Modeling and Quantifying Effects of Different Porous Media on Dendrite Growth in Batteries

Arleen Liu1,3, Aimi Wen2,3, Andrew Cannon1, Emily M. Ryan3

Homestead High School, 21370 Homestead Rd, Cupertino, CA 95014; Pinewood School-Upper Campus, 26800 Fremont Rd, Los Altos Hills, CA 94022; Computational Energy Lab, Boston University, 110 Cummington Mall, Boston, MA 02215

Introduction

Batteries have a wide usage, so their tendency to decrease in cell life and short-circuit wastes huge amounts of power. The problem is caused by dendrites, tree-like structures that divert, trap, and lose lithium from the battery during discharge, which reduces the supply of available lithium in the battery by creating non reactive lithium dendrites (1). Past studies have shown that dendrite growth is significantly affected by the lithium concentration in particular areas, so we aim to look for ways to control local lithium transport. One possible solution for prolonging battery life is to add a porous media, or filter, inside batteries to suppress dendrite growth. Previous studies have found that increasing the filter area has been effective overall in slowing growth, so we expanded upon the idea by testing the effectiveness of different filters, focusing on shape, size, and spacing factors. To compare the effects on the dendrite structure, we wrote two algorithms to quantify the growth rate and branching of dendrites.

Methods

Setup for particles and filter:
We use smoothed-particle hydrodynamics (SPH) to model dendrite growth (3). The code sets up blocks of non reactive particles for filter shapes and then nucleation points (4). Quantifying growth rate:
Setup for finding trunk tips:
A circle detects boundary particles that determine locations of trunk bases (5). Rectangle bounds are used to detect the branch ends and eliminate noise (6). We then group potential branch tips with a trunk (7), using particle slopes to match a branch with a trunk (8). Backtracking from detected trunk tips:
We iterate backwards through timesteps detecting previous trunk tips using sectors in each one, used to calculate the growth rate (9). Quantifying branching:
We set up a circle centered on the nucleation point that increases in radius size every iteration to determine the ratio of solid to total particles as a means to quantify the density of branches for that particular radius size (10). The algorithms were run for different Damkohler numbers (reaction to diffusion rate ratio), to obtain dendrites with different branching properties as test cases. Lower Damkohler numbers tend to result in shorter, thicker branches.

Results

Quantifying growth rate:
This graph displays the average length of the trunks, on the y-axis, over time, on the x-axis for different Da numbers. Growth rate is found from the slope of the line. The Da value of 1600 is shorter due to time constraints in collecting data. The Da value of 64 has some negative growth due to the difficulty for the algorithm to detect the ends of extremely thick branches (13).

Quantifying branching:
This graph shows the results of the density algorithm for different Da numbers. The y-axis represents the number of solid particles detected within the corresponding radius value on the x-axis. Both the x and y values are rescaled using natural log to compare against values obtained from prior related research (14).

Discussion/Analysis:

For the growth rate algorithm, the different Damkohler (Da) numbers demonstrated that it was fairly accurate because the length increased as the Da numbers increased, which can be qualitatively observed from the simulations. According to the graph, the overall growth seemed to slow down towards the end, possibly due to the decreased amount of available lithium. As for the branching algorithm, we also found that it was fairly accurate because as the Da numbers increased, the branching density decreased due to the tendency for the branches to become thinner and longer with higher Da numbers. In future research, since the current methods only attempt to quantify two factors — branching and growth rate — they do not tell us everything about the dendrites. As a way to improve on the current algorithms, we can use a different approach such as image processing on the branches.

In the different filter cases, the triangle filter case grew more evenly than the others, which grew fastest near the corners. It seemed that the shape had a significant impact on growth rate because the dendrites with the square filter took the longest to reach the other end, meaning that it grew the slowest. This could indicate that the path for lithium flow created by the squares is more effective for suppressing dendrite growth than the others. We can then use the collected results to narrow down the factors to test more extensively, possibly creating an even more effective filter to make longer-lasting batteries.

References


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