

Optimizing Lithium-Ion Batteries - Tailoring Electrodes for Microhybrid Vehicle Applications

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ABSTRACT

Design of batteries for automotive applications requires a careful balance between vehicle requirements - as driven by automakers - and cost. Typically, for batteries, the goal is to meet the most stringent requirement at a competitive cost. The real challenge in doing so is understanding how the battery-level requirements vary with changes in the vehicle, powertrain, and drive cycle.

In this work, we consider the relationship between vehicle-level and battery-level requirements of microhybrid vehicles and their linkage with battery design. These vehicle platforms demand high-power pulses for impractical durations - over 60 seconds on some drive cycles.

We demonstrate a method for optimizing the battery design for fuel economy against any specific drive cycle, whether regulatory, consumer, or otherwise. This method allows for a high degree of customization against manufacturer or consumer value. Electrochemical modeling and vehicle modeling, coupled with experimental validation, is used to investigate the effects of key battery design parameters - such as particle size and coating thickness - on the energy and power capability of lithium ion batteries.

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INTRODUCTION

Microhybrid vehicles based on a 48V architecture have recently emerged as a means of achieving significant fuel economy savings - as much as 20% in some cases - with minimal impact to the vehicle architecture or cost [1, 2, 3, 4]. These fuel economy improvements are necessary to meet consumer preference for improved fuel economy as well as regulatory requirements for the same. In the United States, Corporate Average Fuel Economy (CAFE) requirements will reach approximately 54.5 mpg by 2025 [5]. Many different improvements will be required to achieve these government-mandated fuel economy standards, and technologies such as microhybrid will help achieve them.

Microhybrid vehicles, and similar mild-hybrid vehicles, typically consist of a more powerful motor/generator, provide for regenerative braking energy, and may provide traction power to the wheels via electrical power [6]. To accomplish these tasks, microhybrid (and mild hybrid) vehicles can operate at higher voltage levels, such as 48V, that reduce electrical currents and thus IR-based losses.

One of the primary functions of a microhybrid system is to recover energy when possible, through the means of regenerative braking, and to distribute that energy later to electrical consumers or to electrical propulsion. The time-shifting nature of energy consumption in a microhybrid system requires an energy storage device. The energy storage device must, of course, be optimized for the task; it must provide the power necessary while not being over-engineered, which would drive excessive cost.

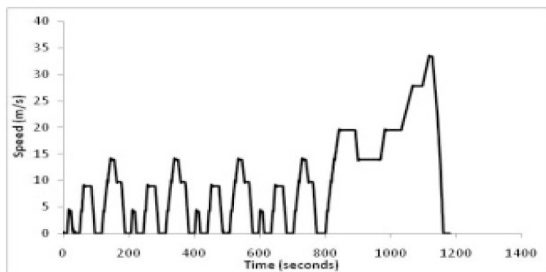
Toward that end, in this paper we explore the optimization process for lithium-ion batteries that would be used in a microhybrid application. We propose a new class of metrics that can be directly linked to the performance vs. cost tradeoffs that frame the microhybrid optimization process. We explore one example metric, the density of recovered braking energy, Wh_{recov}/L .

Finally, we consider how vehicle design choices, including component selection, affect the optimization. We also explore how the choice of regulatory drive cycle affects the result of optimization, and how the battery might be engineered for specific drive cycles.

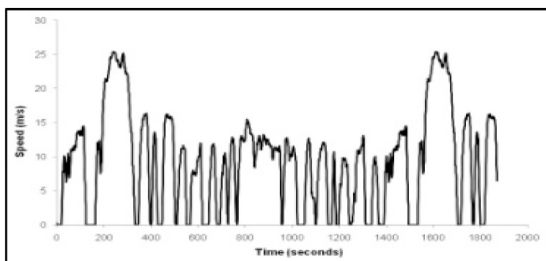
EXPERIMENTAL

Drive Cycles Used in this Work

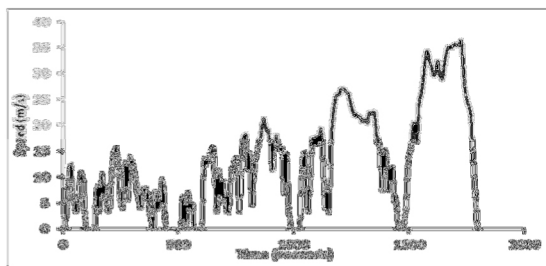
Three drive cycles were used to characterize vehicle demand for this work: The New European Drive Cycle (NEDC), Federal Test Protocol - 1975 (FTP75), and the full World Light-Vehicle Test Protocol (WLTP). Each of these cycles is used to determine regulatory compliance and provide fuel economy information to consumers. Vehicle speed vs. time profiles are shown for each cycle in Figure 1 a), b), c) below.



(a)



(b)



(c)

Figure 1. Drive cycles used in this analysis: a) the New European Drive Cycle used in much of Europe, b) the Federal Test Procedure (FTP75) used in the United States, and c) the World Light Vehicle Test Protocol (WLTP) that has been proposed.

These three drive cycles exhibit substantially varying characteristics, as shown in Table 1. The US FTP75 displays frequent stops, but for very short time periods. It exhibits fairly low speeds for most of the cycle, with the exception of two periods of higher speed, and shows a great deal of speed variation. The NEDC is a “mechanical” cycle, in that it has periods of constant speed and constant acceleration. The NEDC has longer stop events, but much less speed variation.

Finally, the WLTP is a test still under proposal that mixes characteristics of many different drive cycles and different types of driving.

Table 1. Characteristics of drive cycles

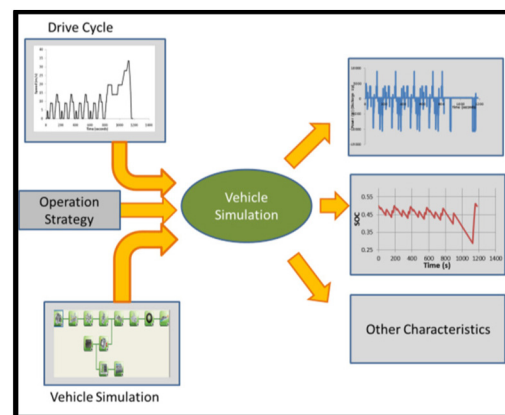
Parameter	NEDC	FTP75	WLTP
Duration	1180s	1877s	1800s
Total Regen Possible	289Wh	655Wh	630Wh
Longest Regen Peak	36 s	37 s	80s
Largest Regen Peak	88Wh	65Wh	97Wh
%Stopped	25.0%	21%	13.2%
Max. Speed	33.5m/s	25.4m/s	36.5m/s

These three cycles will be explored in more detail during the following sections of this work.

Vehicle Simulation

Vehicle simulation was performed using the Autonomie software package developed by Argonne National Laboratory [7-8]. Simulation was conducted by applying the test vehicle to a drive cycle, consisting of a vehicle speed vs. time plot. For this work, we used regulatory drive cycles as described in the section above. The time interval for the drive cycles was 0.1 second. The physics simulation embedded in Autonomie determined how much brake regeneration power would be available during a braking event, accounting for factors such as air resistance, rolling resistance, limitations of the motor/generator, and component losses.

Autonomie simulations were used to develop a power vs. time profile for a mid-size (C segment) vehicle with a 48V microhybrid architecture. This microhybrid contained a 8 or 12kW motor/generator. The powertrain architecture of this is shown in Figure 2, with details provided in Table 2.



(a)

Figure 2. Vehicle Simulation. a) Process used in Autonomie vehicle simulation, b) Vehicle architecture including powertrain and electrical components used in vehicle simulations

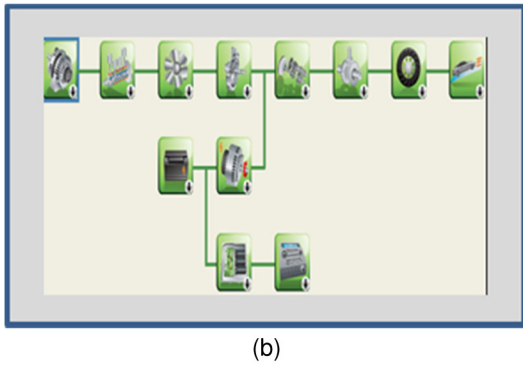


Figure 2. (cont.) Vehicle Simulation. a) Process used in Autonomie vehicle simulation, b) Vehicle architecture including powertrain and electrical components used in vehicle simulations

Table 2. Vehicle characteristics

Engine Displacement	2.2L
Combustion Engine Power	110 kW
Electric Motor Power	8kW or 12kW
Vehicle mass	1706 kg
Cross-sectional area	2.09 m ²
Coefficient of drag	0.26
Battery size	6Ah or 12Ah
Nominal Voltage	48V
Cell Configuration	13SP1

This research focuses on regenerated braking energy as a source of fuel economy benefit rather than on hybridization schemes. The power profiles included in this work did not optimize the usage of electrical propulsion. The method used in these simulations is agnostic to the method of electrical propulsion.

Figure 3 displays power profiles derived from application of the vehicle simulation process described in Figure 2 against the vehicle described in Table 2 and the drive cycles described above. The large spikes correspond to regenerative braking events.

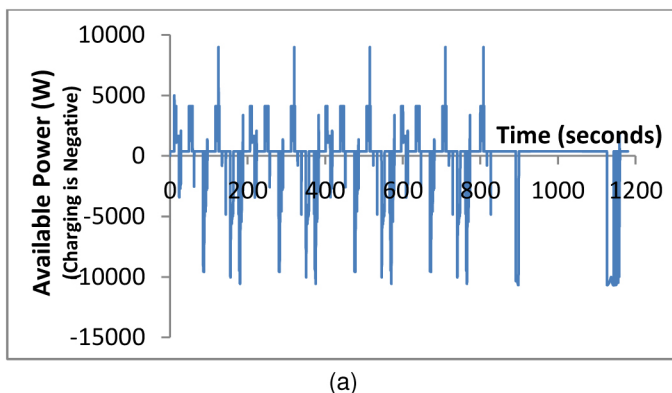


Figure 3.

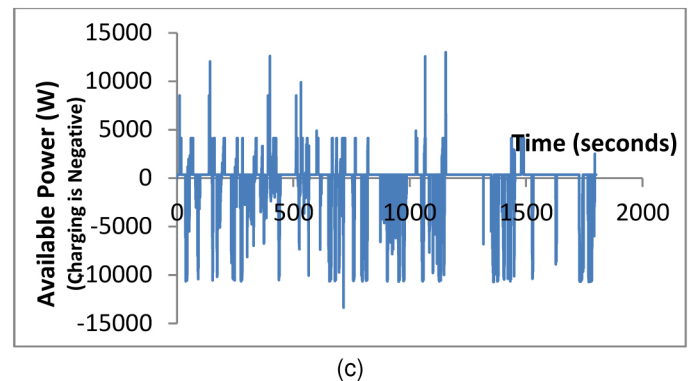
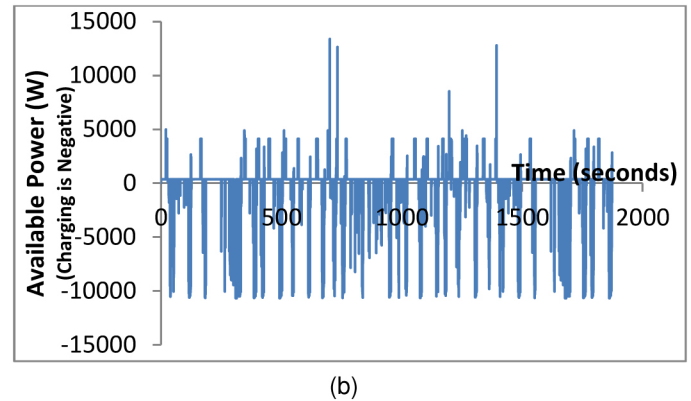


Figure 3. (cont.) Power profiles from NEDC, FTP-75, and WLTP in a)-c).

Electrochemical Simulation

COMSOL Multiphysics was used for physics-based modeling of coin cell data to identify material properties responsible for observed cell characteristics. The Doyle-Fuller-Newman model included with COMSOL was used for the simulations included in this work [9].

A 1-D electrochemical model was used to describe the chemical and physical processes that occur in the cell.

Conditions for simulation are shown in Table 3. Conditions for cathode material - including porosity, particle size, and diffusion characteristics - were chosen from NMC 1:1:1 intrinsic parameters as determined from literature, and simulate Umicore MX-6 cathode material [10]. Cathode and anode porosities were selected as typical for lithium-ion batteries [11].

Cathode diffusivity was fit to experimental data collected from cycling an 8Ah cell comprised of NMC 1:1:1 cathode combined with a graphite anode. For the purposes of this work, we have used a value for D that varies with SOC, because it is known in the literature that D varies with SOC [10,13]. In practice, SOC will be very specific to the choice of vehicle operating strategy, making it important to represent cathode diffusivity as a variable as we have done in this work. Anode Li diffusivity was selected from Guo et al [12].

Table 3. Electrochemical parameters used in this work

Cathode Thickness	Varies per experiment
Anode Thickness	Varies per experiment
Separator Thickness	20 μm
Cathode Particle Radius	3 μm
Anode Particle Radius	4 μm
Cathode Li Diffusivity [10]	Function of SOC: $\sim 10^{-15} \text{ m}^2/\text{s}$
Anode Li Diffusivity [12]	$4 \times 10^{-14} \text{ m}^2/\text{s}$
Cathode Conductivity	1.0 S/m
Anode Conductivity	100 S/m
Electrolyte	1:2 EC+DMC, 1.1M LiPF ₆
Cathode	Li-ion Ni:Mn:Co, 1:1:1
Anode	Carbon (graphite)
Cathode Porosity [11]	0.4
Anode Porosity [11]	0.4

RESULTS

Defining Metrics and Targets for Microhybrid

Optimizing a battery for microhybrid - or any other application - requires proper metrics and targets for which the device should be optimized. This combination of metric and target can be a cost function, or simply a particular characteristic that should be maximized or minimized.

Here, we explore three possible options, energy density, power density, and a new metric that we define, "recovered energy density".

Energy Density

Energy density of a battery is a commonly-used characteristic that is used to describe the capability of a battery to store energy. Lithium batteries have long been described on the basis of their volumetric energy density (Wh/L) and gravimetric energy density (Wh/kg) [14]. Of particular note is how inclusive the denominator is; whether it includes the mass and volume of just the active material, or whether it includes other components, including void volume, conductive material, binder, and current collector, among others. These additional components do not add energy storage capability but are critical to battery function [15].

The energy content of a drive cycle for this application can be determined by integrating under the heaviest braking pulse. For NEDC, this provides up to 88Wh for the vehicle and architecture described here. Assuming no other energy-based requirements are made, this value becomes the notional energy requirement for the battery.

However, this energy must also be collected at high power, and variable power - meaning that the recovered energy content cannot be used to directly size the battery. Figure 4 displays

energy utilization as a function of SOC. This figure illustrates that the usable energy is a small fraction of the total energy in the battery, if that battery is sized such that it can take the full braking pulse, even for 10 seconds.

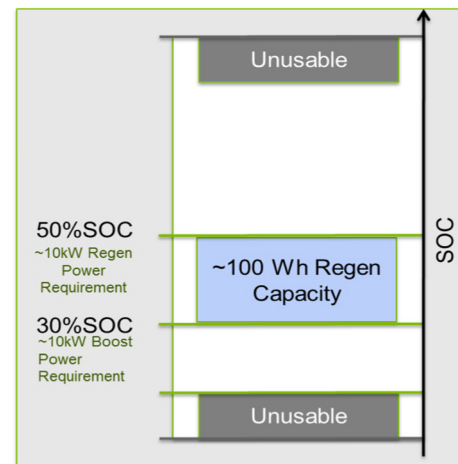


Figure 4. Sizing schematic in which a notional NMC 1:1:1 microhybrid battery is designed to provide 10kW of pulse power. The total energy content is much greater than is used to store a braking pulse.

Other requirements may contribute to the overall energy requirement of the battery. These include reserve capacity for long-term maintenance of hoteling loads and accessory support during start-stop events. However, these requirements are significantly lower power than braking loads, representing a few mA or amps, respectively - much less than the braking loads which can reach well over 100A at 48V [16]. As a result, much of the energy requirement is a low-power requirement.

Given these requirements, it is not reasonable to make energy density a primary driver for system-level optimization of a microhybrid system.

Power Density

Having ruled out energy density, power of a microhybrid becomes the clear enabling characteristic. However, determining a power density can be challenging. This is because power capabilities must be qualified much more so than energy content, as they depend heavily on the state of the battery at any given time [17]. Previous work has shown that pulse performance of a battery is limited due to solid state diffusion, a process that causes the power capability to continuously change [13].

Figure 5a) displays the maximum charging capability of the NMC 1:1:1 system studied in this work. Here, such a battery was modeled under peak voltage charging, in which the battery is charged and held at 4.2V. As can be seen, the power capability fades during the pulse. The reason for this power fade is shown in Figure 5b)-c), which displays the concentration of lithium over time at the separator/cathode and separator/anode interfaces (b), and in electrolyte (c). This result shows how mass-trans port limitations slow lithium