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Water Quality Modeling for Aquaculture Water Reuse Systems

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Introduction

A modeling system is being developed to simulate water quality and fish growth in intensive aquaculture production systems that include a variety of water treatment units for water recirculation. The purpose of this model is twofold: 1) to increase and integrate the scientific knowledge in intensive aquaculture, and 2) to make this knowledge accessible to and usable by non-experts for educational and practical purposes. Improving the efficiency and predictability of intensive aquaculture operations are major goals of farmers, researchers, and system designers. Improvements in efficiency and predictability are contingent upon: 1) more accurate quantification of metabolic rates of the fish under intensive production conditions; 2) quantification of the relationship between water quality and fish growth and health; and 3) improvement and refinement of water reuse technology. A computer model is an effective tool for analyzing the effects of water treatment units and fish metabolic responses on overall system performance. Such a model can predict the performance of several water reuse processes and configurations while also simulating water quality, resource requirements, and production capabilities of aquaculture systems. The predictions will be useful in the design of new systems, the evaluation and selection of system components, the implementation of changes to existing systems, and in the management of water quality and production schedules in existing farms.

The Modeling Tool

The model is being developed using a modeling software package (Extend™) that allows for the creation of "blocks", each of which simulates a separate unit operation. Once created, the blocks are stored in a library and can be accessed and connected on the screen to create a model for a particular system configuration. The model can simulate water quality changes and fish biomass production in an aquaculture system over any desired duration (e.g. 60 day period with a 0.05 day time-step) as well as account for feed and oxygen consumption, based on assumptions in each block. Unlike some simulation model programs, Extend does not automatically perform numerical integration, so differential equations must be handled within each block separately. Rate changes have been programmed using Euler's method. After configuring the culture system by connecting the desired blocks, the modeler can input specific operating and design data into each block through dialog boxes. Then a desired simulation period and time-step are chosen and the model is executed. Time steps used for model execution should be less than one day since most state variables fluctuate daily and to prevent possible instability in the numerical integration calculations. Output is presented within Extend in graphs and tables.

Three terms can be used to describe the type of model being developed (Thornley and Johnson, 1990). The model is dynamic, which means it predicts how a system changes over time (e.g. fish size, water quality, feed consumed). The model is deterministic in that it makes definite predictions for state variables based on input conditions and model assumptions without any associated probability distribution. Thirdly, all the components of the model are mechanistic or reductionist in nature, concerned with the physical laws (e.g. conservation of energy and mass), chemistry, biology, and the environmental conditions of a process. Consequently, the models contribute understanding and theories for how systems work and inter-react.

The water quality variables considered in the model include dissolved gases (oxygen, carbon dioxide), solids (suspended solids), dissolved nutrients (total ammonia, combined nitrite and nitrate, total phosphorus), nutrients in suspended solids (nitrogen, phosphorus), organic matter (dissolved, in suspended solids), alkalinity, pH, salinity, and temperature. Other state variables are fish size, total fish biomass, and oxygen consumption.

Aquaculture System Library of Blocks

The blocks currently available in the aquaculture system library include: 1) water supply; 2) flow mixers and splitters; 3) fish culture tank (hierarchical block including fish metabolism, tank design, and husbandry data); 4) generic biofilter; 5) trickling biofilter; 6) fine-screen solids removal (drum filter); 7) settling tank; 8) granular media filter; 9) in-line diffused oxygenation; 10) pure oxygen air stone; 11) multi-stage low head oxygenation (LHO); 12) packed column aerator; 13) chemical addition; and 14) output blocks. A brief description of each of the blocks is presented below.

Water Supply Block

The water supply block is used to input the characteristics of the make-up water in the culture system. A dialog box allows the modeler to input information about the quality and flow rate of the water source. Some calculations related to the carbonate system are carried out in the block to complement data that would normally be available to the model user. These calculations are performed using generalized relationships that are valid for both fresh and salt

water (Piedrahita and Seland, 1995). Seasonal fluctuations in water quality and flow rate of a source can be taken into account.

Flow Mixers and Splitters

Flow splitter blocks allow a flow stream to be divided into two flow streams at any ratio desired, without affecting the water quality. The flow splitter may be used to send water to different locations (e.g., multiple fish tanks in parallel), to bypass a fraction of the flow around a unit process, or to discharge a fraction of the recycle flow along any point in the system. Flow mixers combine two flows and mix them into one flow stream. Flow mixers calculate the water quality resulting from mixing two separate flows. For calculating the pH of a mixture, first the alkalinity and total carbonate carbon are calculated based on mass balances and then the pH is calculated from these values (Piedrahita and Seland, 1995). The influent flow mixer verifies the hydraulic balance of the entire aquaculture system by checking that the influent flow equals the combined effluent flows.

Fish Culture Tank (Hierarchical)

The fish culture tank is a hierarchical block consisting of a total of four blocks, the fish tank block and three blocks nested within it: the fish species characteristics block, the tank design block, and the fish husbandry block. A hierarchical block simplifies the model by allowing complex sub-models to be nested within one block icon on the screen. The fish species block allows the user to input metabolic and growth rate data for a specific species for various size ranges. Blocks for various species of fish (striped bass, sturgeon, tilapia, Atlantic salmon) are currently being developed based on available data. The tank design block specifies the size and shape of the fish tanks and the fraction of solids removed in a side-stream flow (if any). The fish husbandry block contains information regarding the operating characteristics of the fish tank, such as feed type, feed rate, stocking density, initial fish size, etc. All the calculations regarding growth rates of the fish and the effects of wasted feed and metabolic activity on water quality in the fish tanks are carried out in the fish tank block. A modified version of the fish culture tank was developed to simulate changes in water quality during fish transport events ("Fish Transport Tank" block).

Generic Biofilter

This block simulates either a closed system (e.g. fluidized bed) or open system (e.g. trickling filter) biofilter based on inputs from the user regarding specific ammonia and dissolved organics removal rates in units of $\text{g TAN m}^{-2} \text{ day}^{-1}$ (TAN = total ammonia nitrogen) and $\text{g BOD}_5 \text{ m}^{-2} \text{ day}^{-1}$ (BOD_5 = five day biochemical oxygen demand), respectively. The possible limitation of dissolved oxygen (DO) on filter performance is ignored in an open system and an effluent DO is calculated based on a packed column equation. No contact between the biofilter media and the atmosphere is assumed for a closed biofilter, and oxygen consumption by bacteria within the filter is calculated. Treatment performance is modified based on limiting DO concentrations within the filter. For a closed biofilter system, a pure oxygen air stone block may be attached to the biofilter block to add oxygen to the system and increase treatment capacity in oxygen limited scenarios.

Trickling Biofilter

Nitrification and BOD removal in the trickling biofilter block are calculated using theoretical and empirical formulas. The nitrification calculations are based on work primarily from Hochheimer (1990) and Gujer and Boller (1986). The BOD removal component is based on the empirical formulas of Eckenfelder and O'Connor (1966). Ammonia removal is calculated based on oxygen and ammonia concentrations and diffusion rates, nitrification kinetics, water temperature, media surface area and void fraction, and hydraulic loading rate.

The model divides the trickling filter into several completely mixed reactors in series. Ammonia and BOD (biochemical oxygen demand) removal are calculated within each section of the filter. The effluent from one section is the influent to the section immediately below. Oxygen is consumed by both heterotrophic bacteria, which remove BOD, and nitrifying bacteria, which remove ammonia. Consequently, there is competition for oxygen and oxygen may become a limiting factor. Based on literature in wastewater treatment, the assumption has been made that heterotrophs are more successful at obtaining oxygen than nitrifiers. Consequently, the model first calculates BOD removal in a section, then calculates remaining dissolved oxygen, then calculates nitrification. For gas transfer calculations, air is assumed to be well mixed within the biofilter and oxygen saturation concentrations are calculated based on temperature and on an atmospheric oxygen partial pressure of 0.21 throughout the reactor. This assumption may not be valid for some trickling biofilters and the gas transfer code from the packed column aerator may be included in this block in the future.

Fine Screen Solids Removal (Drum Filter)

The drum filter block is in its initial stages of development. This block simulates the removal of suspended solids from the water, based on screen pore size and particle size range (Figure 1). Initially, the water quality array passed between the blocks considered total suspended solids (solids larger than about 1 μm) without regard to particle size; however, this was inadequate for the theoretical modeling of solids removal systems. Consequently, consideration of three solids particle size ranges was added by including the following categories in the water quality array and in solids removal calculations: solids between 1 μm and 30 μm ; solids between 30 μm and 60 μm ; and solids larger than 60 μm . These ranges were chosen based on experimental protocols developed for a separate aquaculture solids research project.

Currently, the drum screen filter model is designed to simulate solids removal with continuous rotation of the drum filter. Changes in the particle sizes due to shearing or pressure effects are not considered in the current model. The model will assume straining of particles larger than the screen pore size, followed by cake filtration due to a build-up of solids over the screen, which will allow removal of smaller particles and improved overall removal efficiency.

Settling Tank

The settling tank simulates the removal of suspended solids from water depending on particle size and specific density of solids. Suspended solids are divided into the same three particle size distributions as for the drum filter block. This block currently assumes ideal flow and Stoke's Law for particle settling, but will be upgraded to account for hydraulic scouring and re-suspension effects due to non-ideal reactor hydraulics.

Granular Media Filter

A granular media (sand) filter is being developed to simulate solids removal in non-pressurized depth filters. The model assumes steady state removal of particles based on a trajectory analysis and mass balance approach (Yao, et. al., 1971). This is a conservative assumption for depth filters, since removal efficiency tends to improve as particles accumulate in the filter (ripening). The model will be extrapolated to account for filter ripening in the future (Darby, et. al. 1992). Data required for the model include collector diameter, depth and area of filter, collector efficiency, flow rate into filter, and solids concentration and size distribution of influent. The model will predict solids removal for the three particle size ranges listed above. Very little information is available on the solids removal performance of sand filters in aquaculture applications.

A more common granular media filter in aquaculture is the "bead" filter, which uses plastic beads as the collector media rather than sand. The basic filtration mechanisms are the same as for sand filters, but the beads are significantly larger in diameter, which influences removal efficiencies and ripening effects. Depending on the operation of the filter (backwash frequency), bead filters also may serve as nitrifying biofilters.

Parameter	Value
Number of filter units in parallel	1
Drum Diameter (m)	1.6
Filter area (m ²)	5.4
Length of drum filter (m)	
Screen Mesh Size (um)	60
Rinse water flow rate per unit	10
Specific gravity of suspended solids	1.19
Drive motor size (kw)	1.6
Temp Change in Tank (°C)	0
Drum rotation rate (rpm)	1
Liquid level control (off = 0, on = 1)	<input checked="" type="checkbox"/>

Figure 1. Sample dialog Box of the Fine Screen Solids Removal Block.

In-Line Diffused Oxygenation

This block is not related to a particular technique for oxygen addition, but more to a control strategy for maintaining a target oxygen concentration. In the dialog box for this block, the user specifies the range within which DO concentration in the fish culture tank is to be maintained, the maximum flow of gaseous oxygen into the system, the partial pressure of oxygen in the system, and the base-line transfer efficiency of the system. The flow of oxygen into the system is regulated in the model as a function of the DO level in the fish tank. The oxygenation block outputs the quantity of oxygen used over the simulation time period. Since the user inputs the overall base oxygenation efficiency and partial pressure of oxygen in the reactor, this block could theoretically be calibrated to virtually any in-line oxygenation system.

Pure Oxygen Air Stone

This block uses similar code to the in-line oxygenation block; however, the air stone block is designed to simulate the addition of oxygen directly into a fish tank by diffused bubbles. The control strategy for this block is identical to the in-line oxygenation block.

Multi-Stage Low Head Oxygen (LHO) System

The multi-stage LHO simulates a common oxygenation device used in aquaculture which consists of a group of short (normally less than one meter) packed columns, through which water flows in parallel but oxygen flows in series (Watten and Boyd, 1990). In this block, the oxygen concentration within each column is calculated by considering the gas to liquid flow ratio, the mole fraction of oxygen, and the water temperature using packed column formulas for completely mixed reactors (Hackney and Colt, 1982). Each column is assumed to have a homogeneous gas concentration, but the mole fractions of oxygen are adjusted through iteration within each column to reflect the transfer of oxygen. The user can input the depth of the LHO, the number of columns, the influent mole fraction of oxygen, the maximum flow of oxygen, and a desired range of oxygen to maintain in the fish tanks.

Packed Column Aeration

This block simulates a counter-current packed column aerator (PCA) used to "strip off" supersaturated levels of carbon dioxide (CO_2) and to add oxygen. The PCA model uses a multi-step approach to calculate CO_2 removal and oxygen addition, including gas transfer equations, mass balance equations, gas flow characteristics, and equilibrium reaction kinetics. The column is modeled as a series of completely mixed reactors, with the number of "sections" depending on the gas to liquid flow ratio. The PCA model is based on experimental work carried out at UC Davis and on a model derived from that work by Grace and Piedrahita (1993).

Chemical Addition for Alkalinity and pH Control

In intensive aquaculture systems employing high levels of water recirculation, alkalinity may be continually diminished by nitrification. In addition, accumulation of CO_2 produced by fish stocked at high densities, may result in low pH levels. Furthermore, nitrifying bacteria perform more efficiently at neutral or basic pH levels. Aeration helps control the concentration

of carbon dioxide in the system, but it does not affect the alkalinity. One control strategy for restoring lost alkalinity and raising the pH (shifting CO_2 to bicarbonate) is the addition of chemicals, such as NaOH (sodium hydroxide), NaHCO_3 (sodium bicarbonate), and various forms of CaCO_3 (lime). The chemical addition block allows the modeler to increase the alkalinity of a flow stream to a desired level or to manually control the rate (mass time^{-1}) of chemical added to a flow stream. The block will calculate the changes in alkalinity, total carbonate carbon, pH, and CO_2 , as well as account for the cumulative quantity of chemical added over the simulation period, based on the characteristics of the chemical added.

Output Blocks

Output blocks present the results of a model execution in graphical and tabular formats. Values from the tables may be transferred into other software applications, such as spreadsheets.

Sample Aquaculture System Models

Sample aquaculture system models are shown in Figures 2 and 3. Figure 2 depicts a flow through culture system, while Figure 3 shows a model for a recirculating aquaculture system. The flow through system consists of a water supply, a packed column aerator which could be used to remove excess gases (supersaturation) and add dissolved oxygen, and a fish tank with an oxygen diffuser system. The recirculation system consists of a water supply block, an influent mixer, a fish culture tank, a solids removal unit, a nitrifying biofilter, and an in-line oxygenation unit. Water flows from one block to another as indicated by the lines connecting the blocks. In the flow through system, water goes through a packed column aerator before entering the fish tank. An oxygen diffuser system is installed in the fish tank itself. In the recirculating system, water leaving the in-line oxygenation system is returned to the influent mixer, where it is combined with the supply water and recirculated back into the fish tank. Waste solids are discharged from two locations: the fish culture tank side-stream and the solids removal effluent. Discharge flows for a given system model are hydraulically balanced by the supply water flow to prevent the overall system volume to fluctuate over time: the rate at which water leaves the system equals the rate at which water enters the system from the water supply.

To illustrate the capabilities of the modeling system, the recirculating system model was executed for a 30 day time period with a time-step of 0.1 days. A sample of the fish tank water quality output plot is shown in Figure 4. The parameters shown include water temperature (T), total ammonia nitrogen (TAN), dissolved oxygen (DO), and pH. In this particular case, temperature remains constant over time, since the supply temperature is uniform, and heat losses across any of the units are neglected at this time. TAN increases over time, as a result of ammonia production by the fish. The rate of TAN increase is very high initially as the system comes to a pseudo equilibrium status. At time zero, fish are introduced into a fish culture system in which TAN equals zero. After some time (around five days in this example, Figure 4), the initial TAN build up results in a TAN concentration that rises slowly as a result of the continuously increasing rate of ammonia excretion by fish. The speed with which curves such as the TAN curve come to a pseudo equilibrium state depends not only on the physical characteristics of the system being modeled (i.e. flow rates, volumes, etc.), but also on the size of the time step being used. A large time step tends to prolong the time required to reach a pseudo steady state condition in addition to making it difficult or impossible to consider diel fluctuations in metabolic rates or in system performances.

The dissolved oxygen curve on Figure 4 results from the control strategy used to maintain oxygen concentration within a prescribed range. In this case, DO is to remain within the range

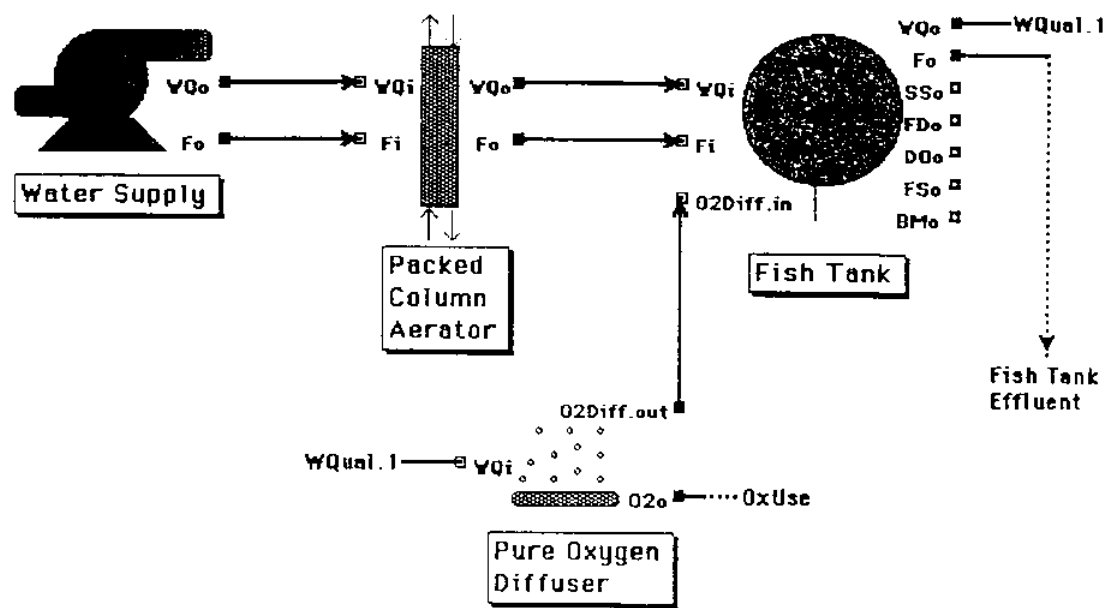


Figure 2. Sample model for a flow through system.

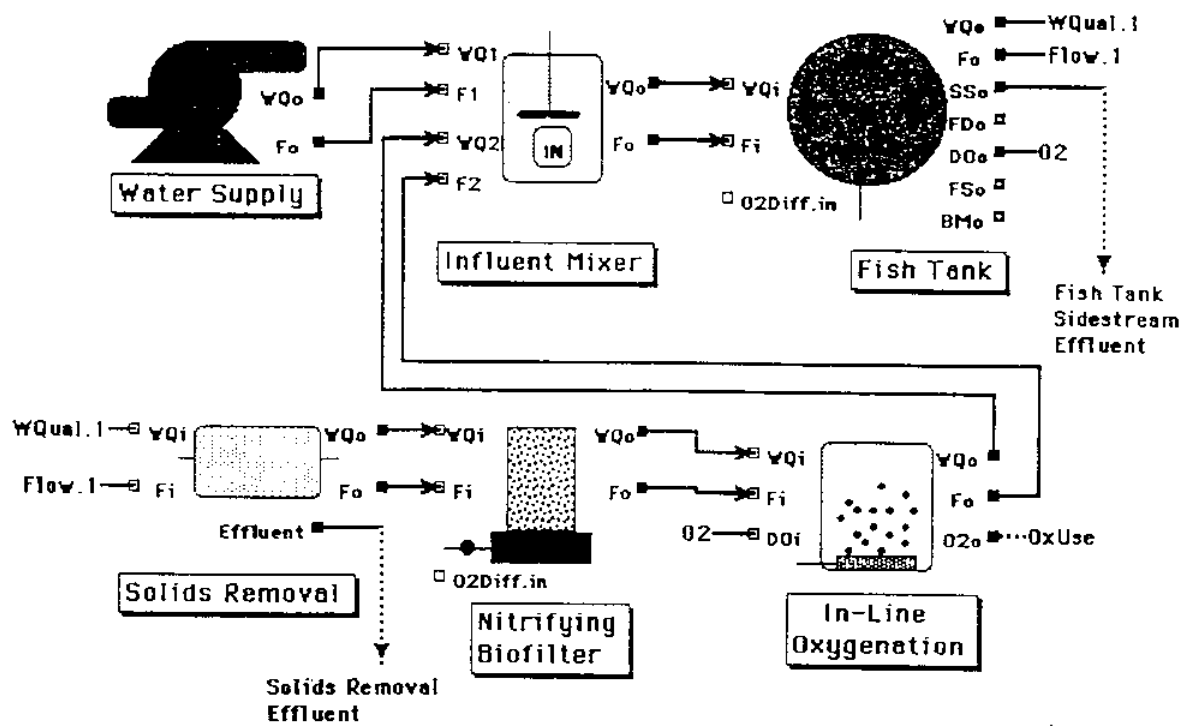


Figure 3. Sample Recirculation System Configuration

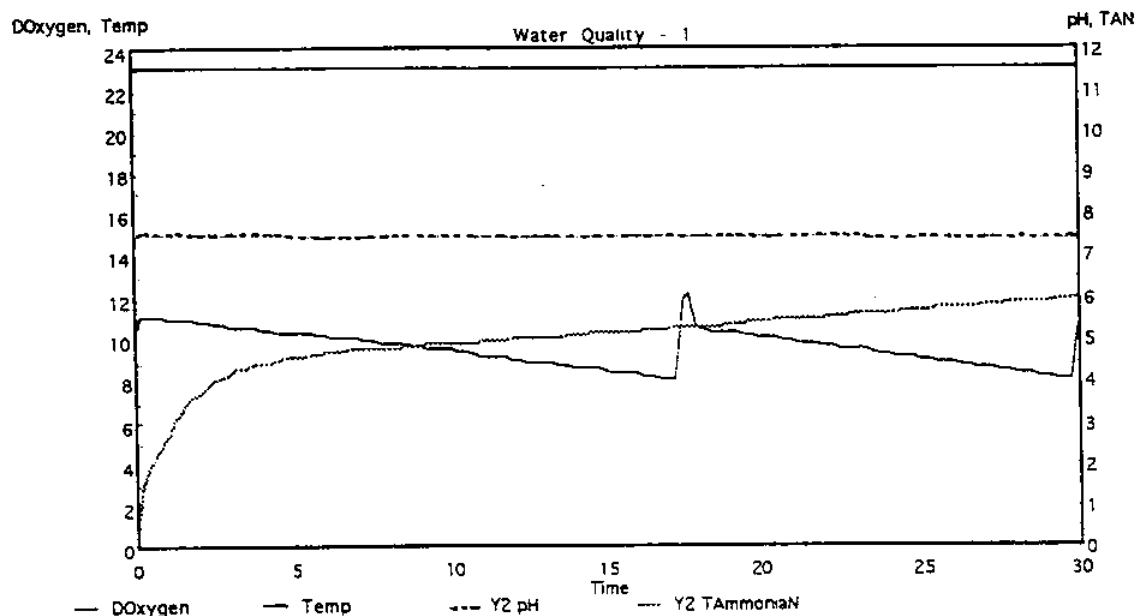


Figure 4: Sample Water Quality Output Plot (DO, pH, Temp, TAN). The step change in the dissolved oxygen curve is caused by the control strategy of the oxygenation system, which is designed to maintain dissolved oxygen concentration within a specified range (8 to 12 mg l⁻¹ in this case).

of 8 to 12 mg l⁻¹. As the demand for oxygen increases to the point where DO drops below the threshold level (8 mg l⁻¹) in this case, the flow of oxygen to the in-line oxygenation system increases as a step function (analogous to opening a valve). The result of this sudden increase in oxygen inflow to the system is an increase in concentration over time up to the point where oxygen demand once again exceeds the new supply rate, and oxygen concentration begins to drop. As the concentration drops below the prescribed limit, further increases in total oxygen flow are attempted up to the point where the maximum oxygenation capacity of the system is reached. At that point, a message would be shown on the screen of the model indicating that the total oxygen demand exceeds the maximum oxygenation capacity available.

The pH of the water declines slightly over time. The decline is caused by the production of CO₂ by the fish, and by the destruction of alkalinity (production of hydrogen ions) in the process of nitrification. The rate at which pH declines will depend on the activity of the fish, on the type and efficiency of the treatment units included, and on the flow rate and characteristics of the make up water.

Curves similar to those shown in Figure 4 can be displayed for the influents or effluents to any treatment operation. In addition to water quality information, fish growth, and cumulative feed and pure oxygen consumption can be plotted.

Future Work

The modeling framework being developed, and the library of models for treatment operations used in aquaculture, are a starting point for what will be a design, research, and management tool. Calibration and validation of the various blocks will be carried out using data collected in experimental and commercial installations. New blocks and calibration data will be developed for additional unit operations, and for particular treatment units and species. Data from several

systems containing various water treatment operations will be used to validate system models constructed from model blocks in the aquaculture model library.

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