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# Battery Thermal Management Simulation - 1D+1D Electrochemical Battery and 3D Module Modeling on Vehicle System Level

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## Abstract

Approaching engineering limits for the thermal design of battery modules requires virtual prototyping and appropriate models with respect to physical depth and computational effort. A multi-scale and multi-domain model describes the electrochemical behavior of a single battery unit cell in 1D+1D at the level of intra-cell phenomena, and it applies a 3D thermal model at module level. Both models are connected within a common vehicle simulation platform. The models are discussed with special emphasis on battery degradation such as solid electrolyte interphase layer formation, decomposition and lithium plating. The performance of the electrochemical model is assessed by discharge cycles and repeated charge/discharge simulations. The thermal module model is compared to CFD reference data and studied with respect to its grid sensitivity. The temperature evolution of a module is simulated for enabled and disabled degradation equations revealing a very high impact of the degradation equations when approaching engineering limits, which is demonstrated for the outbreak of a thermal runaway. A dedicated cold-start simulation additionally highlights the importance of multi-scale and multi-domain models when predicting the rate of lithium plating.

## Introduction

Global concerns on sustainable energy use and environmental protection call for a widespread use of innovative energy conversion technologies. Batteries are one of the key enablers for complying with the Paris Declaration on Climate Change, United Nations [1]. They facilitate more sustainable mobility and more user-friendly leisure applications, and with the introduction of renewable energy sources, they are gaining significance in energy applications.

When focusing on automotive applications, batteries are integrated in battery electric vehicles (BEV), plug-in hybrid electric vehicles (PHEV) and hybrid electric vehicles comprising either the internal combustion engine (HEV) or the fuel cell (FCEV) as the main energy provider. What all these applications have in common are maximum requirements in view of higher energy and power density, prolonged life and increased safety. However, this broad range of applications also imposes several application-specific objectives, which cover significantly different load profiles, and thus specific durability and safety criteria. Therefore, a single design of a battery pack cannot optimally comply with all envisaged application areas. Thus, tailoring cell, module and pack design to a specific application with the aim of approaching engineering limits represents a significant challenge.

One of the crucial approaches to tackle the outlined challenge relies on virtual prototyping with predictive models in the early development phases of future batteries. Virtual prototyping and model-based development with predictive models is one of the key enablers to frontload the development process, Zhu et al. [2]. This is even more important in the light of the outlined challenges, which cover a broad range of spatial and temporal scales. This is reasoned by the fact that energy and power density as well as degradation rates and safety aspects of batteries inherently reflect the entire spectra starting from the basic material properties, over electrode and cell designs to module and pack design including its electric and thermal boundary and operating conditions.

Current battery models are not yet capable of providing credible answers to all these challenges by modeling all relevant scales spreading from atomistic to macro and vehicle scales in a coupled manner, Franko et al. [2]. Therefore, there is a strong push to develop advanced and innovative multiscale approaches, e.g. [2, 3, 4, 5, 6, 7, 8, 9, 10, 11], to answer urgent needs of the industry and society. In addition to the multiscale nature of the models, a high level of prediction capability and generality as well as short computational times are very important attributes of such models. The latter is key to efficiently simulate numerous design configuration variants and to assess aspects of the battery lifetime. A high level of prediction capability is required since in early development phases

- These features of the applied modelling framework characterize it as an advanced MSMD early stage development tool with high prediction capability suitable to efficiently explore the vast design space of material, geometry, domain specific design and vehicle as well as battery operation parameters.
- Therefore, the proposed methodology significantly contributes to more accurate virtual prototyping, since it enables more efficient frontloading and allows for approaching engineering limits with higher certainty.

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# Nomenclature

## Latin Letters

$\boldsymbol{a}$ - Specific surface area ($m^2/m^3$)
$\boldsymbol{c}$ - Molar concentration ($mol/m^3$)
$\boldsymbol{c_p}$ - Specific heat capacity (J/(kg·K))
$\boldsymbol{D}$ - Diffusion coefficient ($m^2/s$)
**F** - Faraday constant, 96485 (A/mol)
$\dot{\boldsymbol{F}}$ - Flux (variable)
$\boldsymbol{\Delta h}$ - Heat of reaction (J/mol)
$\boldsymbol{I}$ - Current (A)
$\boldsymbol{j}$ - Specific mole flux (mol/(m2.s)
$\boldsymbol{k}$ - Transfer coefficient ($W/(m^2 \cdot K)$)
$\dot{\boldsymbol{N}}$ - Mole flow (kmol/s)
$\dot{\boldsymbol{q}}$ - Heat source ($W/m^3$)
**R** - Ideal gas constant 8.3144 (J/(mol·K))
$\boldsymbol{r}$ - Spherical coordinate (m)
**Δs** - Entropy
$\boldsymbol{T}$ - Temperature (K)
$\boldsymbol{t}$ - Time (s)
$\boldsymbol{t^+}$ - Cation transference number (-)
$\boldsymbol{x}$ - Spatial coordinate (m)
$\boldsymbol{\Delta x}$ - Length of finite volume (m)
$\boldsymbol{y}$ - Spatial coordinate (m)
$\boldsymbol{z}$ - Spatial coordinate (m)

## Greek Letters

$\boldsymbol{\beta}$ - Split factor (-)
$\boldsymbol{\eta}$ - Activation over potential (V)
$\boldsymbol{\kappa}$ - Ionic conductivity (A/(V·m))
$\boldsymbol{\rho}$ - Density ($kg/m^3$)
**σ** - Electric conductivity(A/(V·m))
$\boldsymbol{\phi}$ - Potential (V)
$\boldsymbol{\Phi}$ - State vector (variable)

## Indices

**D** - Decomposition
**deg** - degradation
**e** - Electrolyte
**eff** - effective
***i*** - index over heat sources
**irrev** - irreversible
**Li** - Lithium
**Li-el** - Lithium electrolyte
**LPL** - Lithium plating
**ohmic** - Ohmic
**p** - Particle
**pol** - Polarization
**r** - Coordinate direction r
**r** - reaction
**rev** - reversible
***s*** - Solid