Modelling biological processes in water treatment: the integrated biofiltration model

Bruce E. Rittmann and Douglas Stilwell

ABSTRACT

Biofiltration is a form of biofilm process used to make drinking waters biologically stable, which means that the water does not support excessive bacterial growth when it is distributed. Biofiltration avoids the many quality problems associated with biological instability: high chlorine doses, disinfection by-products, accelerated corrosion, taste and odours, high turbidity, and increased plate counts or coliforms. Most designs of biofilters have been empirical. However, using a mechanistic model as a design tool can improve process reliability and the effectiveness of pilot and laboratory studies on biofiltration. Unfortunately, models that include the critical phenomena have been quite complex; they are good research tools, but are not easily used for routine design and analysis.

The Integrated Biofilm Model (IBM) is a spreadsheet program that includes all the key phenomena for biofiltration of drinking water, but is simple to use. Specifically included in the model are the consumption and production of chemical species (input substrates, end products and soluble microbial products); heterotrophic and nitrifying bacteria; inert biomass; physical processes, such as transport and detachment; and the relationships between all of the different organisms and chemical species. An example shows the inputs to the model and the kind of trends that it predicts for original substrates, soluble microbial products, and biofilm biomass. The IBM makes iterative design and analysis of biofiltration processes straightforward.

Key words | biodegradable organic matter, biofilm, biofiltration, detachment, nitrification, soluble microbial products

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BIOFILMS IN DRINKING WATER TREATMENT

The use of biofilm processes in drinking water applications, relatively common in Europe (Rittmann and Snoeyink 1984; Rittmann and Huck 1989), is beginning to emerge in North America. The current interest in North America is due in large part to the Disinfectant/Disinfectant-By-Product Rule, which is placing tighter restrictions on disinfection by-products, such as trihalomethanes and haloacetic acids (Pontius 1993).

An alternative to the traditional North American practice of adding high levels of chlorine to the distributed water is to make the water biologically stable by eliminating bacterial substrates, which support the growth of microorganisms in the distribution system (Rittmann and Snoeyink 1984). Most natural waters contain some levels of biodegradable organic matter (BOM), and some also contain reduced nitrogen, iron, or manganese, all of which have the potential to support the growth of microorganisms. Excessive growth of microorganisms can lead to serious water-quality problems: high heterotrophic plate counts or coliforms, increased turbidity, survival or growth of pathogens, accelerated corrosion, accelerated loss of chlorine residual, and creation of tastes and odours (Rittmann and Huck 1989).

Water made biologically stable by the removal of these substances has much less potential for bacterial growth than does unstable water, thereby greatly reducing the

amount of chlorine residual required during distribution. For example, the levels of residual chlorine used in Europe, where biological stability is already a treatment objective, are often 10 times lower than typical levels found in North America, and some European cities do not maintain a chlorine residual at all (Rittmann 1996). In addition to achieving a biologically stable water, the removal of BOM helps to meet other water quality and aesthetic goals, such as the removal of taste and odour-causing compounds and hazardous micropollutants in the raw water source (Rittmann *et al*. 1995; Rittmann 1995*b*).

The best method for removing biodegradable material is biological filtration (Rittmann and Snoeyink 1984; Bouwer and Crowe 1988; Rittmann and Huck 1989; Rittmann 1995*a*; Bouwer *et al*. 1995; Rittmann and McCarty 2001). Some biofiltration technologies are used for *biofilm pretreatment*, in which elimination of bacterial substrates is the primary objective of the process: (1) Raw water is passed through fixed beds of stone, plastic, or expanded clay media (often accompanied by aeration) prior to conventional treatment. (2) Raw water is passed upflow through a bed of fine media causing fluidization of the bed prior to conventional treatment.

Another method of biofiltration is *hybrid biofiltration*, in which particle filtration and biodegradation take place together. Because most treatment facilities already employ sand, anthracite, GAC, or mixed-media filters for the removal of turbidity, hybrid biofiltration can be successfully integrated into the treatment scheme at these facilities through modifications of rapid-filter design and operation (Rittmann and McCarty 2001). When the loading of biodegradable substrates is not too great, hybrid biofiltration allows the benefits of biofiltration without a large capital investment for a special biofilm process (Rittmann 1996; Rittmann and McCarty 2001). Slow sand filtration is another example of hybrid biofiltration.

THE ROLE OF BIOFILM MODELS AND GOAL OF THIS WORK

Although biofilm processes are in wide-scale use throughout the world, design often is based on empirical loading factors or trial-and-error experimentation at particular sites. On the other hand, a properly constructed model serves vital functions in research and practice by incorporating all major physical, chemical and biological phenomena. By identifying and quantifying the important factors in a process, models help us to optimize experiments so that unproductive measurements or trials are avoided, while critical measurements are emphasized. Models are especially valuable in a design setting, where they provide insight into mechanisms underlying results obtained in laboratory or pilot research. A proven model provides simulations that are completed in a minuscule fraction of the time required for an actual experiment. In this way, modelling leads to a reduction in laboratory expenses and time invested in data collection and design testing.

The goal of this work is to present a simple biofilm model that captures the main phenomena that control the performance of a biofilter used to treat drinking water, but also can be solved easily with a spreadsheet. We begin by reviewing the basic phenomena that need to be included in a biofiltration model. Next, we present the model itself, including the spreadsheets used for input and output. We then illustrate how the model works and what it predicts with a series of examples.

BASICS OF BIOFILM MODELLING

Certain key phenomena must be captured in the formulation of a model to accurately describe biofiltration. Prior to presenting the mathematical formulation of these phenomena, we describe these key phenomena qualitatively. This overview highlights the issues that are common to all biofilm models and those that apply particularly to biofiltration of drinking water.

The most fundamental reactions in all biofilm processes are the oxidation, or consumption, of electron-donor substrates by bacteria and the resultant bacterial growth fuelled by this oxidation. The transformation of substrates into either an oxidized product or bacterial cell mass is the driving force behind biological treatment (Rittmann and McCarty 2001). A biofilm model necessarily

must start with the reactions describing this consumption and growth. For biofiltration of drinking water, the substrates are the components of biological instability.

Also of fundamental importance to most biofilm models are the physical processes that transport substrate to and within the biofilm (Williamson and McCarty 1976; Rittmann and McCarty 1980). Biofilms are characterized by limited mass transport and substrate concentration gradients (Brusseau *et al*. 1997; Rittmann and McCarty 2001). Transport and consumption occur simultaneously and must be linked quantitatively to describe concentrations and rates in the biofilm.

In addition to bacterial growth due to substrate consumption, the bacteria also experience losses: physical detachment and self-oxidation. Physical detachment of biomass from the biofilm depends on the viscoelastic properties of the biofilm and the outside forces exerted on the film (Gantzer *et al*. 1989; Rittmann 1989; Rittmann and Laspidou 2002). These forces can include liquid shear stresses, pressure fluctuations brought on by turbulent flow regimes, or the abrasive action of solids coming into contact with the biofilm. Self-oxidation of bacterial cell mass is a normal function of bacterial metabolic activity. It is often called endogenous respiration or decay. Whereas self-oxidation occurs relatively constantly for the biomass, physical detachment can be either continuous or periodic. In fixed-bed biofiltration processes that employ backwashing, the detachment rate is very high for the few minutes of backwashing, but relatively low at other times.

The normal metabolic reactions of bacteria release a suite of organic by-products referred to as *soluble microbial products* (SMP), which constitute a significant flow of carbon and electrons within the biofilm. SMP are also substrates for some bacteria in the biofilm. SMP must be included in any complete biofilm model, because SMP often constitute the bulk of the effluent BOM (Woolschlager and Rittmann 1995; Rittmann and McCarty 2001). SMP are divided into two distinct categories: UAP (substrate utilization-associated products) and BAP (biomass-associated products) (Namkung and Rittmann 1986; Rittmann *et al*. 1987; Noguera *et al*. 1994). This division of SMP into two categories is an important piece of complexity to add to the biofilm model, because UAP and BAP have quite different biodegradation kinetics.

The coexistence of multiple species or bacterial types is unavoidable in natural and engineered settings. Incorporating the coexistence of different groups of organisms into a biofilm model is a challenge, because separate types of biomass grow from oxidation of separate substrates. Each microbial group and each substrate must be included in the model. Beneficial or competitive relationships often exist between different groups. An example of a beneficial relationship is the cooperation between the autotrophic ammonia oxidizers and the autotrophic nitrite oxidizers. These organisms are often found in the same communities, since oxidation of ammonia to nitrite provides the substrate for the nitrite oxidizers. Competition for space or oxygen may be important in defining the population distribution of heterotrophs and nitrifiers, especially when these factors are limiting. Another potential feedback between species involves SMP. All types of microorganisms produce SMP, but only certain types are able to consume the SMP as substrate. Again, the heterotrophs and nitrifiers provide a good example of this type of feedback. Although both groups produce SMP, only the heterotrophs can consume the SMP as an organic substrate. Therefore, through consumption of SMP generated by nitrifiers, a heterotrophic population may be supported in the absence of any input organic substrate (Rittmann *et al*. 1994).

The normal processes of cell metabolism lead to the production of inert (or metabolically inactive) biomass (Rittmann and McCarty 2001). This occurs because, as the cells undergo self-oxidation, a portion of the biomass is resistant to oxidation and is converted to inert biomass. In biofilms with low rates of detachment, the inert biomass can build up to become a substantial fraction of the total biomass in the reactor (Rittmann and Manem 1992).

In summary, a comprehensive biofilm model for drinking water biofiltration must account for:

- the consumption and production of chemical species (input substrates, end products, and metabolic by-products);
- multiple groups of active organisms;
- inert biomass;
- physical processes, such as transport and detachment;

- the relationships among all of the different organisms and chemical species.

Different levels of sophistication have been introduced in previous biofilm models in terms of describing this suite of important phenomena (Williamson and McCarty 1976; Rittmann and McCarty 1980; Kissel *et al*. 1984; Wanner and Gujer 1986; Rittmann and Manem 1992; Furumai and Rittmann 1994; Piciorneanu *et al*. 1999; Noguera *et al*. 1999; Rittmann *et al*. 1999). The rigour with which accurate portrayal is pursued determines the complexity of the model. Requiring more phenomena and components makes the model more complex and leads to greater computational demands. In the ideal situation, the model contains just enough complexity to capture the important phenomena.

THE INTEGRATED BIOFILM MODEL (IBM)

The Integrated Biofilm Model, or IBM, is a multi-species biofilm model that we designed to be a practical tool for the analysis and design of biofilters used in drinking water treatment. It includes all the bulleted features (above) at a level that balances completeness with usability. Figure 1 identifies the IBM's components and how they are connected. The IBM is a steady-state model with a pseudo-analytical solution that builds on previous efforts to bring biofilm modelling out of the realm of research-based, numerical solutions and into engineering practice.

The IBM begins with an idealized, one-dimensional biofilm, which is illustrated schematically in Figure 2 and has these features:

- The biofilm has a uniform biomass density X_f.
- The biofilm has a locally uniform thickness L_f.
- External mass transport may be represented by an effective diffusion layer of thickness L_w.

Substrate transport and utilization

Transport of substrate from the bulk liquid to the biofilm surface is represented by diffusion across a hypothetical liquid layer, or effective diffusion layer, of thickness L_w, which is the distance across which the actual mass transport resistance may be approximated solely by molecular diffusion. Fick's First Law describes the flux across this effective diffusion layer:

$$J = D\left(\frac{\partial S}{\partial z}\right) = D\left(\frac{S - S_s}{L_w}\right) \quad (1)$$

Where:

J = the flux of substrate across the diffusion layer ($ML^{-2}T^{-1}$)

D = the molecular diffusion coefficient of the substrate in water (L^2T^{-1})

L_w = the thickness of the effective diffusion layer (L)

S, S_s = the concentration of substrate in the bulk liquid and at the surface of the biofilm, respectively (M/L^3).

Within the biofilm, the accumulation of substrate due to molecular diffusion is represented using Fick's Second Law,

$$r_{diff} = \left(\frac{\partial S_f}{\partial t}\right)_{diff} = D_f \frac{\partial^2 S_f}{\partial z^2} \quad (2)$$

Where:

r_{diff} = the rate of accumulation of substrate due to diffusion ($ML^{-3}T^{-1}$)

D_f = the molecular diffusion coefficient of the substrate in the biofilm (L^2T^{-1})

S_f = the concentration of substrate at some location, z, in the biofilm (ML^{-3})

z = distance perpendicular to the biofilm surface (L).

The synthesis rate for new biomass is represented by Monod kinetics, which is a saturation function in which the dependent variable, the specific growth rate, is bounded by zero and a maximum rate value and depends on the concentration of the substrate used by the biomass type (Rittmann and McCarty 2001).

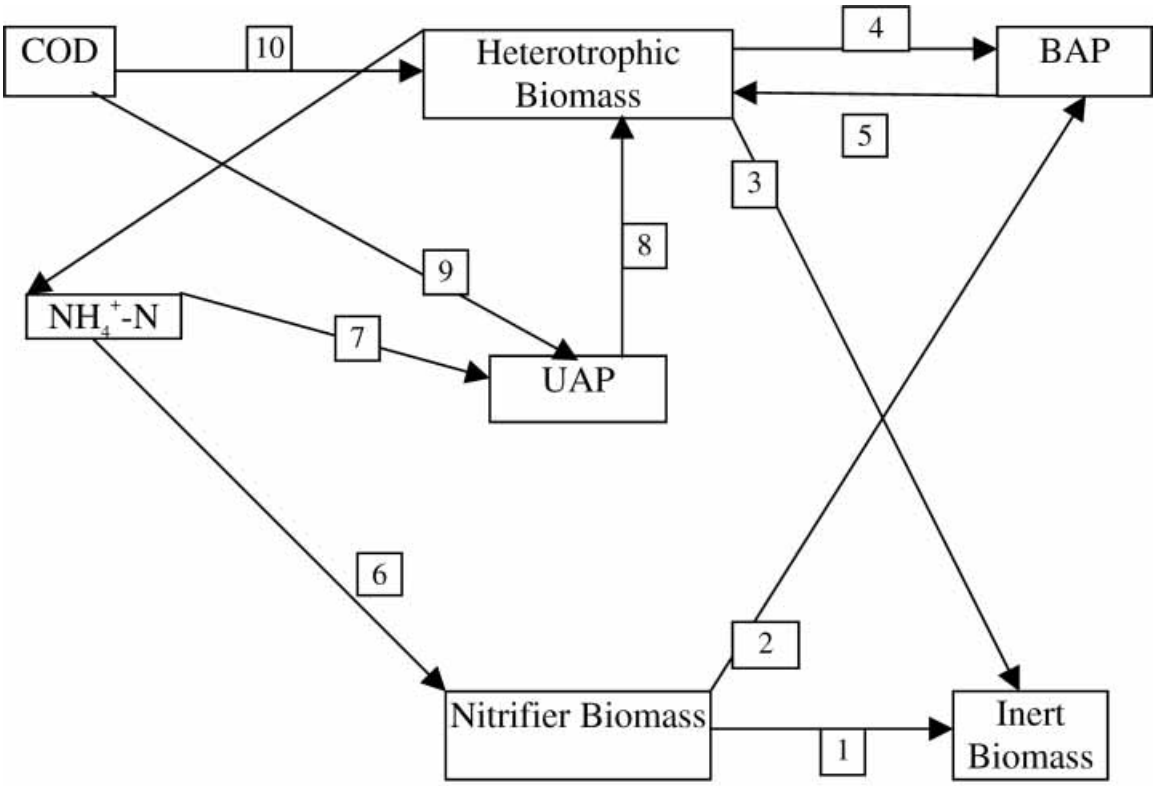
$$\mu = \mu_m\left(\frac{S_f}{K + S_f}\right) \quad (3)$$

Where:

μ = specific growth rate (T^{-1})

μ_m = maximum specific growth rate (T^{-1})

K = half-maximum rate concentration (ML^{-3}).



1	Production of inert biomass by nitrifying organisms
2	Production of BAP by nitrifying organisms
3	Production of inert biomass by heterotrophic organisms
4	Production of BAP by heterotrophic organisms
5	Consumption of BAP by heterotrophic organisms (does not support growth)
6	Production of nitrifier biomass through the consumption of NH_4^+-N
7	Production of UAP as a function of NH_4^+-N flux into the biofilm
8	Consumption of UAP by heterotrophic organisms (does not support growth)
9	Production of UAP as a function of COD substrate flux into the biofilm
10	Production of heterotrophic biomass through the consumption of reduced organic (COD)

Figure 1 | Schematic of the Integrated Biofilm Model (IBM) that identifies its components.

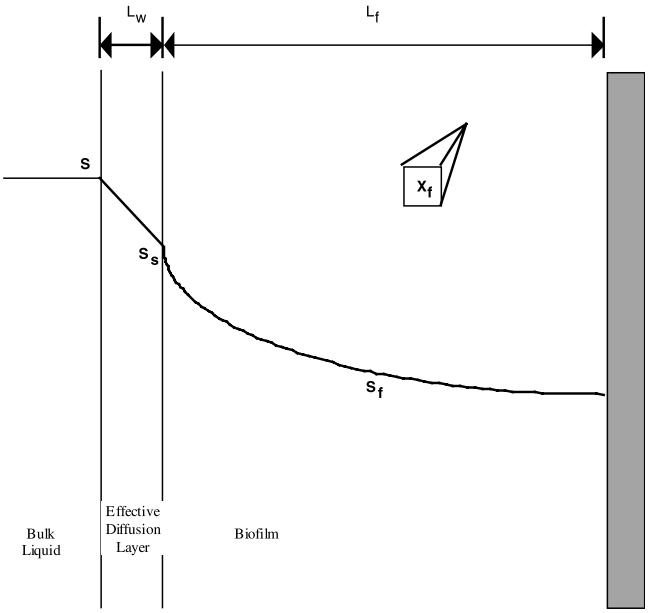


Figure 2 | Schematic of an idealized one-dimensional biofilm. The z-dimension is perpendicular to the substratum and positive from left to right.

The Monod relationship also applies to the utilization of the bacteria's substrate. The maximum specific rate of substrate utilization (q_m) is directly related to the maximum specific growth rate μ_m by the relationship:

$$q_m = \frac{\mu_m}{Y} \tag{4}$$

Where:

q_m = maximum specific rate of substrate utilization ($M_{substrate}M_{cells}^{-1}T^{-1}$)

Y = true yield for cell synthesis ($M_{cells}M_{substrate}^{-1}$).

The term Y is the biomass true yield, and it depends on the thermodynamic potential of the reactions through which microorganisms are able to conserve energy and electrons in newly synthesized biomass (Rittmann and McCarty 2001). The substrate utilization rate at some position in the biofilm is then:

$$r_{ut} = \left(\frac{\partial S_f}{\partial t}\right)_{reaction} = -q_m\left(\frac{S_f}{K+S_f}\right)X_f \tag{5}$$

Where:

r_{ut} = rate of substrate utilization ($ML^{-3}T^{-1}$)

X_f = concentration of active biomass in the biofilm ($M_{cells}L^{-3}$).

The mass balance on substrate that defines the substrate gradient within the biofilm is determined by the combined action of molecular diffusion and the substrate-consuming reaction taking place within the biofilm. This dual action is represented by combining Equations 2 and 5 to give Equation 6 for the net rate of substrate accumulation in the biofilm.

$$0 = \frac{\partial S_f}{\partial t} = D_f\frac{\partial^2 S_f}{\partial z^2} - q_m\left(\frac{S_f}{K+S_f}\right)X_f \tag{6}$$

Because the time constant for Equation 6 is normally small compared with the other times of interest for modelling (Kissel *et al.* 1984), the left side of Equation 6 can be set to zero, giving a steady-state concentration profile in the biofilm (as in Figure 2). The substrate flux (J) is then computed from the concentration gradient at the biofilm/liquid interface,

$$J = D_f\left.\frac{\partial S_f}{\partial z}\right|_{z=L_f} \tag{7}$$

Biofilm growth and loss

A mass balance on the active biomass in the biofilm couples biomass growth and loss with the substrate profile and flux. The growth for a type of biomass (Equation 8) utilizes Y and the Monod expression for utilization of the corresponding substrate:

$$\left(\frac{d(X_f dz)}{dt}\right)_{synthesis} = Y\left(\frac{q_m S_f}{K+S_f}\right)(X_f dz) \tag{8}$$

The left-hand term represents the increase in biomass due to synthesis for a location in the biofilm experiencing substrate concentration S_f.

In the IBM, the loss of active biomass in the biofilm is quantified with the term $b'(T^{-1})$, an overall, first-order loss term, which is the sum of decay (b) and detachment (b_{det}). The term b represents loss due to biomass auto-oxidation to supply maintenance energy needs; b generally is a constant for a given type of bacteria and a fixed

temperature. The term b_{det} represents the loss of biomass due to physical detachment. In a fixed-bed process requiring backwashing, the actual loss rate might be low during a filter run, but extremely high during the backwash. For a steady-state model like the IBM, these periodic loss rates are represented by a single b_{det} value that is the weighted average of b_{det} over time.

Adding biofilm loss to Equation 8 gives the total mass balance on active biomass for a position in the biofilm.

$$\frac{d(X_f\,dz)}{dt} = Y\left(\frac{q_m S_f}{K+S_f}\right)(X_f dz) - b' X_f\,dz \tag{9}$$

A steady-state biofilm

A steady-state biofilm is one for which the sum of the new growth of biomass due to substrate utilization is just balanced by the sum of all biomass losses (Rittmann and McCarty 1980). Within a steady-state biofilm, portions of the biofilm may be in a state of growth or decay on a local scale; however, when the entire biofilm is considered, there is no net growth or decay when the biofilm is at steady-state. Mathematically, this condition is represented by setting the integral of the mass balance on active biomass (Equation 9) over the entire biofilm to zero.

Because the flux of substrate into the steady-state biofilm is equal to the sum of the reactions occurring within the biofilm, the flux of substrate into the biofilm (J) can be substituted for the integral of substrate utilization over the entire reactor. Furthermore, the integral of the losses over the entire biofilm is simply $b'X_fL_f$. Then, the integrated form of the steady-state mass balance on active biomass is given as (Rittmann and McCarty 1980):

$$0 = YJ - b'X_fL_f \tag{10}$$

Pseudo-analytical solution

The IBM employs the pseudo-analytical model of Sáez and Rittmann (1992) to compute J and X_fL_f for any substrate. It is called a pseudo-analytical solution because it is an algebraic approximation based on thousands of numerical solutions of the biofilm equations (Equations 1, 6 and 10). The non-linearity of the substrate profile equation (Equation 6) makes a direct analytical solution impossible, except for special, limiting situations. The pseudo-analytical solution converts the task of biofilm modelling from a highly non-linear group of differential equations demanding numerical solution techniques to an algebraic expression requiring iteration on one variable, the substrate concentration at the biofilm liquid interface (S_s). Details of the pseudo-analytical solution and its solution (in a dimensionless domain) are detailed in Sáez and Rittmann (1992) and in Rittmann and McCarty (2001). For a given bulk-liquid substrate concentration (S) and parameters for the biomass (q_{max}, K, Y, D, D_f, L_w, b, and b_{det}), the pseudo-analytical solution determines the steady-state flux of substrate into the biofilm (J) and the accumulation of biofilm mass ($X_fL_f = YJ/b'$ from Equation 10).

Substrate mass balance in a reactor segment

The IBM combines the output of the pseudo-analytical solution with a steady-state mass balance on substrate in a completely mixed biofilm reactor (CMBR) segment:

$$0 = Q(S^o - S) - JaV \tag{11}$$

in which Q = the liquid flow rate (L^3T^{-1}), V = the segment volume (L^3), a = the specific area of biofilm (L^{-1}), and S^o = the influent substrate concentration (M_sL^{-3}). Equation 11 states that the change in substrate concentration across the biofilm reactor segment is equal to the flux of substrate into the biofilm. Solving Equation 11 simultaneously with the pseudo-analytical solution for J yields the effluent substrate concentration, the flux of substrate into the biofilm, and the biomass accumulation as outputs. Equation 11 ignores substrate consumption by suspended bacteria.

For the heterotrophic bacteria, the IBM allows only one organic substrate. This is a simplification that allows a simple spreadsheet solution. The organic matter in natural waters has a range of biodegradation kinetics (Woolschlager and Rittmann 1995).

To solve Equation 11, the IBM requires input values for parameters describing the physical conditions of the reactor (Q, a, V, S^o) and the kinetic parameters (q_m,K,b, b_{det},Y) for the substrate of a given type of bacteria. Based on these input data, the IBM performs iterations on the values of S and S_s until the calculated and trial values converge to give the steady-state solution for the biofilm reactor. Then, J and the active biomass accumulation (X_fL_f) are determined from S_s.

Multiple species

The IBM accounts for multiple species by assuming that each species can be considered separately. The total biofilm is then the combination of the separate species. The IBM employs the separate solution approach for heterotrophic and nitrifying bacteria. The nitrifiers are not subdivided into ammonium and nitrite oxidizers in the IBM. Thus, ammonium oxidized goes to nitrate, with no build-up of nitrite.

By determining two separate steady-state solutions (one for each group of organisms), competition for space and oxygen is not considered. The importance of these effects depends on the substrate loading conditions in the reactor. With a low loading and a thin biofilm, spatial competition does not greatly influence diffusion resistance for the electron donors or acceptors. With high loading or with substrate ratios that strongly favour the growth of one type of organism over another, the assumption may lead to errors. Our evaluation indicates that separate solution introduces only minor errors for conditions relevant to drinking water biofiltration.

Soluble microbial products

The IBM uses the steady-state biomass and substrate flux to determine the production and consumption of soluble microbial products. The approach employed by the IBM is well suited to model usability in that the SMP generation and consumption are approximated based only on the steady-state results of the pseudo-analytical solution. This novel approach eases the computational burden, while at the same time including the production of products by multiple species and the consumption of products by the heterotrophic population.

A review of the products literature by Rittmann *et al*. (1987) found that the kinetics of SMP formation is often divided into two classes: growth-associated and non-growth-associated. Because the growth of microorganisms depends directly on the utilization of substrate, the growth-associated products are more accurately termed substrate utilization associated products, or UAP. Because UAP are present when complete mineralization of a simple substrate is observed, the UAP are of microbial origin, and not simply intermediates from the breakdown of the input organic material (Grady *et al*. 1972; Noguera *et al*. 1994; Rittmann *et al*. 1994). The formation of non-growth-associated products is related to the base metabolism and decay of active biomass; thus these products are termed biomass-associated products, or BAP. BAP are composed of a range of substances associated with cellular macromolecules including fragments of DNA, portions of cell walls, and proteins released as a result of cell lysis (Rittmann *et al*. 1987; Noguera *et al*. 1994).

The production rate of UAP is proportional to the rate of substrate utilization (Rittmann *et al*. 1987; Noguera *et al*. 1994). The IBM, therefore, approximates the production rate of UAP through proportionality to the steady-state substrate utilization rate. At steady state, the substrate utilization rate is equal to Ja, where a is the specific surface area of the biofilm (L^{-1}). When heterotrophs and nitrifiers are active,

$$r_{UAP} = (k_1 Ja)_{heterotrophs} + (k_{1n} J_n a)_{nitrifiers} \quad (12)$$

Where

r_{UAP} = total rate of UAP formation ($M_{product} L^{-3} T^{-1}$)

k_1 = UAP-formation coefficient ($M_{product} M_{substrate}^{-1}$), where the subscript n refers to nitrifiers and no subscript refers to heterotrophs.

BAP are produced in proportion to the active biomass concentration, represented by the X_fL_fa terms.

$$r_{BAP} = (k_2 X_f L_f a)_{heterotrophs} + (k_{2n} X_{fn} L_{fn} a)_{nitrifiers} \quad (13)$$

Where

r_{BAP} = rate of BAP formation ($M_{product} L^{-3} T^{-1}$)

k_2 = BAP-formation rate coefficient ($M_{product} M_{biomass}^{-1} T^{-1}$).

In the IBM, all bacteria are capable of producing UAP and BAP. For each group of organisms represented in the model, a steady-state substrate flux (J) and biofilm concentration ($X_f L_f a$) are generated through use of the pseudo-analytical solution. The BAP and UAP produced by the different groups of organisms are treated as common pools of UAP and BAP.

BAP and UAP are biodegradable, although the kinetics of their degradation is not completely resolved. For example, Gaudy and Blachly (1984) demonstrated that approximately 90% of the SMP generated in their study were degradable. Rittmann *et al.* (1994) grew heterotrophic bacteria solely through their utilization of SMP generated by nitrifiers. The fact that SMP are degradable makes sense intuitively, because both categories of SMP are natural, metabolic by-products. Although both categories of SMP are degradable, research has demonstrated that the degradation kinetics of BAP and UAP are distinct from one another and that BAP is more slowly degraded than UAP (Noguera *et al.* 1994).

In the IBM, the degradation kinetics of UAP and BAP are represented with Monod expressions (Noguera *et al.* 1994). To capture the differences in degradation kinetics between UAP and BAP, two different half-maximum-rate concentrations (K_{UAP} and K_{BAP}, $M_{product}L^{-3}$) and maximum utilization rates ($q_{m,UAP}$ and $q_{m,BAP}$, $M_{product}M_x^{-1}T^{-1}$) are employed.

$$r_{degUAP} = \frac{q_{m,UAP}UAP}{K_{UAP} + UAP} X_f L_f a \tag{14}$$

Where r_{degUAP} = rate of UAP degradation ($M_{product}L^{-3}T^{-1}$).

$$r_{degBAP} = \frac{q_{m,BAP}BAP}{K_{BAP} + BAP} X_f L_f a \tag{15}$$

Where r_{degBAP} = rate of BAP degradation ($M_{product}L^{-3}T^{-1}$).

Because the SMP are organic compounds, only the heterotrophic organisms are capable of degrading them. Therefore, only the steady state, active, heterotrophic biomass concentration ($X_f L_f a$) is used to determine the degradation of SMP in the IBM. Synthesis of new heterotrophic biomass due to the degradation of SMP is not directly included. Likewise, loss of either biomass due to the release of SMP is not included in the IBM. In most cases, these omissions roughly balance each other, and errors are minor. When the NH_4^+-N:BOM ratio is large, SMP produced by nitrifiers can be the major substrate for heterotroph synthesis. In that case, the IBM underestimates the heterotrophic biomass and the removal of BOM.

Steady-state mass balances on UAP and BAP are:

UAP:

$$0 = QUAP_{in} + k_1 JaV + k_{1n} J_n aV - \frac{q_{m,UAP}UAP}{K_{UAP} + UAP} X_f L_f aV - QUAP \tag{16}$$

BAP:

$$0 = QBAP_{in} + k_2 X_f L_f aV + k_{2n} X_{fn} L_{fn} aV - \frac{q_{m,BAP}BAP}{K_{BAP} + BAP} X_f L_f aV - QBAP \tag{17}$$

Equations 18 and 19, obtained by solving Equations 16 and 17 for UAP and BAP, respectively, provide the steady-state concentrations of BAP and UAP. The solutions are in quadratic form, with steady-state SMP concentrations as functions of the model input (the kinetic parameters for SMP production and consumption: k_1, k_2, K_{UAP}, K_{BAP}, $q_{m,UAP}$, $q_{m,BAP}$) and the steady-state pseudo-analytical solution output (active biomass concentrations, $X_f L_f a$, and substrate fluxes, J). The term θ is the hydraulic retention time and is equal to V/Q. X_h and X_n refer to the biofilm concentrations in the reactor and are of the form $X_f L_f a$.

Steady-state UAP concentration in a CMBR:

$$UAP = \frac{UAP_{in} + k_1 Ja\theta + k_{1n} J_n a\theta - q_{UAP} X_h \theta - K_{UAP}}{2} + \frac{\sqrt{(UAP_{in} + k_1 Ja\theta + k_{1n} J_n a\theta - q_{UAP} X_h \theta - K_{UAP})^2 + 4(UAP_{in} K_{UAP} + K_{UAP} k_1 Ja\theta + K_{UAP} k_{1n} J_n a\theta)}}{2} \tag{18}$$

Steady-state BAP concentration in a CMBR:

$$BAP = \frac{BAP_{in} + k_2 X_h \theta + k_{2n} X_n \theta - q_{BAP} X_h \theta - K_{BAP}}{2} + \frac{\sqrt{(BAP_{in} + k_2 X_h \theta + k_{2n} X_n \theta - q_{BAP} X_h q - K_{BAP})^2 + 4(BAP_{in} K_{BAP} + K_{BAP} k_2 X_h \theta + K_{BAP} k_{2n} X_n \theta)}}{2} \tag{19}$$

Inert biomass

The production of inert biomass depends on the steady-state active biomass. Inert biomass is produced through the natural course of the bacterial life cycle because a portion of the biomass synthesized is refractory to self-oxidation. The term f_d denotes the fraction of the active biomass that is susceptible to self-oxidation (Rittmann and McCarty 2001); therefore, $(1 - f_d)$ represents the portion of the active biomass not susceptible to self-oxidation. As endogenous decay takes place and biomass is oxidized, the refractory portion of the biomass accumulates in the form of inert biomass.

The decay loss of active biomass, represented by b, accounts for the oxidation of biomass and the production of inert biomass:

$$-b(X_a) = (-f_d b(X_a)) + (-(1-f_d)b(X_a)) \quad (20)$$

The mass balance on inert biomass in a CMBR is given by Equation 21, which contains the second term on the right-hand side of Equation 20 (the production of inert biofilm biomass due to the decay of active biomass) and the loss of inert biomass due to inert biomass detached from the biofilm. The IBM uses the same value of b_{det} for active and inert biomass.

$$0 = (1-f_d)bX_f L_f aV - X_{fi} L_f aV b_{det} \quad (21)$$

Solving Equation 21 for the accumulation of inert biofilm biomass ($X_{fi}L_f a$) gives

$$X_{fi}L_f a = (1-f_d)\left(\frac{b}{b_{det}}\right) X_f L_f a \quad (22)$$

Reactor segmenting and information flow in the IBM

As shown in Figure 3, the IBM divides biofilm reactors into up to three sections, each section representing a completely mixed biofilm reactor (CMBR). Segmenting simulates a plug-flow nature in the reactor, while allowing the use of equations describing a CMBR. If the reactor is completely mixed, only one segment is needed. The choice of up to three segments allows the user to incorporate a plug-flow nature without introducing too much computational demand. For reactors with a high length-to-width ratio and little mixing (e.g. mixing due to bed aeration), more than three segments may be warranted, but this is not the normal circumstance in biofiltration of drinking water.

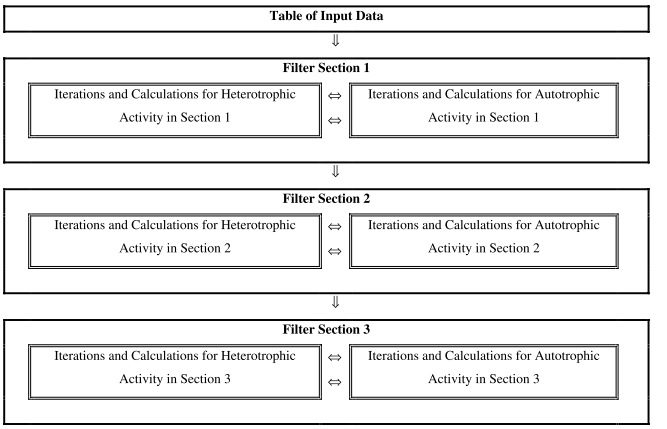


Figure 3 | IBM organization into three segments and the flow of information.

The steady-state solution for the first (influent) section is determined iteratively using the equations and method described above. Then, the information (e.g. effluent substrate and product concentration) is passed along, becoming the influent data for the second section. The same pattern occurs between the second and third sections. This approach describes substrate and biomass levels throughout the reactor.

The IBM spreadsheets

The IBM is solved via an Excel spreadsheet.† The user specifies operating conditions and trial values for the iterations. The kinetic parameters for biological activity and substrate flux, and the physical conditions of the reactor (flow rate, volume and surface area), are first input to a spreadsheet table at the top of the model. A copy of the input information to the program is shown in Table 1. For each simulation, the experimental conditions are

†The Excel spreadsheet for the IBM, as well as guidelines on parameter values, can be obtained by contacting Dr Rittmann at b-rittmann@inorthwestern.edu.

Table 1 | Input information for the IBM with typical parameter values

Term	Units	Reactor	UAP*	BAP*	NH_4-N	BOM*
Q	$m^3\ day^{-1}$	3.2	—	—	—	—
V	m^3	0.0033	—	—	—	
a	$m^2\ m^{-3}$	5,625	—	—	—	
S^o	mg subst. (as COD or N) l^{-1}	—	—	—	0.6	3.2
L	μm	—	—	—	100	100
X_f	mg Vsact l^{-1}	25,000	—	—	—	
K	mg subst. l^{-1}	—	100	85	1.5	1.25
q_m	mg subst. per (mg VSact.*day)	—	1.8	0.10	3.1	3.0
D	$cm^2\ day^{-1}$	—	—	—	1.9	1.25
D_f	$cm^2\ day^{-1}$	—	—	—	1.7	0.75
Y	mg Vsact. per mg subst.		—	—	0.33	0.45
b_{det}	$1\ day^{-1}$	—	—	—	0.05	0.05
b	$1\ day^{-1}$	—	—	—	0.09	0.09
b′	$1\ day^{-1}$	—	—	—	0.14	0.14
k_1	mg CODprod per mg CODsubst.	—	0.12	—	—	
k_2	mg CODprod per mg VS*day	—	—	0.09	—	

— no parameter exists for that entry.
*BOM, UAP and BAP are expressed in units of mg COD l^{-1}; the typical conversion to BDOC is 2.8 g COD per g BDOC.

entered into the input spreadsheet, and they are subsequently referenced throughout the program. Altering one or more of the input parameters creates new simulations.

Table 1 contains generic kinetic parameters for the biodegradation of the NH_4^+-N, SMP and original BOM (biodegradable dissolved organic carbon). They were taken from values reported in the literature (Rittmann 1990; Woolschlager and Rittmann 1995; Furumai and Rittmann 1994; Bouwer *et al*. 1995). The IBM uses mg COD/l as the units for BOM, UAP and BAP to ensure consistency in units among and to allow relevant comparisons between the different forms of BOM. The conversion between COD and BDOC (biodegradable organic carbon) is approximately 2.8 mg COD per mg DOC, a value that varies within a narrow range of 2.5 to 3.0 for natural organic matter.

Given the flow rate, filter specifications, kinetic parameters, and an influent substrate concentration, the IBM returns the steady-state effluent concentrations of original substrate and both soluble microbial products for each segment. It also returns the biomass accumulation (active and inert) and substrate flux into the biofilm. Two iterative

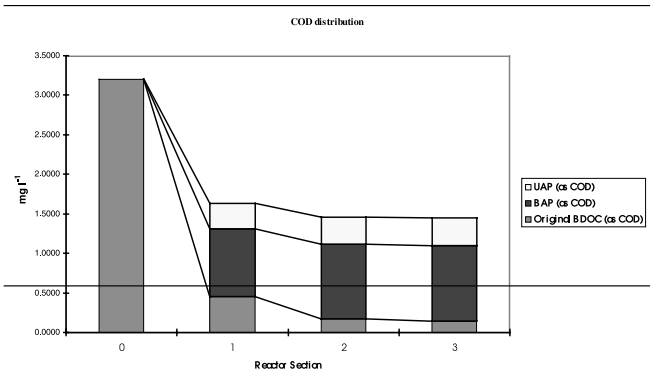


Figure 4 | COD distribution in the reactor for the conditions of Table 1.

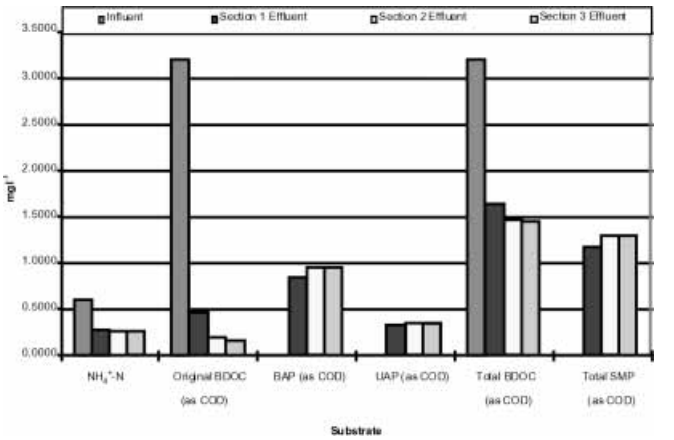


Figure 5 | Changes in the concentrations of the soluble components across the biofilter for the conditions of Table 1.

solutions are performed for each section of the reactor (Figure 3), one for heterotrophs and one for nitrifiers. The IBM, therefore, contains two separate data windows in which iterations are performed for each reactor section. These solutions are performed on each section sequentially, and the values for BDOC, NH_4^+-N, UAP and BAP are passed to the next section.

Graphical output

In addition to the spreadsheet tables, the IBM provides graphical output in a format convenient for analysis of reactor performance and observation of trends in the data. These figures show the changes in concentration of important materials across each section.

SAMPLE RESULTS

Figures 4 to 6 are examples of the graphical output of the IBM. They use the inputs listed in Table 1. These sample results show trends typical of biofilm processes used for drinking water biofiltration.

Figure 4 displays two trends common to soluble organic species in biofilm processes: specifically, the rapid consumption of original BOM (noted as original BDOC) and the dominance of SMP in the effluent distribution of BOM components. The most dramatic changes in BDOC, BAP and UAP concentrations occur in the inlet portion of the filter. As is typical of biofilm reactors subject to low-loading situations, S is rapidly driven to values near S_{min}, the minimum substrate concentration capable of supporting steady-state biomass (Rittmann and McCarty 1980, 2001). S_{min} is approximately 0.15 mg COD l^{-1} for the original BDOC in this example. Therefore, original-BDOC concentrations in the lower levels of the reactor are not capable of supporting a large biomass. A build-up of BAP relative to UAP is shown in Figure 4. The difference in concentration between the two species of SMP is a result of the difference in their biodegradation kinetics: BAP is consumed slowly relative to UAP.

Figure 5 provides more information on soluble species. Added to Figure 5 are NH_4^+-N, total SMP, and the sum of all soluble organic components (noted as total BDOC). Like original BDOC, NH_4^+-N is driven close to its S_{min} value, approximately 0.25 mg N l^{-1} for this example, in the first segment. SMP gradually increases in the second and third segments, and its effluent concentration is about 1.3 mg COD l^{-1}. The total BDOC, which is the sum of original BDOC and SMP, is just under 1.5 mg COD l^{-1} in the example effluent. This corresponds to about 54% net removal of BOM.

Figure 6 displays the total heterotrophic biomass present (given as $X_f L_f$ in mg volatile solids per cm^2) for the different reactor sections, as well as the flux of substrate into the biofilm at each section (given as J in mg COD

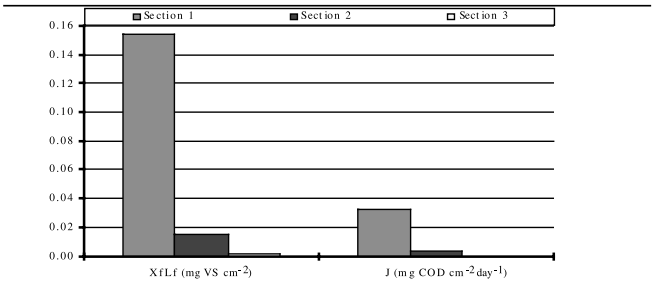


Figure 6 | Changes in biomass concentration and substrate flux across the biofilter for the conditions of Table 1.

transferred per cm^2 per day). Because of the low level of biomass present in the later sections of the filter and the correspondingly low value of substrate flux, SMP and original BDOC concentrations do not change greatly after the first section of the filter. The nitrifier biomass is much smaller than is shown in Figure 6. For example, the total nitrifier accumulation is 0.012 mg VS cm^{-2} in segment 1, compared with 0.14 mg VS cm^{-2} for heterotrophs.

CONCLUSIONS

The Integrated Biofilm Model (IBM) is a spreadsheet program that includes all the key phenomena for biofiltration of drinking water, but is simple to use. Specifically included in the model are the consumption and production of chemical species (input substrates, end products, and soluble microbial products); heterotrophic and nitrifying bacteria; inert biomass; physical processes, such as transport and detachment; and the relationships among all of the different organisms and chemical species. An example shows the inputs to the model and the kind of trends that it predicts for original substrates, soluble microbial products, and biofilm biomass. The IBM makes iterative design and analysis of biofiltration processes straightforward.

ACKNOWLEDGEMENTS

This work was supported by a grant from the Irvine Ranch Water District. We specially thank Mr Carl Spangenberg, the project collaborator from the Water District. The paper was originally presented at the IWA Workshop on Modelling of Conventional Drinking Water Production Processes, held at the Technical University of Delft, 16–18 March 2000.

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First received 1 June 2000; accepted in revised form 24 October 2001