Sensitivity-Analysis for Polymer Filter Design Using Derivative-Free Optimization

by

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A Thesis Proposal by

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Introduction

Fiber spinning is a process that uses polymers to create fibers. Polymers are pumped through an extrusion filter and through a spinneret that produces thin strands of fiber that are converged into a larger fiber product. Upon solidification, these fibers can be used in many diverse ways. For instance, fibers can be used as a component of composite materials or matted into sheets to make products like paper. Hence, to use these fibers, it is essential that the fibers don’t contain any debris as a result of the fiber spinning process; engineers determine a bound that represents the maximum amount of debris that is acceptable in fiber strands for proper handling [1].

Producing pure fibers depends on the performance of the filter. To measure filter performance, two objectives are necessary to consider. First, the lifetime of the filter must be considered. Because filters are expensive to replace, it is desirable for a filter to last as long as possible; hence, the filter lifetime should be maximized. Second, the filter must capture the maximum amount of debris to ensure that a consistent fiber product is produced; hence, the amount of debris leaving the filter should be minimized [1].

Given the two objectives stated above, the goal of our research is to maximize the performance of the filter subjected to specific filter parameters. The two filter parameters that we will be analyzing include the porosity, $\eta$, and pore diameter, $d_p$. Finding optimal parameter values and understanding how these parameters interact to affect filter performance are the key contributions of this research. We will analyze two and three layer filter configurations.

Because the function we seek to minimize requires a computationally expensive computer simulation to describe the filter-extrusion process, gradient information is unavailable. Thus, to find these optimal parameter values, derivative-free optimization (DFO) methods are used, which guide the minimization using only function values [2]. DFO methods are often referred to as sampling methods. Two sampling methods that are used include the implicit filtering method [2] and the genetic algorithm (GA) [2]. The implicit filtering method is considered a fast local method but can depend on a good initial guess at the solution. The GA is a population-based approach known to exhaustively search for the solution, but has the drawback of requiring a large number of function evaluations. For this work, that is a major drawback since one simulation can take roughly three hours [2].

In order to investigate how the interaction between the filter parameters $\eta$ and $d_p$ affects filter performance, it is necessary to conduct a sensitivity analysis using an analysis of variance (ANOVA) [3]. A sensitivity analysis examines how an output response varies when the model parameters change. Some statistical approaches to consider when performing a sensitivity analysis include a main effects analysis and a two-way interaction analysis. Since DFO methods sample a significant number of design points during the optimization phase, that information can be stored and used in a statistical analysis to help gain insight into the relationships between the decision
variables and the objective function values (i.e. filter performance). This approach was taken in [4] in which 17 model parameters were determined to fit a mathematical model of heart-rate to actual data taken from patients. In that work, a GA, implicit filtering, and the Nelder-Mead method were used [5]. Over 6,058 design points were examined and stored during the optimization and studied using the ANOVA tools in Minitab [4]. Example plots generated from the ANOVA approach in that study are shown below to demonstrate the approach.

In a main effect analysis, the output of the model is analyzed to observe how the output changes when its input parameters change. To do this analysis, each parameter is placed in a group; group numbers are assigned according to the value of the parameters, and groups with higher numbers contain parameters with higher values. For each group, the average value is calculated and then plotted. When the average value remains nearly constant across the groups on a plot, then it can be implied that the parameter has no significance on the model. A main effect plot is depicted in Figure 1 [2].

Two-way interaction analysis examines how the model output changes when there are variations in two or more parameters working together. Two-way interaction plots show how much overlap exists between each group for a specific parameter, as displayed in Figure 2. For interaction to exist between two parameters, the two graphs must cross or must not be parallel to each other; if two graphs are parallel, then there is no interaction between the two parameters. This statistical analysis is particularly important in my research because one goal is to determine how the interaction between porosity and pore diameter affect filter performance [2].

![Parameter Main Effects](image)

Figure 1: A Main Effects Plot
Background

Polymers have been used to generate many products. One such use for polymers has been in the creation of fibers through polymer processing, known as the fiber-spinning process; this process is detailed in Figure 3 [5]. In this process, molten polymer, unmelted polymer gel particles, and other debris enter an extrusion filer, which is used to remove the debris particles before this material enters the spinneret to be spun into a fiber. When the material enters the spinneret, small holes allow for the production of a thin set of fibers that are later joined together to create the final fiber product. Upon exiting the spinneret, the fiber solidifies when it is exposed to quench air [5]. During this process, it is important that debris particles be removed from the polymer; if debris particles remain in the fiber, this could lead to an inconsistent fiber and degradation in fiber properties [6].

Figure 3: Fiber melt-spinning process
The filter consists of pores with small diameters that confine debris particles that are a few microns in diameter. As the material flows through the filter, and as the debris particles accumulate inside the filter, the volume of empty space decreases, thus decreasing the permeability [5]. However, it is important that the mass flow rate is constant throughout the system so that the material enters and exits the filter at the same rate; thus, in order to ensure this continuity, the pressure drop must increase between the entrance and exit of the filter. However, the pumping instrument that pushes the polymer through the filter can be damaged if the pressure drop exceeds a certain value; if the pressure drop does exceed this threshold value, the filter must be replaced, which is a costly endeavor [7]. Hence, it is advantageous to not replace the filter as often.

Research done with polymer filtration is of great interest to researchers at the Center for Advanced Engineering Fibers and Films (CAEFF). They have developed a computational tool that simulates the stages of a fiber-spinning process, discussed above, and have created a three-dimensional model of an extrusion filter [6]. This simulator has been previously been used to help process engineers understand the importance behind debris removal. This simulator has been extended for use in the context of this problem, which is to find design parameters that will improve filter performance.

Filter performance can be measured in two different ways. The primary measure is looking at the lifetime of the filter [6]. Since filters are costly to replace, it is essential that the filter lifetime is maximized. Another way to measure filter performance is the effectiveness of debris removal [6]. Debris caught in the fiber leads to destruction in the fiber product; hence, it is crucial to minimize the amount of debris that escapes the filter.

In order to measure filter performance, design parameters must be considered. Filters can consist of one layer, or of multiple layers. Hence, important considerations include the number of filter layers and the characteristics in each layer. The characteristics that are important in this research include the porosity and the pore space diameter. For each layer in the filter, there is an associated porosity and pore diameter. These design parameters result in competing objectives when the goal is to maximize the lifetime of the filter while minimizing the amount of debris that escapes the filter. An example of this competing objective is as follows. If the filter is completely permeable, then none of the debris is trapped inside the filter. Therefore, the filter lasts forever, but the fiber product will not be consistent. However, if the filter is not permeable, then none of the debris escapes the filter. Hence, the filter lifetime will have to be replaced continuously, although a consistent fiber product has been produced [6]. Thus, the optimization problem is presented as

\[
\text{Maximize (or minimize) } F(x) \quad (1)
\]

subject to \( x, \ x \in \Omega \),

where \( F(x) \) represents the lifetime of the filter or the measure of debris escaping the filter, \( x = \{ \eta, d_p \} \), and \( \Omega \) represents the bounds on \( \eta \) and \( d_p \) [8].
Three different problems are considered, each using a different measure of filter performance. The problem formulations include the following: to maximize the filter lifetime, $F_1(x)$, to minimize the maximum rate of change of the pressure drop across the filter, $F_2(x)$, and to measure the total pressure change over the lifetime of the filter, $F_3(x)$ [8]. Each of these problem formulations is described below.

$F_1(x)$: Filter lifetime

In this optimization problem, the primary objective is to maximize the lifetime of the filter while minimizing the amount of debris that escapes the filter. In analyzing the amount of debris that is allowed to escape the filter, a bound must be defined that represents the level of debris that an engineer would deem acceptable to be included in the final fiber product. If $b$ represents this limit, and $\xi(x)$ represents the total mass of debris that escapes over the lifetime of the filter, then it is best to construct a function such that $\xi(x)$ is far away from $b$. The following function characterizes this situation:

$$B(\xi) = \frac{\xi(x)}{b - \xi(x)},$$

This function is defined on the interval $[0, b)$. It then follows that $t(x)$ should be defined as the lifetime of the filter. Then

$$F_1(x) = -t(x) + \rho_1 B(\xi),$$

where the lifetime of the filter is being minimized and $\rho_1$ is a constant. Based on the function for $B(\xi)$, $F_1(x)$ is defined for $\xi(x) < b$ [8].

$F_2(x)$: Pressure drop across the filter

Once the pressure drop across the filter reaches a specific threshold, the filter must be replaced. Hence, the main objective is to minimize the rate of change of pressure drop across the filter, which contributes to maximizing the lifetime of the filter. To mathematically describe this situation, $p_n$ represents the pressure difference from the entrance of the filter to the exit of the filter at the $n^{th}$ timestep, $t_n$. Hence, the pressure change between any two consecutive time steps is

$$\Delta p_n = \frac{p_n - p_{n-1}}{t_n - t_{n-1}}.$$  (4)

Over any time step, it is optimal to have a small pressure change. If $P$ is the set of all pressure changes, denoted as $P = \{ \Delta p_1, \Delta p_2, \ldots, \Delta p_k \}$, from time step $1$ to $k$, then a function can be written to minimize the amount of debris leaving the filter as

$$F_2(x) = a_{\text{min}}(x) + \rho_2 B(\xi),$$

(5)

(2)
where $\rho_2$ is constant and $\alpha_{\text{min}}$ is the smallest upper bound for $P$. $F_2(x)$ is also defined for $\xi(x) < b$ [8].

$F_3(x): \text{Overall Pressure Change}$

For this situation, we are considering the total change in pressure over the lifetime of the filter, consisting of $N$ time steps. To measure the total change in pressure, the two points of significance are the first time step, $(t_0, p_0)$ and the last time step, $(t_N, p_N)$.

Minimizing the slope of the secant line between the first and last time step, $(t_0, p_0)$ and $(t_N, p_N)$ is an approach to this objective. The slope is denoted as

$$m = \frac{p_N - p_0}{t_N - t_0},$$

where $t_0 = 0$. Hence, the filter lifetime is measured by $t_N$ and $t = t(x)$. By denoting $p_N = p_N(x)$, an objective function can be described as

$$F_3(x) = \frac{p_N(x) - p_0}{t(x)} + \rho_3 B(\xi),$$

where $\rho_3$ is also constant. $F_3(x)$ is also defined for $\xi(x) < b$, $t(x) \neq 0$ [8].

To solve the optimization problem stated above in equation 1, two types of sampling methods have been used. The first is called a genetic algorithm, and the second is called an implicit filtering method. These sampling algorithms were chosen because the information obtained for the parameter sets can be analyzed to further understand how the mathematical model depends on the parameters; additionally, no derivative information is needed [2].

**Genetic Algorithms**

Genetic algorithms belong to a group of evolutionary algorithms known as population based global search heuristic methods. Genetic algorithms are based on biological processes, including survival of the fittest, natural selection, inheritance, mutation, and reproduction. Design points are depicted in binary as strings of zeros and ones. Based on the biological processes mentioned above, a population evolves through each generation. In each generation, the fitness (i.e. objective function value) of every individual in the population is evaluated, individuals are selected from the current population, and these individuals are modified and then accumulated to form a new population. This new population is used in the next iteration. The algorithm ceases when a smaller fitness value has been reached [9]. The steps in this algorithm are included below.

1) Initialize the population randomly, or through an engineering prospective.
2) Evaluate the fitness of each individual in the population by evaluating the objective function at each of the design points in the initial population.

3) Iterate, to produce new generations.
   (a) Select individuals to reproduce by ranking the design points according to fitness values. Randomly select fitter individuals.
   (b) Produce crossovers and mutations, giving birth to offspring, producing a new generation.
   (c) Determine the fitness of the new individuals.
   (d) Replace the worst part of the population with new offspring.

   When selecting individuals, fitter individuals are randomly arranged to form a mating pool so that further operations can be executed. During the crossover process, information is traded between two design points that produces a new point that preserves the top attributes of the “parent points.” The mutation process is executed to preserve the new, optimal point and to further explore the design space; this phase is also significant because it prevents the algorithm from choosing a point that is not optimal from being selected. For the algorithm to terminate, either a specific number of generations must be selected or the highest ranked individual’s fitness has reached a level of stability. Often, researchers disapprove of using genetic algorithms due to their computational complexity and dependence of optimization parameter settings, which are unknown prior to the calculations. However, genetic algorithms are useful in that they help gain insight into the parameter design space and can rapidly locate good solutions for difficult search spaces [9].

**Implicit Filtering Method**

The implicit filtering method is another sampling method that performs optimization analyses without requiring knowledge of derivatives. This type of method is guided solely by objective function values that build approximate gradients of \( F(x) \). The implicit filtering method uses finite difference gradients that get smaller as the optimization proceeds. With this method, the goal of reducing the difference increment is to avoid local minima from being selected at the beginning of the optimization; functions containing a large number of local minima that are not known in advance are known as noisy functions. Using a large difference interval at the beginning of the optimization process can avoid these local minima and close in on the global minima. This algorithm requires a means to compute the objective function, an initial starting point, difference increments, and termination criteria; a function terminates based upon a function evaluation budget or a scaling budget, which consists of reducing the difference increment a fixed number of times [10].

**Previous Work**

A multiobjective genetic algorithm was used to examine the competing objectives of maximizing filter life, \( t(x) \), while decreasing the amount of debris that escapes the
Two representations of this goal were analyzed, $\xi(x)^I$ and $\xi(x)^{II}$. In $\xi(x)^I$, the goal was to minimize the percent of total debris escaping the filter; this percentage is the ratio of the mass of escaped debris compared to the mass of incoming debris. For $\xi(x)^{II}$, the goal was to minimize the total mass of the debris that escapes the filter. Since a genetic algorithm was used, an initial population size was set to 20 with 5 generations [11].

For $\xi(x)^I$, the parameters that were found to maximize $t(x)$ were $[\eta, d_p] = [0.7, 32 \mu]$, leading to a filter lifetime of 102.5 hours and allowing 6% of the debris to escape. Figure 4 depicts the filter profile, showing that most of the debris was trapped at the entrance of the filter [11].

The parameters found to minimize the percentage of escaped debris through the filter were $[\eta, d_p] = [0.61, 25.4 \mu]$, which resulted in a filter lifetime of 62.3 hours, allowing 5% of the debris to escape. Before it was stated that the more permeable a filter is, the less debris that is trapped inside, leading to a longer filter lifetime. However, further results show that the parameters that resulted in allowing the most debris to escape the filter did not correlate to a longer filter lifetime. These parameters were $[\eta, d_p] = [0.59, 36.2 \mu]$ which gave a filter lifetime of 77.9 hours while allowing 9% of the debris to escape the filter. Figure 5 shows the tradeoff curve for optimizing equation 1 using $\xi(x)^I$. This scatter plot shows the design points that an engineer can choose to create a suitable filter for his process; however, as the figure indicates, it was concluded that it is difficult to make a decision regarding what points to use based on the wide range and nonlinear trend of the values [11].
The parameters found to maximize the filter lifetime, while optimizing $\xi(x)^I$ were $[\eta, d_p] = [0.68, 38.7 \, \mu\text{m}]$, leading to a lifetime of 110.2 hours, while allowing $1.2302 \times 10^{-4}$ kg of debris to escape. Minimizing the total mass of debris that was lost leads to parameter values of $[\eta, d_p] = [0.1, 28.5 \, \mu\text{m}]$. Figure 6 shows a linear trend between the lifetime of the filter and the total mass of the debris leaving the filter [11].

More research was further done, using the implicit filtering algorithm, first on a one-layer model, 1 cm thick. Under the given conditions discussed above, filter performance was optimized for $F_1(x)$, $F_2(x)$, and $F_3(x)$. Table 1 depicts these results [8]. As displayed in the table, all formulations have the same value for the porosity, but differ in the pore diameter. Through these optimizations, it was found that $F_2$ has the smallest filter lifetime and the smallest value for escaped debris. $F_3$ has the highest value for filter lifetime, as well as the highest value for escaped debris, with $F_1$ being an intermediate.
Table 1: Filter performance comparison for $F_1(x)$, $F_2(x)$, $F_3(x)$

<table>
<thead>
<tr>
<th></th>
<th>$\eta$</th>
<th>$d_p$ ((\mu))</th>
<th>$t$ (hours)</th>
<th>$\alpha_{\text{min}}$ (10(^4) Pa/hr)</th>
<th>$\xi$ (10(^{-5}) kg)</th>
<th>$m$ (10(^5) Pa/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_1$</td>
<td>0.65</td>
<td>29.9205</td>
<td>78.1</td>
<td>7.7934</td>
<td>3.9468</td>
<td>2.0200</td>
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<tr>
<td>$F_2$</td>
<td>0.65</td>
<td>23.0000</td>
<td>65.2</td>
<td>7.2276</td>
<td>2.1475</td>
<td>2.3083</td>
</tr>
<tr>
<td>$F_3$</td>
<td>0.65</td>
<td>30.0850</td>
<td>81.4</td>
<td>7.9401</td>
<td>4.7075</td>
<td>2.0933</td>
</tr>
</tbody>
</table>

This same approach was then extended to a two layer model where $x = (\eta_1, d_{p1}, \eta_2, d_{p2})$. From an engineering standpoint, a multilayer filter should capture larger particles in the top layer and smaller particles in the bottom layer [12]. Table 2 below displays the results from the optimization. These results show that for $F_1$ and $F_3$, the lifetime of the filter is extended by nearly 23%, when compared to the results from the one layer model [8]. Results further show that while $F_2$ has the smallest lifetime, it also allows the least amount of debris to escape. The smaller lifetime suggests that this is due to the fact that the porosity in the first layer for $F_2$ is smaller than that of the other two formulations; hence, to extend filter lifetimes, porosity and pore diameter must be stabilized.

Table 2: Two-layer results using an engineering perspective for optimization parameters

<table>
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<tr>
<th></th>
<th>$d_{p1}$ ((\mu))</th>
<th>$\eta_1$</th>
<th>$d_{p2}$ ((\mu))</th>
<th>$\eta_2$</th>
<th>$t$ (hours)</th>
<th>$m$ (10(^4) Pa/hr)</th>
<th>$\alpha_{\text{min}}$ (10(^4) Pa/hr)</th>
<th>$\xi$ (10(^{-5}) kg)</th>
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<td>$F_1$</td>
<td>38</td>
<td>0.65</td>
<td>23</td>
<td>0.643</td>
<td>96.4</td>
<td>1.7905</td>
<td>9.0344</td>
<td>5.1664</td>
</tr>
<tr>
<td>$F_2$</td>
<td>38</td>
<td>0.51</td>
<td>23</td>
<td>0.64</td>
<td>57.3</td>
<td>2.621</td>
<td>8.3123</td>
<td>4.0229</td>
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<td>$F_3$</td>
<td>32.57</td>
<td>0.682</td>
<td>23</td>
<td>0.605</td>
<td>94.6</td>
<td>1.8419</td>
<td>8.7536</td>
<td>4.2888</td>
</tr>
</tbody>
</table>

To further investigate this two layer model, an optimization was also done with parameters that described the one layer model. Table 3 below displays the results from this optimization. From these results, $F_3$ has an arrangement that leads to a longer lifetime. This is due to the fact that the first layer has a larger pore diameter, while the second layer has a larger porosity [8]; hence, this delays the time it takes to surpass the pressure threshold, leading to a longer filter lifetime. Results for $F_2$ indicate a much smaller lifetime compared to $F_1$ and $F_3$. Pressure drop curves for each objective were analyzed, specifically the slopes. The slope for $F_3$ was smaller than that of the other two objectives [8]. Debris deposition was further explored, resulting in an even distribution of debris over the entire filter for $F_3$ [8]. However, based on these results, a sensitivity analysis must be performed to better understand how changes in the filter parameter values affect the objective functions in the two layer model.
Table 3: Two-layer results using initial one-layer configuration

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<tr>
<th></th>
<th>(d_{p1}) ((\mu))</th>
<th>(\eta_1)</th>
<th>(d_{p2}) ((\mu))</th>
<th>(\eta_2)</th>
<th>(T) (hours)</th>
<th>(M) (10^4) Pa/hr</th>
<th>(\alpha_{\text{min}}) (10^-4)</th>
<th>(\xi) (10^-5) kg</th>
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<td>(F_1)</td>
<td>28.71</td>
<td>0.70</td>
<td>23</td>
<td>0.413</td>
<td>92</td>
<td>1.8840</td>
<td>8.4924</td>
<td>3.4298</td>
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<tr>
<td>(F_2)</td>
<td>23</td>
<td>0.625</td>
<td>23</td>
<td>0.4478</td>
<td>58.9</td>
<td>2.5511</td>
<td>7.3992</td>
<td>2.0578</td>
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<tr>
<td>(F_3)</td>
<td>38.53</td>
<td>0.65</td>
<td>23</td>
<td>0.646</td>
<td>97.5</td>
<td>1.7748</td>
<td>9.0895</td>
<td>5.2819</td>
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Proposed Work

Based on previous research on the two-layer model discussed above, we will conduct a sensitivity analysis. For the sensitivity analysis, we will analyze the data and look for relationships between the filter parameters and the filter performance. Aspects of filter performance to consider include filter lifetime, pressure drop, and the mass of debris that escapes the filter. Some questions to consider include the following: Which parameters drive the optimization? Is the lifetime of the filter sensitive to changes in any parameter? To do this sensitivity analysis, R and ANOVA tools will be utilized. A main effects analysis and a two-way interaction analysis will assist in understanding how the interaction between these parameters affects filter performance. To assist in the sensitivity analysis, we will also produce landscapes that will help identify the behavior of the objective functions. Since our studies involve problems with either four or six decision variables (for a 2 or 3 layer model), we can fix some variables and vary two others while sampling the objective function over a range of values. We can then create a 3-D minimization surface that is a representative snapshot of the objective function landscape to further gain insight to the design space.

Once we gain a better understanding of how the parameters affect the filter performance of a two-layer filter, we will extend these same techniques to a three-layer model. Hence, the proposed problem for a three-layer model is

\[
\text{Maximize (or minimize) } F(x)
\]

subject to \(x\), \(x \in \Omega\),

where \(F(x)\) represents the lifetime of the filter or the measure of debris escaping the filter, \(x = \{\eta_1, d_{p1}, \eta_2, d_{p2} \eta_3, d_{p3}\}\), and \(\Omega\) are the bounds for each \([\eta, d_p]\). Both a genetic algorithm and the implicit filtering method will be used to obtain information regarding the values of the parameter set \([\eta, d_p]\) that maximizes (or minimizes) \(F(x)\). We will optimize performance for \(F_1(x), F_2(x)\), and \(F_3(x)\). Using the same statistical methods for the two-layer model, including a main effects analysis and a two-way interaction analysis, we will perform a sensitivity analysis to determine how the parameters affect the performance of the filter.
## Timeline

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## References


