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, final
  - **Case 2 not presented*
  - **Case 3 presenting, still pending final review*
- Conclusion and Future Work
- References
- Disclaimer Statements
  - This work was inspired by, but is not affiliated with the NASA/Boeing ISS LIB replacement battery project
  - All results are part of on-going research conducted for academic purposes with my graduate advisor (H. Ardebili, co-author)

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

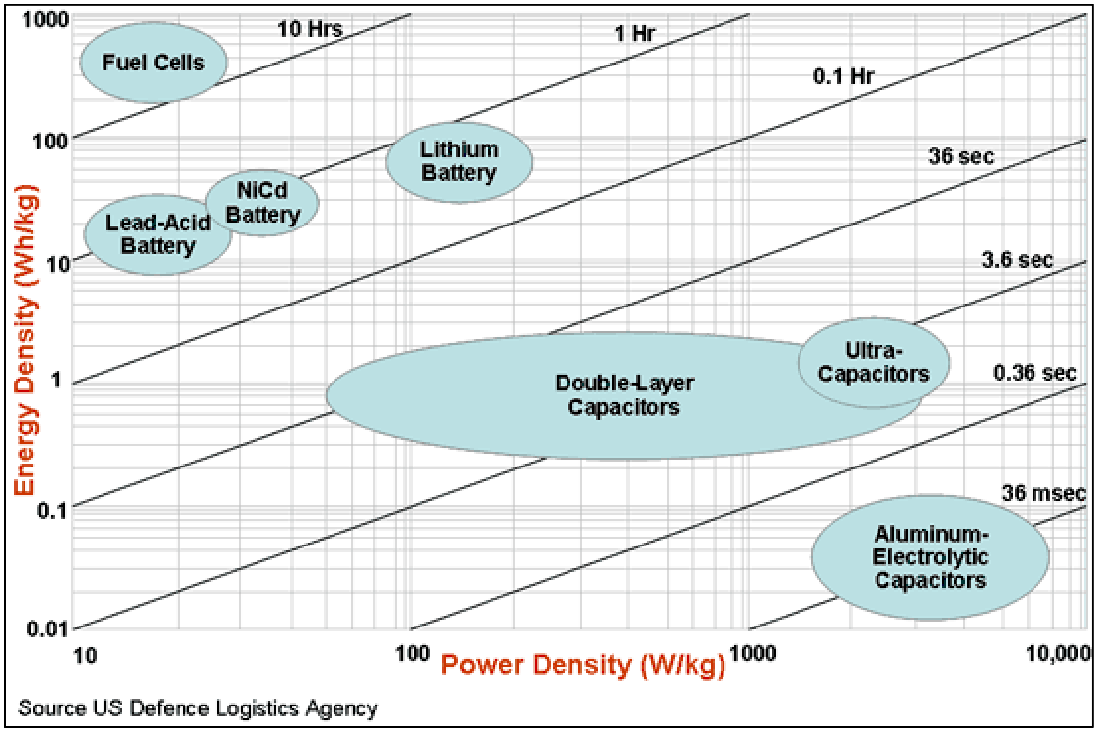


Image retrieved belongs to the US Defense Logistics Agency

Introduction to the Topic Cont…

- LIBs are increasing in popularity and were chosen as replacement batteries for some of the ISS Ni-H_2 batteries because of their superior performance in:
  - Energy density and power density
  - Ionic conductivity
  - Operating and storage temperature ranges
  - Life cycles and shelf life
- The selection of LIBs for use in satellites and now the ISS exemplifies the need to predict thermal performance in orbital environments; for 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)
    - The problem is that TD is not readily set up to incorporate the complexities of local heating from thermo-electrochemical reactions
- 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
  - Rather than a power profile that is provided prior to analysis
  - Essentially, the power profile should be a function of the model itself

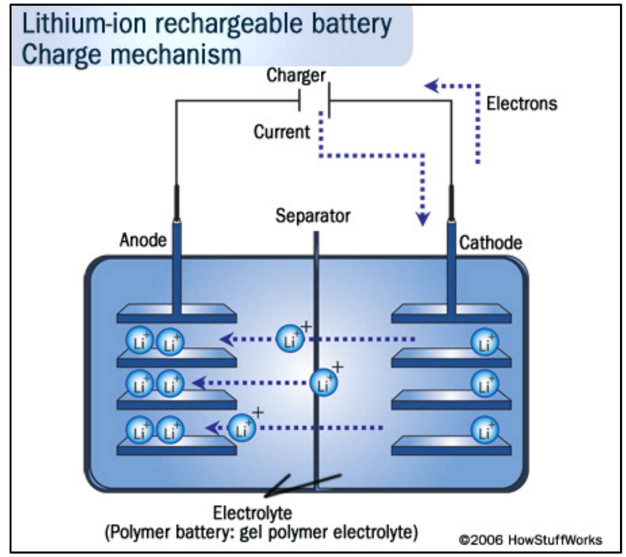
Section 2:
LIB Charge/Discharge Heat Transfer Mechanisms

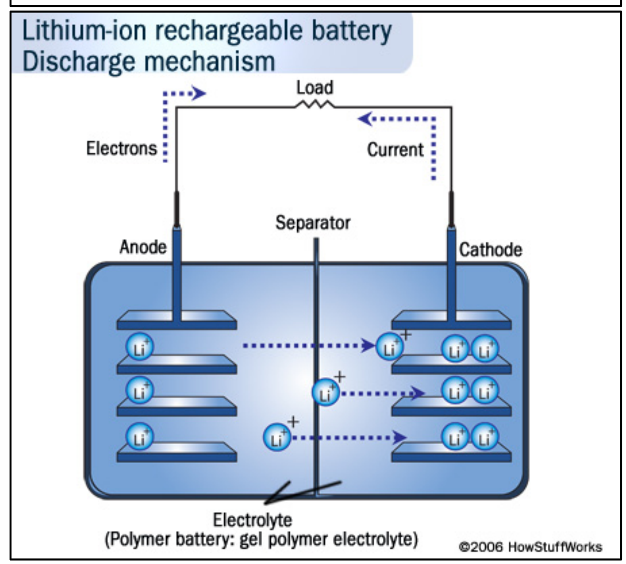
LIB Charge/Discharge Heat Transfer Mechanisms

- LIB Basics:
  - 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
- As with any object, the three modes of heat transfer apply: convection, conduction, radiation
- 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 (captures heat due to Ohmic losses, charge-transfer at the interface, and mass transfer limitations):

$$Q = I\left(E_{OC} - E - T\frac{\partial E_{OC}}{\partial T}\right) \qquad \textbf{(1)}$$

  - I is the total current
  - E_{OC} is the open circuit potential
  - E is the working voltage
  - T is the local temperature





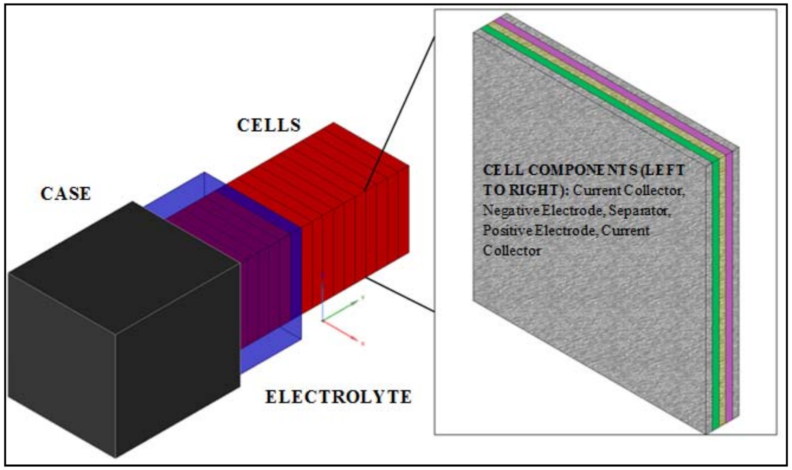
Images retrieved from electronics.howstuffworks.com

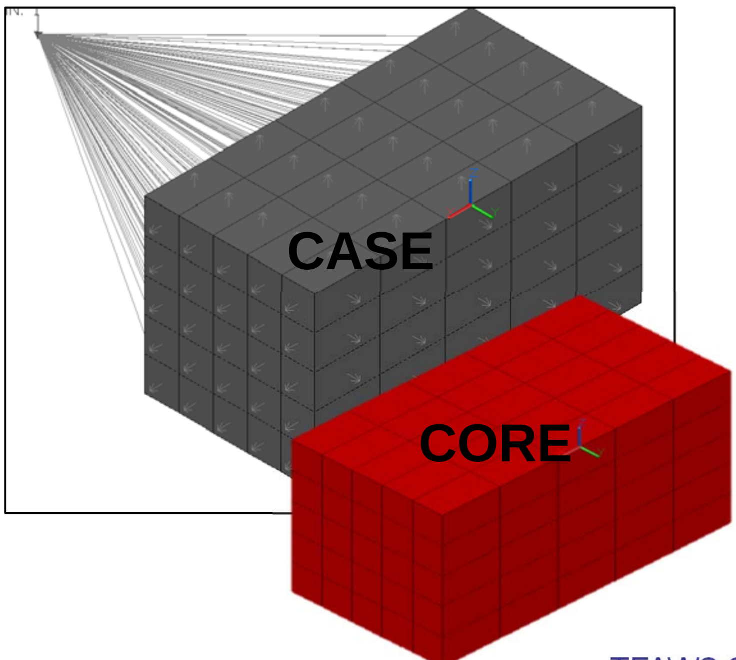
Section 3:
Thermal Desktop Model Development

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 numerically based assessment of a 185 Ah LIB conducted by Chen et. al. (primary source) who also utilized Bernardi's equation for local heating
- In short, 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)

Thermal Desktop Model Development



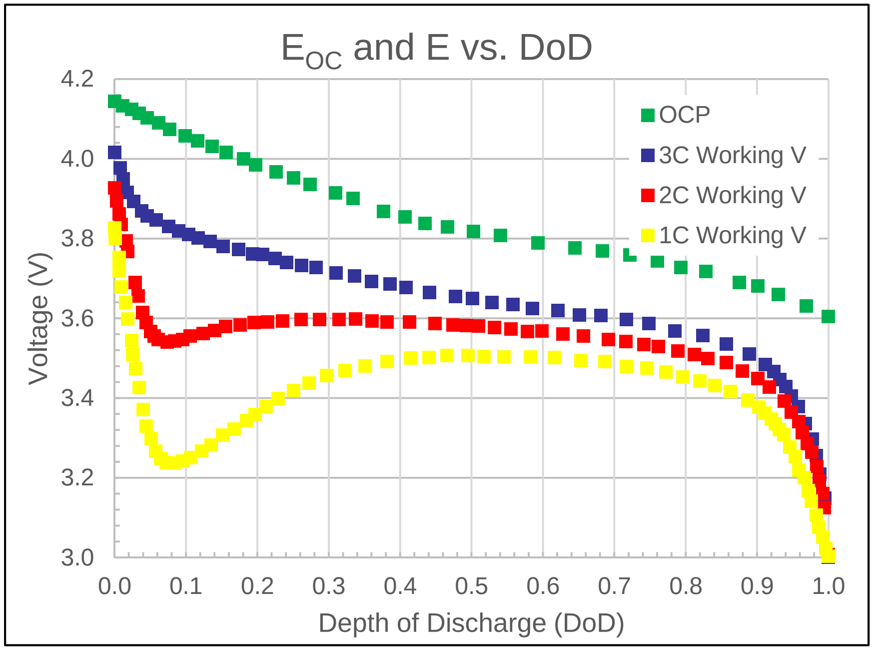


- Thermal Definition:
  - Geometries and material properties provided in table
  - Convection represented through a 300 K boundary node connected to the exterior encasement surfaces with a natural convection conductor (4.3-10 W/m^2K depending on location and DoD)
  - External surfaces set to radiate 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 EOC 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*



$$Q = I\left(E_{OC} - E - T\frac{\partial E_{OC}}{\partial T}\right) \quad (1)$$

Thermal Desktop Model Development

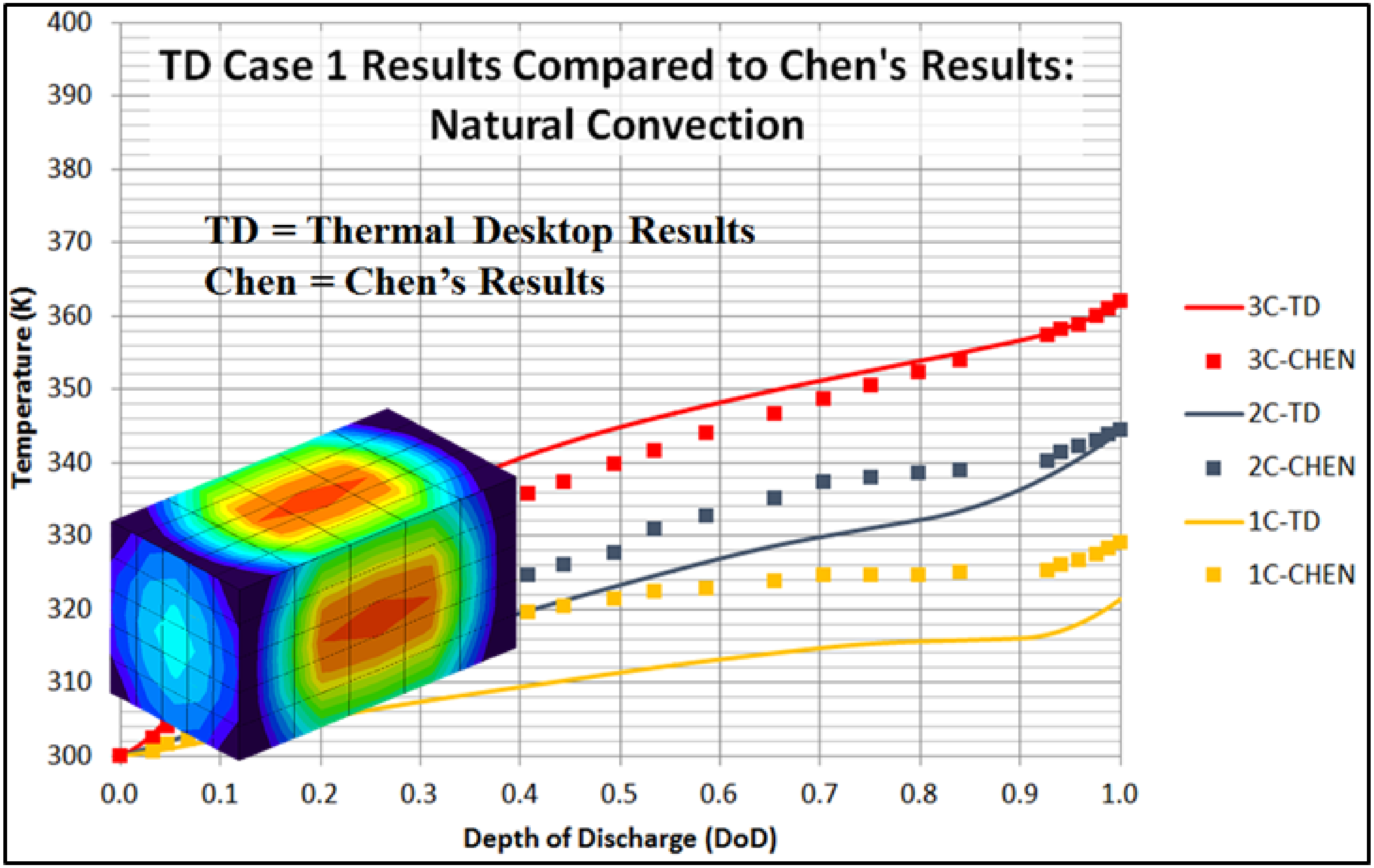
Test Case Matrix

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)

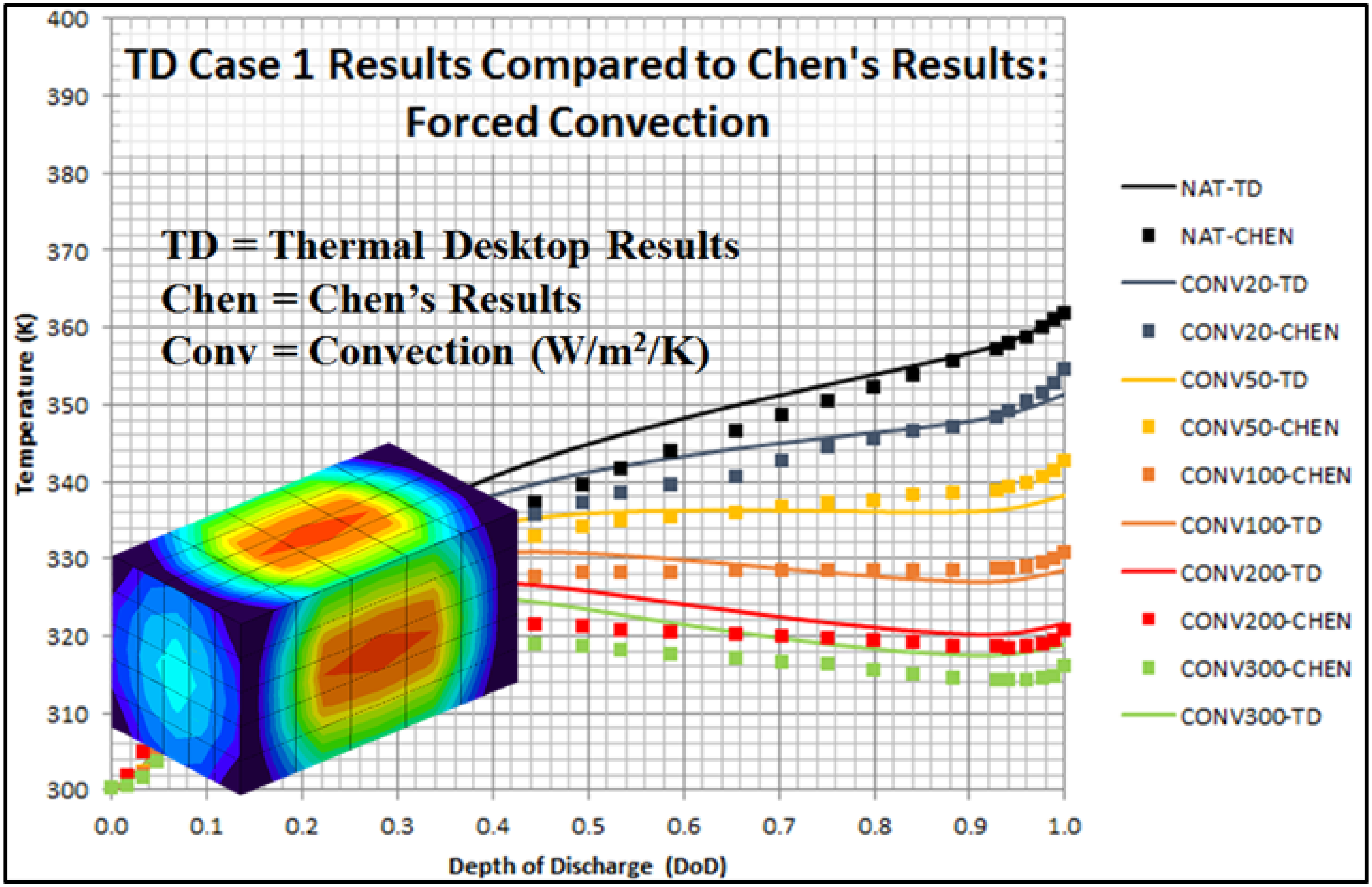
- Case 1: Exact Replication of Chen's Study
  - EOC and E update in the Q equation (Bernardi's) after each iteration. I, T, and $\frac{\partial E_{OC}}{\partial T}$ held constant
- Case 2: No-Logic, Constant/Averaged Local Heating Applied
  - Constant local heating applied based on average of entire 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

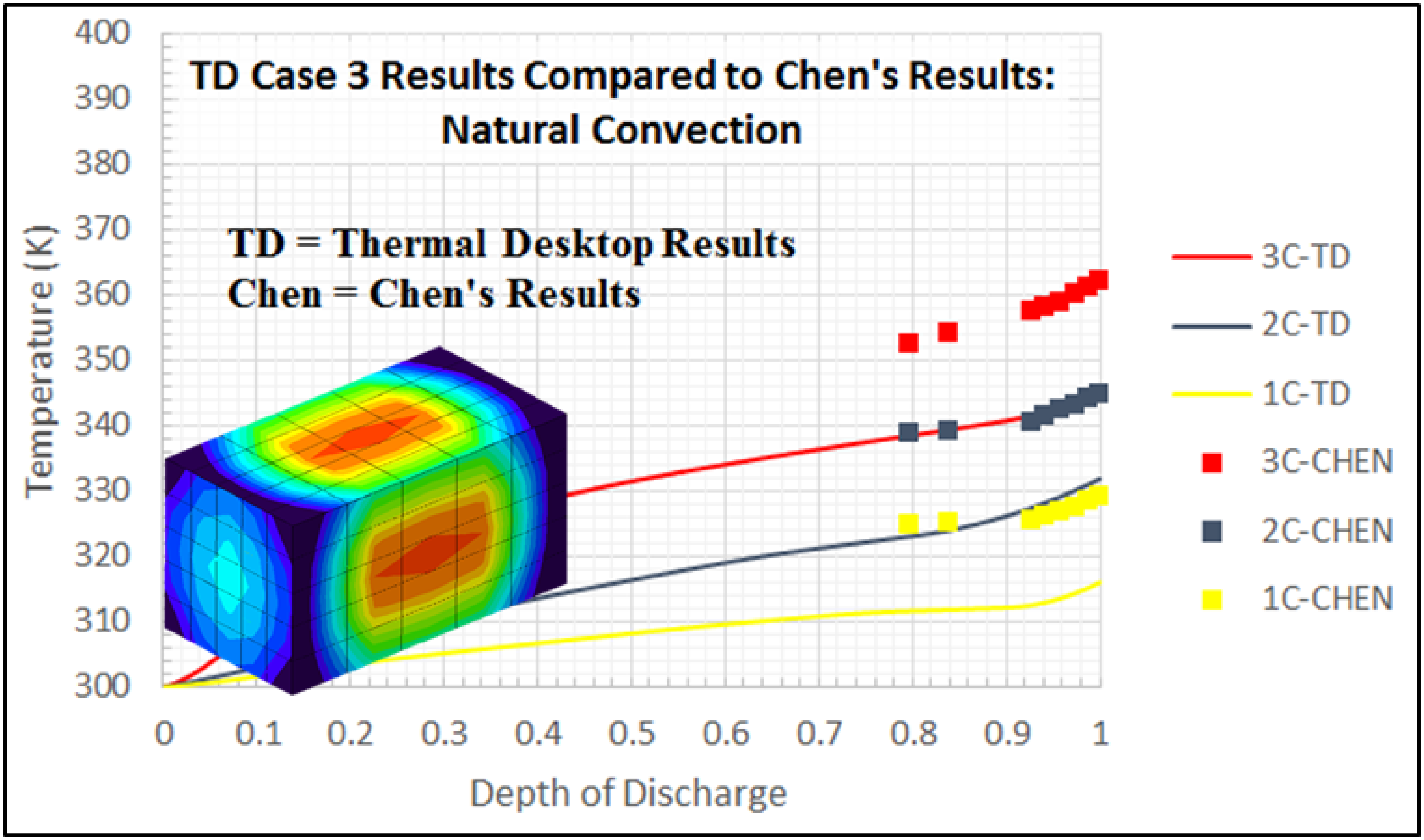
Case 1 Natural Convection Results



Case 1 Forced Convection Results

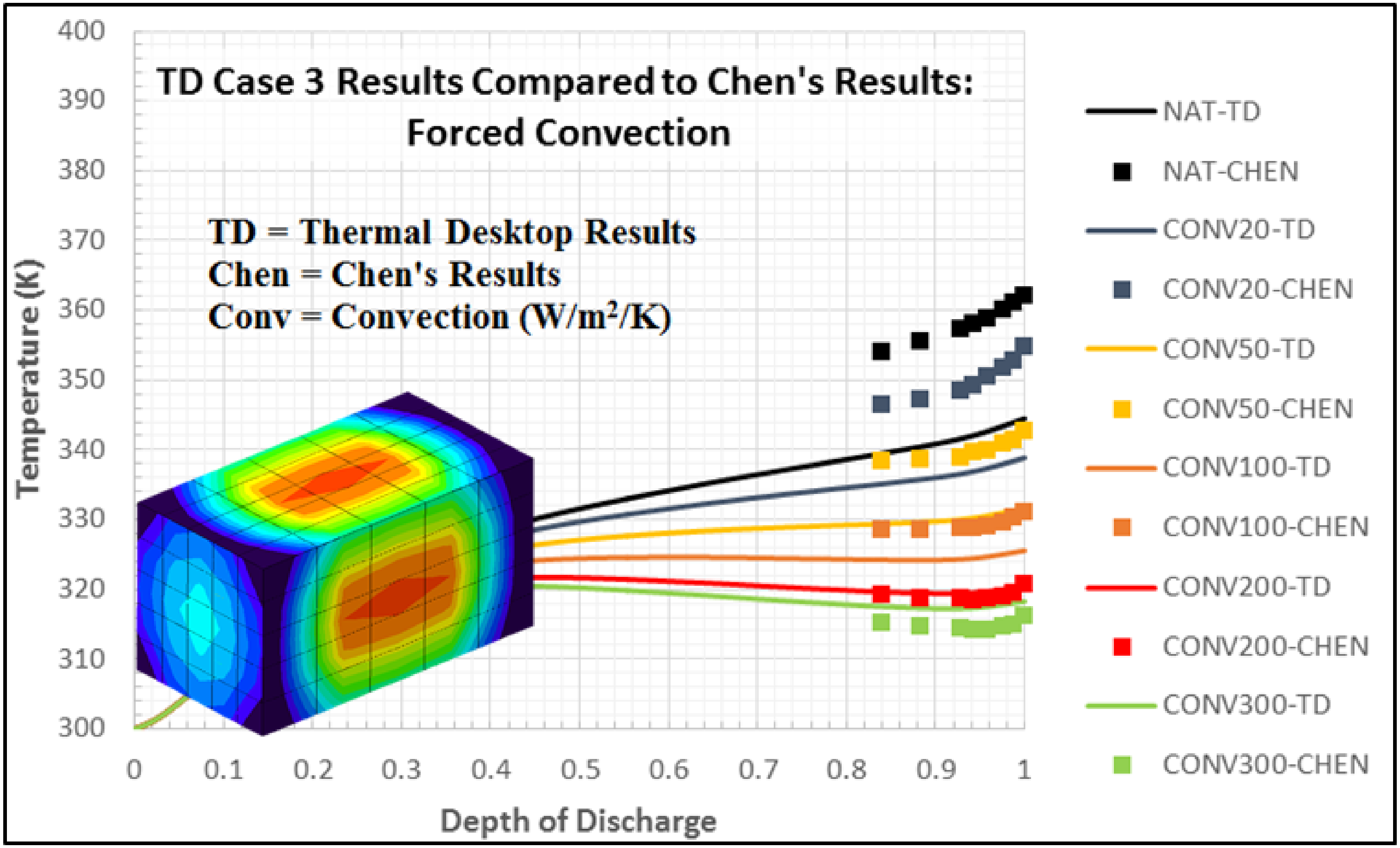


Case 3 Natural Convection Results



Case 3 results pending final review

Case 3 Forced Convection Results



Case 3 results pending final review

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:
  - 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
  - Implement these techniques into an orbital scenario/model (ultimate goal) to investigate the effects of this analysis technique combined with orbital analysis techniques
  - Develop more detailed model to provide better definition of where the hot spots will occur (similar to work being done in COMSOL)
  - Could we then?
    - Predict beta angles and solar conditions which could invoke a thermal run-away condition
    - Make more accurate performance predictions to minimize necessary thermal control/protection
    - Implement thermal considerations into the design of the battery rather than waiting until the battery is complete and then adding passive/active thermal cooling/heating

Section 6:
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