



Pareto fronts for multiobjective optimal design of the lithium-ion battery cell

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ABSTRACT

The objective of this paper is to study the multiobjective optimization problems for the optimal design of lithium-ion batteries. First, a two-objective problem is constructed with the performance measures of energy per unit separator area for the discharge rate of 0.5C and the mass per unit separator area. The reaction zone model and genetic algorithm are employed to solve this problem qualitatively. The resulted Pareto front comes out to be a concave curve in the 2D plane of the two performance measures. Three case studies are guided to illustrate the advantages and applications of employing the multiobjective optimization in the design process. A more sophisticated simulation model is then employed for a three-objective optimization problem with the objectives of energy performance at both low and high discharge rates and mass performance. The problem is quantitatively resolved with the assistance of the electrochemical model and genetic algorithm. The Pareto front comes out to be a curved surface in the 3D space of the three objectives. The properties of the Pareto front are discussed to offer new perspectives on product designs in the industry.

1. Introduction

There are growing efforts to increase the share of sustainable energy sources while decreasing that of fossil fuels. However, sustainable energy sources such as wind energy and solar power have the disadvantage of being intermittent. High performance devices for energy storage are required so that the spare energy during good times can be stored and utilized during bad times. The lithium-ion battery is one of the most promising candidates for this purpose due to its good balance between specific energy and specific power as well as its long battery life. Therefore, there have been increasing attention to the study of lithium-ion batteries in recent years [1–3].

The performance of a battery cell is not only affected by the chemistry of cell materials but also by the cell design. For instance, several design parameters such as the separator area, electrode thickness, and porosity determine the amount of active materials and the resistance of the electrodes. Both the amount of energy and the speed of energy delivery are heavily dependent on the cell design. Therefore, optimal design of the lithium-ion battery cell has been actively sought by many researchers.

It should be noted most approaches to optimal design of the lithium-ion battery cell aimed at minimizing or maximizing a single objective function. The specific energy of a battery cell was maximized [4–6] whereas the ohmic drop across the cell was minimized [7]. The

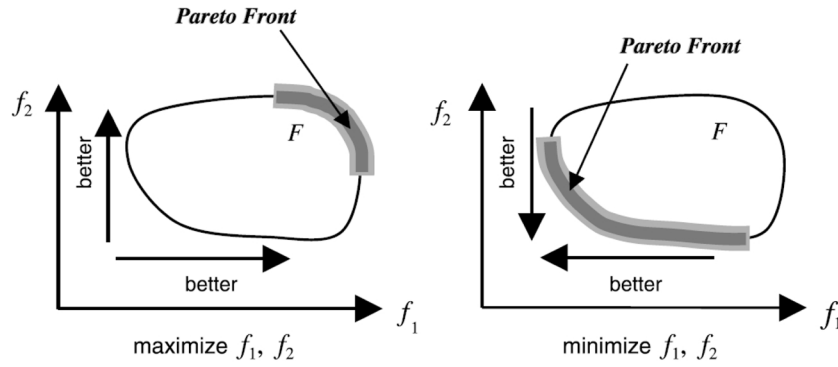
minimum usable capacity of a cell for a range of discharge rates was optimized [8]. These approaches are limited in their utility for practical applications since only a single performance measure can be addressed when a single objective function is employed. However, a trade-off among multiple performance measures such as specific energy, power and weight should be made for typical design problems in practice. A single-objective optimization problem does not offer any flexibility for making such trade-offs. A well-formulated multiobjective optimization problem, in contrast, can allow trade-offs among competing performance measures.

The solution to a multiobjective optimization (MO) problem with multiple contradictory objective functions consists of sets of compromised objectives [9,10]. This set of optimal solutions to a MO problem is referred as Pareto-optimal set, whose members are termed as the Pareto-optimal solutions. Here, the solutions are designs that are not dominated by any other design. A design is considered dominated by another if it is not better than others in any objective and worse in at least one objective [11]. A Pareto-optimal front is constructed by connecting the Pareto-optimal solutions. Fig. 1 gives illustrative examples for Pareto-optimal fronts for two-objective problems.

It is noted both specific power and specific energy were employed as objectives in [11]. However, the problem was constructed rather for the purpose of observing the effect of operating conditions on the battery performance than for cell designs. For instance, the discharge rate,

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Note: f_1, f_2 are different objective functions

Fig. 1. Illustrative examples for Pareto-optimal fronts [10].

which is an operating condition, was employed as an independent variable in [11]. To the best of authors' knowledge, the Pareto-front for battery cell designs with multiple objectives has not been reported.

The objective of this paper is to illustrate and discuss the application of multiobjective optimization to the lithium-ion battery designs and its advantages compared with the traditional design process based on a single objective. First, a two-objective optimization problem demonstrates the advantage of the multiobjective optimization approach. The two objectives are to maximize the energy per unit separator area and minimize the cell mass per unit separator area. After employing the reaction zone model [5] and the genetic algorithm (GA), the Pareto front of the constructed problem and its applications are qualitatively discussed. Then, a more complex three-objective optimization problem is constructed to account for the high-rate performance of the battery in addition. The three-objective optimization problem is quantitatively solved with a differential-algebraic equations (DAE)-based high-fidelity simulation model introduced in [12]. The Pareto front as a concave surface in the 3-D objective space is presented and discussed.

2. Two-objective Pareto front for optimization of capacity, size and weight

Optimization of the battery cell for capacity, size and weight using a two-objective problem is demonstrated in this section. After the simple reaction zone simulation model is introduced, a two-objective design problem, which is referred as the base problem, is formulated. The base problem considers energy generated during discharging and the mass of the battery cell for unit separator areas as objectives. The solution to this base problem is shown to be applicable to three case studies demonstrating the versatility of the base problem for dealing with different design problems

2.1. Reaction zone model

Although simplified, a reaction zone model is capable of offering some perspectives of how the design variables will influence the performance of a battery and, thus, is considered as a proper tool for a qualitative analysis. Fig. 2 shows a schematic of the reaction zone model.

In the reaction zone model, both positive and negative electrodes can be divided into the reacted and the unreacted regions. Between these two regions are the narrow reaction zones. All the chemical reactions are assumed to happen in the reaction zones. While the battery is discharged, the ionic current must flow from the reaction zone in negative electrode to the reaction zone in positive electrode through the porous reacted region in negative electrode, separator, and the porous reacted region in positive electrode. The two reaction zones, during the

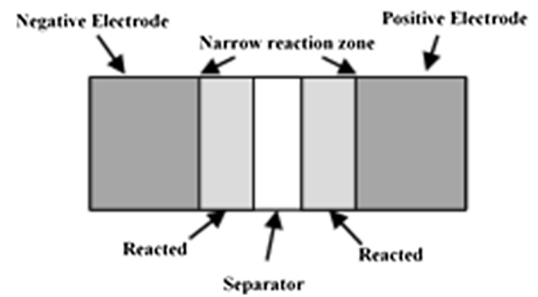


Fig. 2. A schematic of the reaction zone model.

cell discharging, will migrate from the separator toward the current collectors.

In the reaction zone model, the energy per unit separator area E is calculated by the following equation [5]:

$$E = \left(U - \frac{L_s i}{\kappa_s} \right) i t_d - \frac{i^3 t_d^2}{2\kappa_+(1 - \varepsilon_+)q_+} - \frac{i^3 t_d^2}{2\kappa_-(1 - \varepsilon_-)q_-} \quad (1)$$

where U is the open circuit voltage, L_s is the thickness of separator, i is the discharge current density, t_d is the discharge time, κ_s, κ_+ and κ_- are the effective conductivities of the electrolyte in separator, positive, and negative electrodes, respectively, ε_+ and ε_- are the porosity of positive and negative electrodes, respectively, q_+ and q_- are the capacity density of active materials in positive and negative electrodes, respectively. More details about the reaction zone model for this study can be found in [13] and [14].

The mass per unit separator area of the cell is given by Eq. (2).

$$M = M_r + M_s + M_+ + M_- \quad (2)$$

where M_r, M_s, M_+ , and M_- are the mass of remaining parts, separator, positive electrode and negative electrode in a unit separator area domain. For separator, positive and negative electrodes, each of their unit area mass can be obtained by Eq. (3)

$$M_i = [\rho_i(1 - \varepsilon_i) + \rho_e \varepsilon_i] L_i \quad (3)$$

where ρ_i is the density of solid phase in electrode i (can be $s, +$ or $-$), ε_i is the porosity, ρ_e is the density of electrolyte and L_i is the thickness.

The mass of the remaining parts is determined according to Eq. (4). It consists of two parts, one is assumed to be proportional to the mass of separator, and the other is the mass of the current collectors.

$$M_r = bM_s + M_{collector} \quad (4)$$

where b is the assumed proportion, M_s is the unit area mass of separator and $M_{collector}$ is the unit area mass of current collectors. The parameters used in the model are summarized in Table 1.

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