen, J., Baldwin, A., and Levy, S. "A Preliminary Evaluation of Lithium Batteries for Extended-Life Continuous-Operation Applications." Journal of Power Sources. 14 (1985) 167-172.

[7] Gibbard, H.F. "High Temperature, High Pulse Power Lithium Batteries." Journal of Power Sources. 26 (1989) 81-91.

[8] Gilmore, D. "Satellite Thermal Control Handbook." The Aerospace Corporation Press. El Segundo, Ca. 1994.

[9] Gu, W.B. and Wang, C.Y. "Thermal-Electrochemical Modeling of Battery Systems." Journal of Electrochemical Society. January 28th, 2000.

[10] Kim, Ui Seong, et. al. "Modeling the Thermal Behavior of a Lithium-ion Battery During Charge." Journal of Power Sources 196 (2011) 5115- 5121.

[11] Macklin, W.J., et. all. "Development of Lithium-Ion Polymer Battery for Space Applications." Journal of Power Sciences 65 (1997) 275-288.

[12] Megahed, Sid and Scrosati, Bruno. "Lithium-ion Rechargeable Batteries." Rayovac Corporation, Madison, WI. Journal of Power Sources, 51 (1994) 79-104.

[13] Mills, Andrew and Al-Hallaj, Said. "Simulation of Passive Thermal Management System for Lithium-ion Battery Packs." Journal of Power Sources 141 (2005) 207-315. 7 December, 2004.

[14] Rao, L. and Newman. "Heat Generation Rate and General Energy Balance for Insertion Battery Systems." Journal Electrochem. Soc. 144, 2697 (1997).

[15] Rickman, Steve. "Orbital Thermal Environments Training Presentation." Thermal Fluids and Analysis Workshop (TFAWS). August 2011.

[16] Wang, etc. all. "Thermal Runaway Caused Fire and Explosion of Lithium Ion Battery." Journal of Power Sources. 22 March, 2012.

[17] Wu, M.S., Wang, Y.Y., and Wan, C.C. "Thermal Behavior of Nickel/Metal Hydride Batteries during Charge and Discharge." Journal of Power Sources. 74 (1998) 202-210.