# Analytical Modeling and Simulation of Thermoelectric Devices

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### **Outline**

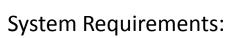


- System level methodology
  - Top-down method of design
- Device level methodology
  - Bottom-up method of simulation
- TE Performance Simulation
  - Defining Operating Conditions
- Thermomechanical Device Simulation
  - Optimizing the couple structure
- System Level Simulation
  - Feedback for integrating simulation tools



## System Level Methodology

From Heat Source to Exhaust



Specific Power/Voltage
Bus/Lifetime/Duty Cycle or Steady

State

Thermal Circuit Model: ChemCAD + CFD

Heat Delivery Requirements:

Heat Exchangers/Flow

Rates/Fluxes/Temperatures/Geomet

ry

**Converter Requirements:** 

Power/Voltage/Thermomechanical

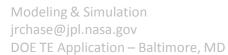
Integration

Thermoelectric
Performance Model:
Analytical/Empirical

Converter Geometry Specifications/Fill Factor/ Modularity/ Heat Concentration/

TE Material Selection





### Device Level Methodology

#### Couple or array thereof



Generic TE Mod Design

**Device Requirements:** 

Demonstrated Efficiency/Life-Time

Material Definition (previous):

Thermal/Mechanical Stability

TE Mod / Semi-Empirical Tools / **COMSOL Transport Model COMSOL** Thermomechanical Simulation

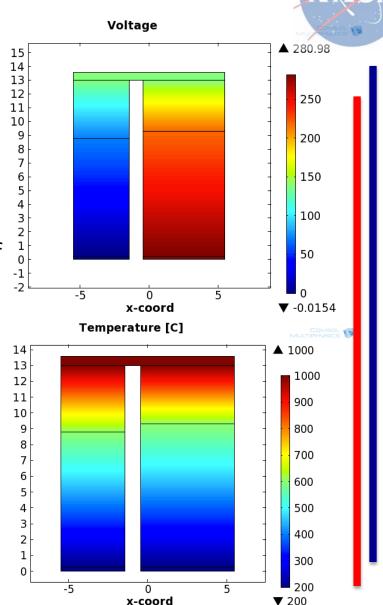
Heat Delivery Requirements: Heat Flux/Leg Footprint/ Packaging or **Encapsulation Requirements** 

Device Geometry Specifications/ Segmentation/Interface Temperatures



### Performance Model Simulation

- TE Mod used as empirical tool to roughly optimize device efficiency and geometry based on segment temperature inputs.
- Several geometric options are catalogued in Excel for selection.
- COMSOL solves for exact, analytical solution of temperature dependent transport equations to provide TE performance conditions: heat flux and open-circuit voltage.
- V<sub>0</sub> and integrated device resistance in COMSOL used for Excel model of predicted Power Curve
- This provides data for comparison to what is actual measured directly from the device once on test

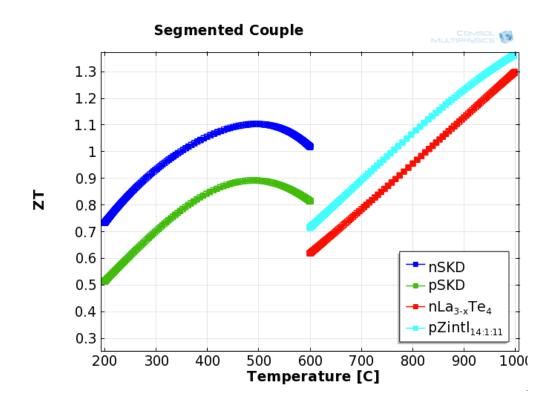




### Performance Model & Simulation

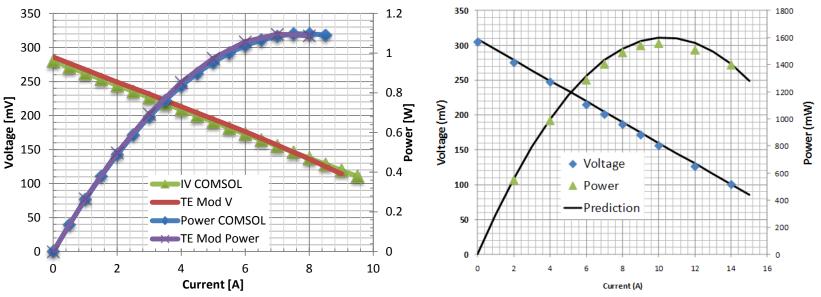


- Tools are highly flexible for use against broad geometries and degrees of system sophistication
- Performance simulation initially performed on TE + electrodes - later compared to final structure



## Comparison with Measurements



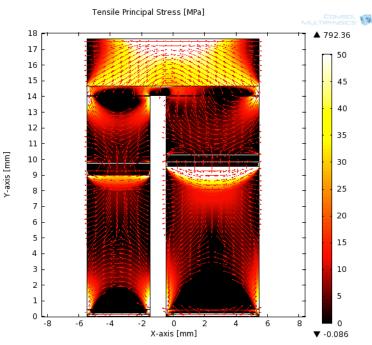


 Comprehensive library of temperature dependent thermal and mechanical properties for thermoelectric, non-TE engineering, and refractory materials/alloys.



### Thermomechanical Device Simulation

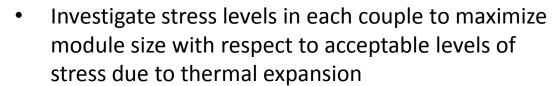
- Temperature Field / Heat flux from performance model is applied to a structural mechanics model to asses stress state in operation of a single couple at each interface.
- Metallization layers, electrodes, insulators, and other mechanical features are included to study robustness realistically.
- Residual stresses from temperature and pressure at each bonding step are included.
- Model is used as parametric tool to show effects of inter-layer thicknesses:
  - Stress increase or relief
  - Voltage drop from additional resistances in series
  - Reduced ΔT across TE segments

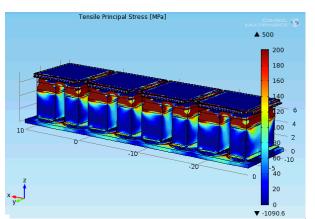


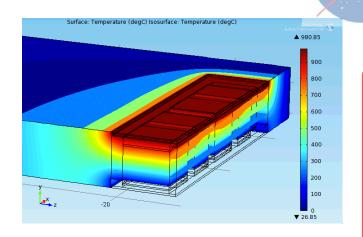


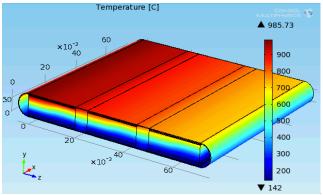
### Thermomechanical Converter Simulation

- Thermal gradient conditions are later applied to a converter level / module model:
  - Couple-couple interactions
  - Thermal losses and shunting define insulation requirements
  - Provide prediction of macroscopic heat flux for feedback to system models









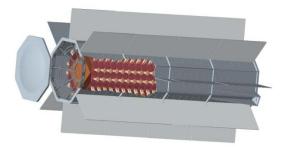
As the true operating conditions / performance of the converter is understood – effects on the balance of plant come into focus.



### **Ongoing Work**

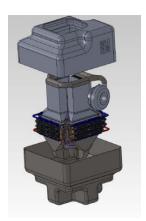
- Coupling of mechanical simulation with equation-based thermoelectric performance to create a more complete system simulation model
- Rapid feedback simulation tools for coupling heat exchangers with TE devices/modules for understanding transients and cycle-time.







kW-class Fission Reactor Power System



Auxiliary and waste heat recovery power systems

### Summary



- A high-level strategy for use of semi-empirical modeling and numerical simulation tools has been outlined
- A top-down approach is typically employed at JPL in order to define operating conditions for the TE device/converter design
- Simulation is then used on a bottom up approach to optimize couple structure and fabrication for implementation in a specific system.
- Iteration and feedback to the system design is then required to optimize on the larger scale – this can be accomplished through coupling of outputs from focused modeling and simulation.



### Acknowledgements



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Thank you.

