

Spring 2017  
Department of Mechanical and Aerospace Engineering  
EMAE 689: Special Topics

Course Title: **Battery Dynamics and Modeling**  
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Large-scale battery packs are needed in hybrid and electric vehicles, utilities grid backup and storage, and frequency-regulation applications. In order to maximize battery-pack safety, longevity, and performance, it is important to understand how battery cells work. The course focuses on developing a mathematical understanding of how electrochemical (battery) cells work, both internally and externally. We will derive physics-based mathematical models of the electrochemical dynamics of battery cells, including thermodynamic and kinematic properties, at multiple scales. We will use discrete-time realization algorithm to convert the physics-based models into high-fidelity approximate reduced order models. We will discuss battery-management system requirements and simulation of battery packs including battery state and health estimation. Modern, lithium-ion chemistries will be emphasized.

The following is a summary of the topics to be covered in the course:

1. Battery Boot Camp

- Introduction to the course
- How electrochemical cells work
- Choice of active chemicals
- Lithium-ion preview; Availability of lithium
- Lithium-ion cell makeup
- Fabrication of electrodes
- Cell Assembly
- Cell failure modes

2. Equivalent-Circuit Cell Models

- Open-circuit voltage (OCV) and the State of Charge
- Linear polarization—departure of cell's terminal voltage away from OCV
- Converting R-C battery models to discrete time
- Hysteresis voltages
- The Enhanced Self-Correcting (ESC) cell model; OCV testing
- Cell testing to determine the OCV relationship
- Determining Coulombic efficiency
- Determining temperature-dependent OCV
- Cell testing to determine the dynamic relationship

3. Microscale Cell Models

- Charge conservation in the solid phase
- Mass conservation in the solid phase

- Energy and thermodynamic potentials
- Thermodynamics; Direction of reaction
- Electrochemical potential; Gibbs-Duhem equation
- Basic characteristics of binary electrolytes
- Electrolyte mass balance equation
- Electrolyte charge balance equation: Electrolyte current.
- Butler-Volmer equation
- Cell-level quantities
- Single-particle models

#### 4. Continuum (Porous-Electrode) Cell Models

- Phase and intrinsic averages
- Volume-averaging theorems
- Continuum models: Charge conservation in the solid
- Mass conservation in the solid and electrolyte
- Charge conservation in the electrolyte
- Cell-level quantities; PDE simulation methods

#### 5. Thermal Modeling

- Micro-scale thermal model
- Continuum thermal model

#### 6. Battery Management Systems

- Introduction and BMS functionality
- BMS Requirements:
  - Sensing
  - High-voltage contactor control
  - Isolation sensing and thermal control
  - Protection and interface
  - State-of-charge estimation
  - Energy and power estimation

#### 7. Simulating Battery Cells and Packs; Battery State and Health

- Battery Cell Dynamics: Equivalent-circuit models (ECMs)
- Battery Cell Dynamics: Physics-based models (PBMs)
- Vehicle dynamics and range calculations
- Lithium-ion aging: Negative electrode
- Lithium-ion aging: Positive electrode
- Sensitivity of voltage to ESR and total capacity
- Degradation as basis for power limits
- Full-order model of SEI formation and growth
- Lithium deposition on overcharge
- Plug-in charging; Fast-charge example
- Dynamic power calculation
- Battery pack simulations