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A method for determining the optimal back-washing frequency and duration for dead-end microfiltration

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A R T I C L E I N F O

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A B S T R A C T

Microfiltration is used in a variety of industrial and municipal water purification settings where one of the main concerns is fouling from the particulate matter that is removed from the water. Our focus has been on developing a unified model that captures fouling behavior in a consolidated manner rather than describing individual blocking regimes using power law models. The unified model provides greater insights into fouling mechanisms so that a deeper understanding of flux decline can be obtained. Moreover, by characterizing both forwards and backwashing behavior together, mathematical theory is available to develop strategies that increase the effectiveness of microfiltration in conjunction with backwashing used to regenerate the filter. We present a very simplified model that was developed to provide details regarding the mathematical analysis and how optimal control theory can be used to predict the timing and duration of backwashing that will optimize the overall water flow through the membrane. We use optimal control theory to derive an analytic solution to the optimal problem and develop a strategy to implement the solution. The model estimates of forward operation are compared with experimental data for constant pressure filtration and indicate that the model is able to capture the basic processes. More interestingly, the optimal control solution and proposed implementation strategy are consistent with empirical demonstrations but provide mathematical evidence that the flux may be increased dramatically by precise timing of the forward and backwashing cycles. Model predictions can be evaluated during pilot-testing that often precedes microfilter regulatory approval and plant design.

1. Introduction

Microfiltration (MF) and ultrafiltration (UF) membranes are commonly installed to purify municipal water and wastewater because of their excellent capabilities to remove difficult to disinfect protozoa, bacteria, and turbidity [1]. MF/UF are also used as pretreatment processes to reduce fouling of reverse osmosis and nanofiltration membranes during desalination, surface water treatment, and water reuse [2–4]. In spite of the widespread implementation of MF/UF, fouling continues to be an important limitation for their continued growth. Various strategies including source water conditioning (i.e. pretreatment), periodic chemically enhanced backwashing, chemical cleaning, and routine hydraulic backwashing are employed to combat MF/UF fouling [5–9].

Early quantitative models of backwashable systems and their experimental verification largely focused on crossflow filtration of biological feed waters and/or frequent flow reversals (order of seconds) [10–13]. In contrast, municipal MF/UF systems are operated in the dead-end configuration, filter a heterogeneous feed water that includes microorganisms, suspended materials, natural organic matter, and dissolved ions, and are backwashed approximately every 10–30 min [14,15]. Under these conditions, hydraulic backwashing does not completely remove the deposited foulants, forcing the effective permeability of the membrane to decline over an extended time frame (order of weeks or months) [16,17].

Most states in the United States mandate an on-site pilot-scale study to provide operational and water quality data in support of the governmental permitting process since membranes are classified as alternative filtration technologies by the Environmental Protection Agency [18]. The high cost of such investigations precludes extensive testing allowing in most cases only a highly truncated experimental matrix to provide operational data in support of system design and regulatory approval. Importantly, in most cases this field evaluation presents the only opportunity to quantify design variables such as process configuration, membrane type, operating flux, backwashing frequency, need for and type of pretreatment, and chemical cleaning interval [19]. An accurate model that captures backwashing effects on fouling kinetics will

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assist in better designing on-site experiments so that the limited time available during regulatory permitting can be better utilized to provide design data for the more optimal design of MF/UF facilities.

The principal objective of this research is to develop such a mathematical model wherein recent efforts to rigorously predict the optimal course of hydraulic backwashing have been extended to maximize the flux of water through the filter. This model is based on previous studies that aimed to describe the fouling process using dynamical systems where the flux decline was functionally related to the filtration process, accumulation of foulants, and contaminant profile (e.g. bacterial type etc.) [20,21].

2. Model development: incorporating forward filtration and backwashing

In this section, a simplified model of dead-end filtration is developed that includes the effects of backwashing on the filtration process. The spirit of previous investigations [20,21] is followed; however, several additions have been made to the model and several important restrictions are indicated. Most importantly, the effects of backwashing have been included in the current formulation of the model. This allows us to study methods for optimizing the fluid filtration using a combination of forward and backwards operation.

Including this effect in the model is quite novel and further supports efforts to move from empirical, power-law like fitting models to more descriptive and flexible differential equation models. In fact, under suitable assumptions (described below), it is possible to determine the optimal backwashing timing and duration analytically. This is a major step in proposing efficient techniques to improve the efficiency of dead-end filtration.

In previous models, the free-filter area depends dynamically on the bacterial foulants, exo-polymeric substances produced by the bacteria. Here the basis is a much simpler model that only includes non-biological foulants and neglects irreversible attachment. In principle, there is no requirement for these restrictions; however, the mathematical techniques that are introduced become much more complicated so the initial focus is on the simplest case. Even with these restrictions, the model captures the experimental observations quite well and is also able to make empirically novel predictions for the backwashing timing.

The model consists of a single ordinary differential equation that describes the accumulation of the foulant, B, on the filter. The focus is on constant pressure filtration where the pressure gradient, ΔP, is constant during the operation. The pressure gradient applied during forward filtration is assumed to be the same as the gradient applied during backwashing, a method that is commonly used by many manufacturers. Thus the pressure drop is equal in magnitude, but in the opposite direction during forwards and backwards operation. The parameter u controls the direction of the pressure drop. The parameter, u, is piecewise constant taking the value 1 during forward filtration and -1 during backwashing. $u(t)$ is referred to as the *control* and $u(t)\Delta P$ describes the filtration protocol and is piecewise constant throughout the filtering process, i.e. forward filtration and backwashing.

The flux of water through the filter as a function of time, $J(t)$, depends on the resistance of the filter which, in turn, depends on the constant membrane filter resistance, R_m and the resistance due to the accumulating foulant, R_b:

$$J(t) = \frac{\Delta P}{\mu(R_m + R_b)}, \tag{1}$$

where μ is the absolute viscosity of the solution.

This is similar to the resistance in series models that have been described previously [25]. The resistance due to foulant accumulation should be a monotonically increasing function of the foulant on the filter during forward filtration. The particular details may be complicated if complete or incomplete fouling are included, so this study begins with the simplest description of the resistance due to the foulant,

$$R_b = \nu B, \tag{2}$$

where ν is the specific resistance per unit of foulant and B is the foulant density on the filter. We construct a model that can incorporate both backwashing and forward filtration based on the value of the control parameter, u. We expect that when the filter is operated in forward filtration, foulants accumulate on the filter which subsequently affects the flux through the filter (as indicated in Eq. (1)). We take a simple model of foulant accumulation that assumes the time rate of change of the foulant density is proportional to the flux through the membrane. The constant of proportionality is denoted, K and describes the amount of foulant in the bulk fluid. Therefore, when the filter is operated in forward mode, $u=1$ and

$$\frac{dB}{dt} = KJ. \tag{3}$$

During backwashing, we assume that the foulant density decreases at a rate proportional to the product of the flux and the current foulant density on the filter, B. The constant of proportionality, denoted $\hat{K}$, represents the effectiveness of the removal. If the foulant was irreversibly attached, $\hat{K}=0$. During backwashing, when $u=-1$, the change of foulant on the filter is described by the differential equation:

$$\frac{dB}{dt} = -\hat{K}JB, \tag{4}$$

We can combine these two modes into a single, piecewise defined differential equation representing the combined effects of accumulation and removal, when $u(t)$ is a piecewise constant function taking values of 1 and -1 during forward operation and backwashing, respectively. Our combined model is

$$\frac{dB}{dt} = \underbrace{\frac{(1+u(t))}{2}KJ}_{\text{fouling}} - \underbrace{\frac{(1-u(t))}{2}\hat{K}JB}_{\text{removal/backflow}}, \tag{5}$$

where K and $\hat{K}$ scale the accumulation (removal) rate during forward filtration (backwashing), respectively and depend on the foulant concentration. u is dimensionless, so K has units of $[B]/[T][J] = \mathrm{g\,m^2\,L^{-2}}$ and $\hat{K}$ has units of $1/[T][J] = \mathrm{m^2\,L^{-1}}$. We assume that the filter is initially clean, which implies that $B(0)=0$.

Observations of backwashing indicate that, while backwashing fails to remove all accumulated foulants, it takes a far shorter time to remove the majority of the foulants from the filter than it does for the foulants to accumulate (i.e. backwashing removal occurs at a faster rate than fouling). This is incorporated into the model by assuming that $\hat{K} \gg K$.

During forward operation, $u=1$, and $dB/dt \geq 0$ and B accumulates on the filter. During backwashing, $u=-1$, and $dB/dt \leq 0$ and, since $J>0$, the foulant is decreasing and tends toward zero. Because u is a piecewise constant, it is either 1 or -1 to describe forwards or backwashing modes of operation. There are other aspects that are neglected in this model including a range of important processes such as physicochemical and biological details of the foulants, irreversible attachment, and flow effects. These are relatively straightforward to include by incorporating extracellular polymeric substances (EPS) and assuming the backwashing efficiency to depend on the EPS density (through $\hat{K}$, for example). However, as shown in Fig. 2, the forward filtration component is able to capture experimental data quite well for the forwards operation. We note that the forward filtration operation model is consistent with our previous methods [21]. The novel aspect of the model, namely the backwashing terms, is the simplest model that can be described that includes only removal of foulant due to fluid passing through the filter (e.g. the flux).

The rest of the manuscript is organized as follows: In the next section, the analytic solution of the forward filtration problem and experimental data are used to determine the best fit parameter values for ν, and K. After that, the mathematical method that is used to determine the *optimal* dosing protocol (e.g. $u(t)$) is briefly discussed. This is described in more detail in the Appendix; however, the analytic value of $u(t)$ that maximizes the total flux through the membrane on the time interval $[0, T_{final}]$ is found to be,

$$u(t) = \begin{cases} 1 & \text{for } 0 \le t \le \hat{T} \\ u^* & \text{for } \hat{T} \le t \le T_{final}, \end{cases} \tag{6}$$

where $0 < u^* < 1$. Because this analytic solution is not consistent with piecewise constant pressure drop operation, we construct a u that is piecewise constant throughout the time interval in Section 5. Briefly, the interval $[0, T_{final}]$ is broken into n equal subintervals, referred to as cycles, and require $u(t)$ to be 1 on a portion of the cycle and -1 on the rest of the cycle. The switching time within a cycle, that describes the fraction of the cycle to be spent in forward/backwards operation, by requiring the average u within a cycle to be equal to u^*. As the number of cycles increases, the average value of u over the entire filtration time is exactly u^*, but consists of rapidly switching between forwards and backwards modes. Numerical simulations of the filtration process for increasing values of n (cycle number) indicate that the method approaches the flux predicted by the analytic method. More importantly, comparisons between the total flux can be made with three relevant values: the first is the flux that would be obtained for constant forward operation (e.g. if $u(t) \equiv 1$ for all time); the second is the flux that is obtained via experimental techniques where the filter is periodically rinsed after forward operation; finally, the optimal flux using the optimal u defined in Eq. (6) can be used. Even though this is not physical, the mathematical analysis proves that this is indeed the optimal solution. Moreover, our constructed approximation approaches the optimal value as the number of cycles increases. The manuscript concludes with some comments about the methods and results.

3. Parameter estimation

With the simplified model, there are several parameters that need to be determined. Typical values of the membrane resistance, R_m, and solution viscosity, μ are used. The value of ΔP is specified by the experiment. This leaves the specific membrane resistance, ν, and the forward/backward accumulation/removal scales $K/\hat{K}$. All of these are determined except $\hat{K}$ using best fit values between the analytic solution and experimental data. $\hat{K}$ is assumed to be much larger than K, but is currently estimated. In this manuscript the change in effectiveness of removal is only incorporated by including the flux contribution in the backwashing term, which is time dependent. However, it is clear that $\hat{K}$ is likely not constant if irreversible attachment is included. We discuss this is some detail below, but only comment that this assumption is likely false in many practical situations but does reflect aspects of the experimental design and allows for relatively simple analysis. Additionally, this points towards refinements of the model that can be addressed in the future.

The forward filtration problem (when $u = 1$),

$$\frac{dB}{dt} = KJ, \tag{7}$$

$$B(0) = 0, \tag{8}$$

can be solved analytically:

$$B(t) = \frac{-R_m + \sqrt{R_m^2 + \dfrac{2\nu t K \Delta P}{\mu}}}{\nu}, \tag{9}$$

and we can choose the parameters ν and K to fit the data. Nelder–Mead optimization is employed and implemented within Matlab's *fminsearch* to obtain best fit estimates for the remaining two parameters.

Two different types of experiments were conducted; one using raw Lake Houston water and the other after electroflotation pretreatment. The source water is moderately turbid (15 NTU), contains 5 mg/L of dissolved organic carbon, and serves as one of the water supplies for the City of Houston. Electroflotation pretreatment was performed at a pH of 6.4 and aluminum dosage of 10 mg/L during which time a portion of the flocs migrated to the surface after attaching to hydrogen bubbles generated during electrolysis. Dead-end, unstirred microfiltration was performed using a modified PVDF disc membrane of nominal pore size 0.22 μm. After filtering 200 L/m^2 of the feed water, the membrane was removed from the filtration cell, surface rinsed with a jet of deionized water, and replaced upside-down in the cell. Backwashing was performed by passing 100 mL of nanopure water through the reversely orientated membrane. After backwashing, the membrane was again removed and replaced in the cell in its original orientation before recording the clean water flux and repeated filtration of 200 L/m^2 feed water. More details on the source water quality, electrochemical pretreatment, and microfiltration protocols can be found in recent publications [34,37]. Instantaneous flux data obtained from duplicate experiments showed no statistical differences at the 95% confidence level. These paired t-tests reveal the reproducibility of our laboratory protocols and allow statistically valid comparison of experiments.

The presumption is that the raw water contains more biologically active material and natural organic matter (NOM) and is therefore less representative of our simplified model. Indeed, we have recently shown that MF, with electroflotation pretreatment removes approximately 50% of total organic carbon and $> 99.9\%$ (3-log) of viruses [38]. Although we did not explicitly measure it, bacteria and turbidity are expected to follow the same trends as viruses since sweep flocculation acts non-specifically on all suspended colloids.

Notice that the behavior of the raw water under repeated forward and backwards filtration is quite different than the electrofloculated water (see Fig. 1). The presumption is that the raw water contains more biologically active material and is therefore less representative of our simplified model. Only the first filtration cycle is used to obtain the fit. As seen in Fig. 2, the model is more consistent with the electrofloculated water, presumably because of reduced biological activity. The best-fit parameters are listed in Table 1. These parameters are used for all simulations for the rest of the manuscript.

Even though only the first cycle is used to estimate the parameters the data can be used to check how well the model fits the repeated cycling by imposing a backwashing cycle based on the *experiment* rather than the mathematical analysis. In Fig. 3a comparison between the experiment using two intermediate cleaning times with a model simulation that uses two backwashing cycles at the same times is shown. Clearly the model is capturing the behavior in both flux and total volume filtered.

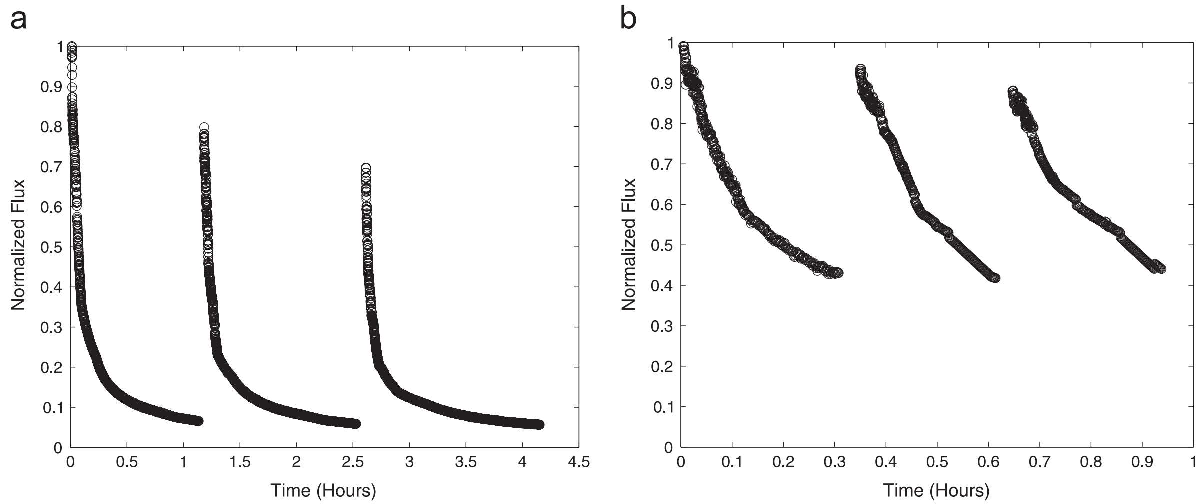

Fig. 1. Normalized flux versus time for the periodic backwashing of raw (a) and electrofloculated water (b). Notice the backwashing does not return the filter to the original flux rate indicating material that is irreversibly bound to the filter. This is neglected in our current formulation.

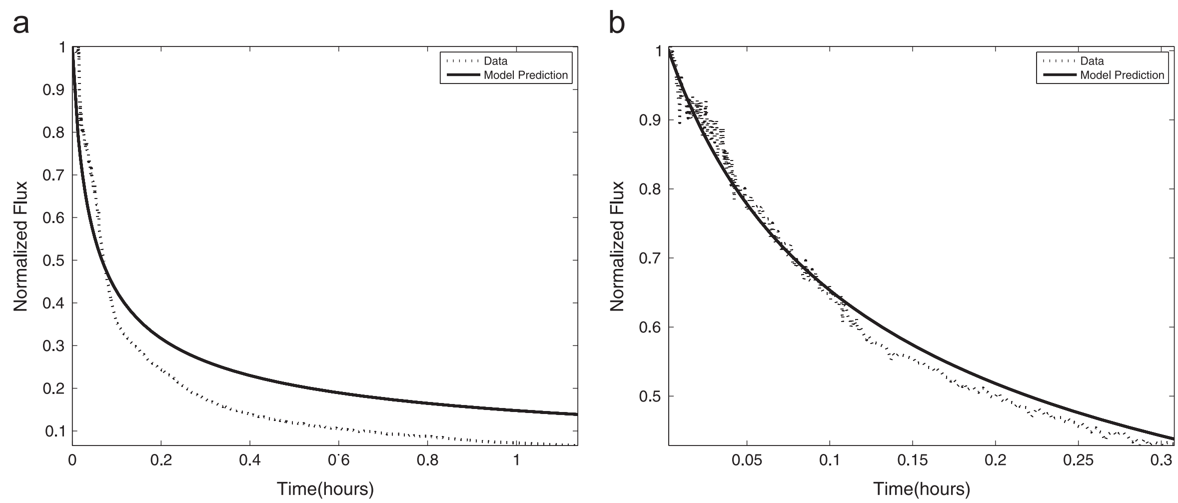

Fig. 2. Comparison between the best-fit model calculations for raw (a) and electrofloculated water (b) where we are comparing the normalized flux to the volume filtered per unit membrane area. Clearly the model is more accurate for the latter experiment.

Table 1
Description of variables and parameters used in this study. The parameters are estimated from fits described here except for the pressure drop, which was given by the experiments and foulant removal, which was assumed.

Model variable	Description (Units)	Value	
B	Foulant density on the filter (g L^{-1})	Variable	
J	Flux (L m^{-2} h^{-1})	Variable	
R_b	Foulant resistance (m^{-1})	Variable	
u	Flow direction, control (dimensionless)	1, −1	
Parameter	Description (Units)	Value	Source
ΔP	Pressure drop (Psig)	2	Experiment
μ	Absolute viscosity (N s m^{-2})	10^{-3}	Experiment
R_m	Membrane resistance (m^{-1})	10^{-10}	Experiment
ν	Foulant efficiency (L g^{-1} m^{-1})	0.003	Estimated
K	Foulant accumulation (g m^2 L^{-2})	10^{-7}	Estimated
$\hat{K}$	Foulant removal (m^2 L^{-1})	0.01	Assumed

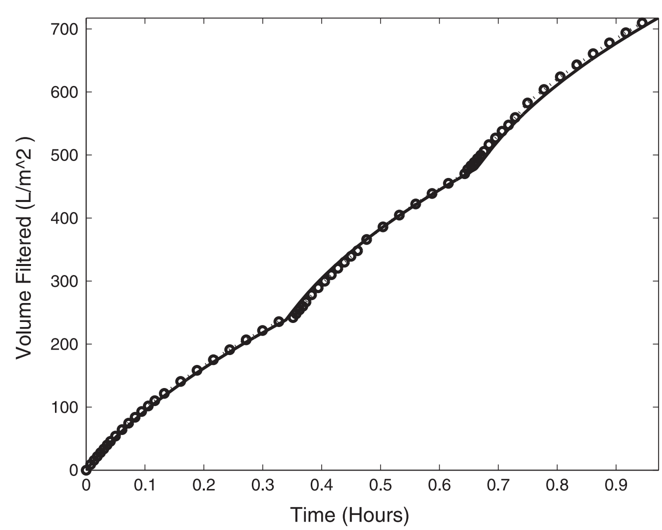

Fig. 3. Comparison between experimental observation of repeated forwards/rinsing filtration with a simulation based on the timing of the experimental backwash duration.

4. Optimal control

The goal of optimal control is to determine the value of a control (here $u(t)$) that optimizes an output (here the total volume filtered), subject to a constraint (e.g. a differential equation). Specifically, we look for $u(t)$ that maximizes the total volume filtered $\int_0^{T_{final}} A_{filter} u(t) J(t)\, dt$, subject to Eqs. (1) and (7). We note that the parameter A_{filter} represents the filter area and has been absorbed into the flux terms. Notice that because backwashing uses filtered water, if $u = -1$ the total volume that is filtered decreases, so there is a penalty for backwashing. At the same time, if $u = 1$, foulants accumulate on the filter, decreasing the flux, J, which lowers the amount of water that can be filtered. The goal is to determine the timing and frequency of backwashing that maximizes the amount of water that is filtered.

The argument uses standard arguments (detailed in the Appendix) that are quite similar to geometric arguments used in basic calculus to optimize a function subject to a constraint (e.g. Lagrange multipliers). The goal of constrained optimization in calculus is to maximize a function, $f(x, y)$ subject to the constraint that $g(x, y) = k$. The geometric solution is found by noticing that gradients of f and g point in the same direction, that is $\nabla f = \lambda \nabla g$, where λ is the Lagrange multiplier.

In optimal control, when the object is to maximize an integral subject to a differential equation constraint, this method is referred to as Pontryagin's principle and we must solve the constraint equations and a related adjoint system that is also defined by differential equations. These are described in detail in the Appendix. This can rarely be done analytically; however, the simplifications that have been made allow us to solve the optimal control problem analytically, as long as the control function may to take values on the interval $[-1, 1]$. In fact, the optimal solution is to allow the filter to foul for a short period of time, (e.g. $u(t) = 1$) and then fix $u = u^*$ where $0 < u^* < 1$ for the remaining time. The details are described in the Appendix, but the main idea is to use the analytic solutions for the forwards and backward filtration and Pontryagin's principle to determine the *switching time*. Although this solution is the analytic solution to the mathematical problem, it requires that the filtration is simultaneously forwards and backwards, since $0 < u^* < 1$. It is evident that, even though the analytic solution is non-physical, it is the optimal solution and presents the upper limit for the filtration. In the next section, an approximation to the optimal strategy is constructed by increasingly frequent, periodic cycling between forward and backwards operation where the switching time between forward and backwards operation is determined so that $1/T_{final} \int_0^{T_{final}} u_{approx}\, dt = u^*$.

5. Approximate control

This prediction can be viewed as a statement regarding the *average* of the direction of operation. The total filtration time is denoted as T_{total}, the time of a single forwards/backwards cycle is denoted as $T_{cycle} = T_{forward} + T_{backward}$. If there are n cycles, $T_{cycle} = T_{final}/n$. During each of the n cycles, it must be that,

$$u^* = \frac{T_{forward} - T_{backward}}{T_{cycle}} \tag{10}$$

since $u = 1$ for $T_{forward}$ length of time and $u = -1$ for $T_{backward}$ length of time. Since our analysis indicates that u^* is positive, more time is spent in forward operation than backwards operation. By allowing the frequency of cycles to increase, while requiring that the fraction of time between forwards and backwards operation satisfies Eq. (10), the optimal control solution can be approximated and still maintain piecewise constant operation.

The analysis indicates that $u^* \approx 0.89$, which implies that only a very short amount of time is needed for reversal to clear the filter. Therefore it is expected that for each cycle less than 90% of the time is spent in forwards operation while the remaining is occupied in backwashing. In Fig. 4 the total volume filtered as a function of time for a run length of ten hours using two cycles is displayed. The numerical estimate is shown along with current experimental data that fits quite well. The regions of decreasing volume show where backwashing is occurring.

Our strategy is to approximate the optimal control with forward filtration punctuated by short, periodic bursts of backwashing with a timing and duration implied by the optimal control solution. Fig. 5 shows what happens if the control is approximated by applying $u = u^*$ by cycling between $u = 1$ and $u = -1$ using increasing frequency of switching and maintaining the average over the period of u^*. The first cycle of the experimental data is shown for comparison. More fluid is filtered as the frequency increases. As the number of cycles increases, the approximation approaches the optimal control solution

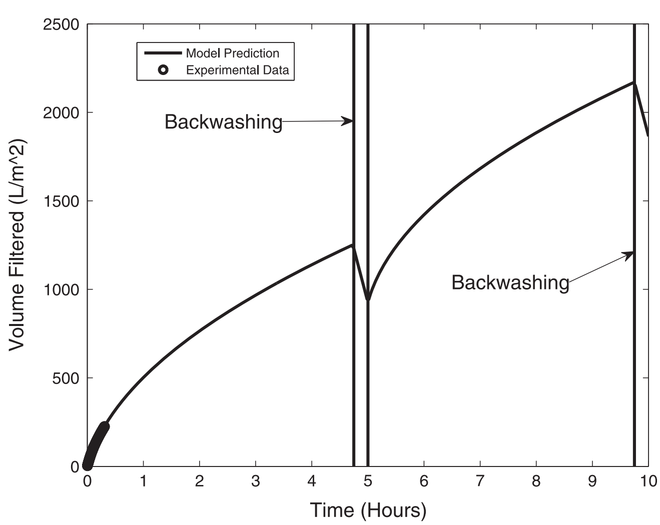

Fig. 4. The predicted volume filtered as a function of time. The volume increases during forward operation and decreases during backwards cycling. The fit with experimental data (represented by dark circles) is quite good.

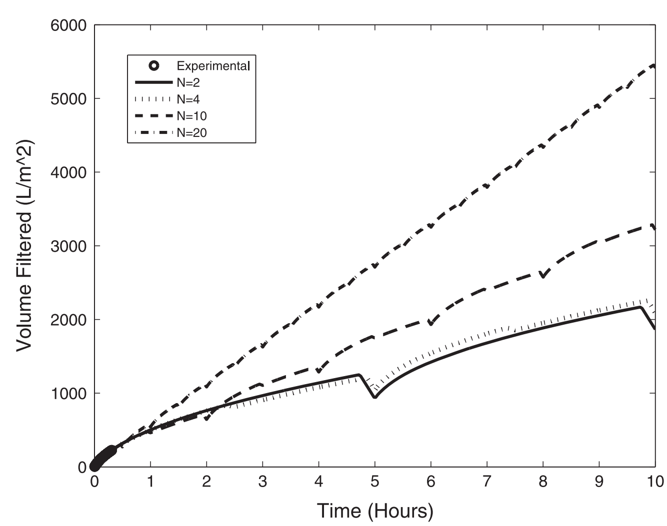

Fig. 5. Comparison if the total volume filtered versus time for varying frequency of cycling where N is the number of cycles. The simulations are performed for the same dimensional time of 10 h while the total volume filtered increases as the frequency increases. The data for the first cycle is shown for comparison purposes.

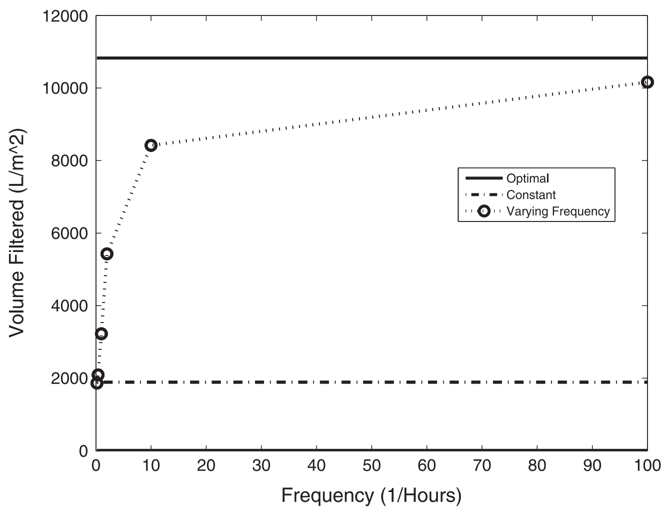

Fig. 6. Comparison of total volume filtered for varying scenarios. For constant forward operation the total volume filtered is approximately 1800 mL while the optimal control solution predicts more than 1.1×10^4 mL within 10 h. By increasing the frequency of backwashing, the physically realistic method of approximating the singular solution is approached.

(i.e. instantaneous cycling). In Fig. 6 where the volume filtered over 10 h for different numbers of cycles is plotted.

Note that the flux over 10 h for the best scenario implied by the data can also be estimated. The methods used to clean the filter of electrofloculated water are clearly not perfect (as seen by the reduction in flux for the initiation of forward filtration shown in Fig. 1). Backwashing was performed after filtering 200 L/m^2 of water, which took 0.31 h for the first cycle after electroflotation pretreatment [34]. Extrapolating these measurements to the entire 10-hour duration of the numerical simulations, this translates to 32 backwashing cycles. Assuming that the filter is instantly cleaned between cycles allows us to make a rough comparison between the optimal flux prediction obtained by the model and the flux obtained in the experiments. The experimental estimate is 7.9×10^3 mL, which is above the volume filtered for constant forward operation (approximately 2×10^3 mL, as estimated from the model), but still far below the optimal flux of 1.1×10^4 mL. It is clear that with increasing frequency the total volume is greatly enhanced and, more importantly, the mathematical theory is able to do a better job than empirically developed strategies.

6. Conclusions

Currently, the timing of backwashes in most municipal and industrial water treatment applications is largely assigned simply based on previous experience of the manufacturer or the design engineer. Most on-site studies are performed almost exclusively for regulatory purposes and do not evaluate backwashing frequency as an independent variable, largely because of the costs associated with piloting. In this manuscript, we attempt to reduce this empiricism by posing the formal optimization problem and developing an approximate solution to maximize the operating flux. Nevertheless, with meaningful assumptions, it is shown that the results are physically meaningful.

This manuscript focuses on the derivation and analysis of a simplified, unified model for constant pressure filtration:

- The model is quite simple but is able to capture dominant aspects of filtration.
- We show how to pose the optimal control problem of optimizing the flux by controlling the timing and duration of the backwashing cycles.
- The model can be attacked analytically and solve the optimal control problem directly.
- We show that by cycling, we can increase the total volume filtered in a physically realistic manner.
- We prove the existence of an optimal control and characterize the implementation procedure that yields the optimal volume filtered.
- Our analysis leads to a quantitative methodology that can be used to predict the optimal duration and timing.

Although it is quite telling that our predictions are in line with observations across a wide range of experiments, that rapid backpulsing can dramatically enhance the permeate flux [35,36] and that the timing and the duration is crucial, there are several aspects of the data that the model does not address currently but will be the subject of our future work. We have neglected irreversible attachment and EPS formation. It is relatively simple to include this in the differential equations, but it is not clear how far the optimal control analysis can be developed. In our previous models we included the production of EPS by the deposited bacteria in a phenomenological way. EPS was not produced until a *quorum* of bacteria had attached to the surface and the EPS added to the resistance terms in the pressure/flux relationship. To add this effect with backwashing we plan to alter the reversing portion of our model (e.g. when $u=-1$) so that the removal rate is lowered as the EPS concentration increases. This extends the utility of the optimal control approach as we can also study how the timing of the backwashing cycles alters the production of EPS. The mathematical structure is quite rich but there is some indication that the problem will be intractable analytically and numerical methods will be applied. We also plan to extend our analysis to focus on constant flux operation where the optimization will focus on reducing the applied pressure.

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Appendix A. Optimal control analysis

The main idea is to determine the value of $u(t)$ to optimize some aspect of the problem. In the context of the current problem, the goal is to optimize the total flux during the filtration time, T_{final}. Mathematically, this means we are trying to optimize

$$L=\int_0^{T_{final}} u(t)J(t)\,dt, \tag{11}$$

subject to the constraint that

$$\frac{dB}{dt}=\frac{(1+u(t))}{2}KJ-\frac{(1-u(t))}{2}\hat{K}JB. \tag{12}$$

The most straightforward method for determining the value of the control is to apply Pontryagin's maximum principle [33]. We form the Hamiltonian

$$H=uJ+\lambda((1+u)/2KJ-(1-u)/2\hat{K}JB) \tag{13}$$

$$H=\left(J+\frac{\lambda J}{2}(K+\hat{K}B)\right)u+\frac{\lambda J}{2}(K-\hat{K}B) \tag{14}$$

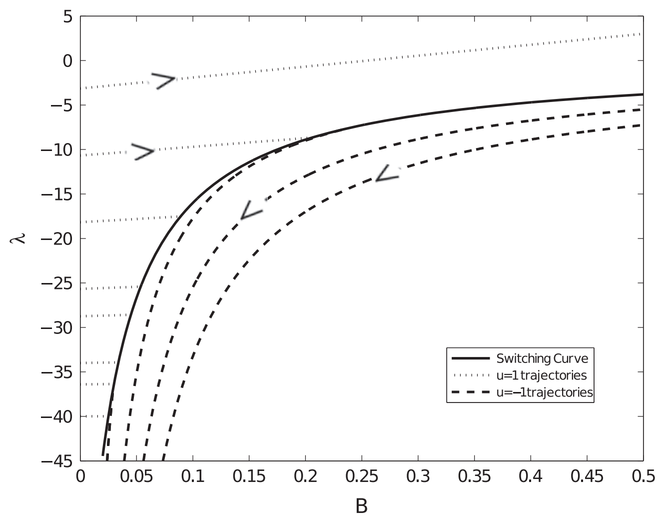

Fig. 7. Trajectories in the (λ, B) plane with directions marked with arrows. Above the curve, the trajectories are straight lines while below the switching curve they are hyperbolas.

$$H = u\Omega + \frac{\lambda J}{2}(K - \hat{K}B). \tag{15}$$

Here, the λ is referred to as the adjoint variables and is equivalent to a Lagrange multiplier. Pontryagin's principle argues that extremizing the functional L is equivalent to extremizing H (under suitable and often easily satisfiable conditions). In calculus one would extremize a function by finding critical points (e.g. where the first derivative is zero), here we are proceeding analogously. Thus we determine the optimal control, u^* by requiring that

$$\frac{\partial H}{\partial u} = 0, \tag{16}$$

when $u = u^*$.

However, when the Hamiltonian is linear in the control, this provides no information for u^*. This is referred to as a bang-bang control and conditions the extreme values are found at the maximum and minimum values of the control [32]. The conditions for extremization are found by noting that the control u should be chosen so that at u^*, we require that,

$$H(u(t)) < = H(u(t)^*), \tag{17}$$

which implies that

$$u^* = \begin{cases} 1 & \text{if } \Omega > 0, \\ -1 & \text{if } \Omega < 0, \\ Unknown & \text{if } \Omega = 0. \end{cases} \tag{18}$$

Since $J \geq 0$, we can write the optimal control in terms of $\lambda(B)$,

$$u^* = \begin{cases} 1 & \text{if } \lambda(K + \hat{K}B) > -2, \\ -1 & \text{if } \lambda(K + \hat{K}B) < -2, \\ Unknown & \text{if } \lambda = \dfrac{-2}{K + \hat{K}B}. \end{cases} \tag{19}$$

The curve in (λ, B) space, $\lambda = -2/(K + \hat{K}B)$ is referred to as the *switching* curve and determines when the filtration should switch between forward and backward operation. At the intersection between trajectories (i.e. solutions to the (B, λ) system) intersect the switching curve, we cannot determine u^* uniquely. This is referred to as a *singular*, *bang-bang* optimal control problem.

We will see, that in our situation the solution to the optimal control problem is either forward operation for all time or forward operation, followed by a singular control, depending on parameter values and the length of the filtration cycle. To determine the value of u^* at the singular state, we have to use a different analysis which is apparent from the geometry of the solution curves in (λ, B) space.

Ω depends on the state variable, B, and the adjoint variable, λ. Clearly, the state and adjoint variables satisfy the differential equations,

$$\frac{dB}{dt} = \frac{\partial H}{\partial \lambda}, \tag{20}$$

$$\frac{dB}{dt} = \frac{(1 + u(t))}{2}KJ - \frac{(1 - u(t))}{2}\hat{K}JB, \tag{21}$$

$$\frac{d\lambda}{dt} = -\frac{\partial H}{\partial B}, \tag{22}$$

$$= \frac{\Delta P\left(2\mu u + \lambda\mu K + \lambda\mu K u + \lambda\hat{K}R_m - \lambda\hat{K}uR_m\right)}{2(R_m + \mu B)^2}, \tag{23}$$

subject to the conditions that,

$$B(0) = 0, \tag{24}$$

$$\lambda(0) = 0. \tag{25}$$

The initial condition on the adjoint variable, λ, is referred to as the *transversality* condition and can be interpreted as a geometric restriction on the couple state/adjoint system [33].

We now turn to the geometric analysis of the optimal control system. When $u = 1$, the system becomes,

$$\frac{dB}{dt} = \frac{K\Delta P}{R_m + \mu B} \tag{26}$$

$$\frac{d\lambda}{dt} = \frac{\Delta P(\mu + K\mu\lambda)}{(R_m + \mu B)^2}. \tag{27}$$

By dividing the two equations we find a single, separable ODE that defines $\lambda(B)$,

$$\frac{d\lambda}{dB} = \frac{\mu(1 + K\lambda)}{K(R_m + \mu B)}. \tag{28}$$

with general solution,

$$\lambda(B) = -\frac{1}{K} + C(R_m + \mu B). \tag{29}$$

Likewise, if $u = -1$, the system reduces to,

$$\frac{dB}{dt} = -\frac{\hat{K}\Delta PB}{R_m + \mu B} \tag{30}$$

$$\frac{d\lambda}{dt} = \frac{\Delta P(-\mu + \hat{K}\mu R_m \lambda)}{(R_m + \mu B)^2}. \tag{31}$$

Which can be written as the single ODE,

$$\frac{d\lambda}{dB} = \frac{\mu - \hat{K}R_m\lambda}{KB(R_m + \mu B)}, \tag{32}$$

whose general solution is,

$$\lambda(B) = \frac{\mu}{R_m\hat{K}} + \hat{C}\left(\frac{R_m + \mu B}{B}\right)^{(\hat{K}/K)} \tag{33}$$

In the (λ, B) plane, we can now describe the possible solution trajectories for the optimal control problem. We begin with points on the λ-axis since $B(0) = 0$ (note that C and $\hat{C}$ are defined by this condition). The optimal solution begins with $u = 1$ as long as we are above the switching curve defined by $\lambda = -2/(K + \hat{K}B)$. Either the trajectory connects with the B-axis (i.e. if the slope of the linear trajectory is large enough) or the trajectory hits the switching curve and switches to the trajectory defined by $u = -1$ (i.e. begin backwashing). It is clear from the trajectories shown in Fig. 7

that there is no possibility of switching back to forward operation. This is clearly not an optimal solution. Instead, if we apply some $u*$ that is between -1 and 1, we can remain on the switching curve for all time, which is the optimal solution.

It is relatively easy to determine u^* by determining the value of B at the intersection between the positive trajectory and the switching curve. This is equivalent to determining the time at which the optimal control problem would predict a switch away from forward cycling. We then determine the u that will keep B at that level by solving $dB/dt=0$ for $u=u^*$.

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