A SYSTEM DYNAMICS COMPUTER MODEL FOR LONG-TERM WATER QUALITY PLANNING

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(ABSTRACT)

The objective of this study was to develop a comprehensive, basin-wide, water-quality-planning model using system dynamics methodology. Later, the model was to be interfaced with a more conventional system dynamics model: one simulating social, technological, economic, and political interactions. By doing so, it is envisioned that such management policies as zoning, abatement facilities, and best management practices may be simulated together.

A water quality model was developed for the Occoquan basin in Northern Virginia, simulating four parameters: dissolved oxygen, sediment, phosphorus compounds and eutrophication. The model performs a steady-state water quality analysis, and yet is capable of simulations into the long-term future. In addition, all significant factors relating to the transport and transformation of pollutants are included.

The model is designed to simulate the four situations important from a basin-wide planning perspective: 1) pollutant concentrations during low-flow events, 2) pollutant concentrations during runoff events, 3) long-term buildup of pollutants in aquatic sediments with subsequent leaching into the water column, 4) long-term, physical alteration of the stream due to changes in the sediment load.

The lake dissolved-oxygen model has been calibrated for 1979, tested with a sensitivity analysis, and applied; the methodology works. In addition, a substantial amount of data has been collected for verification and application.

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CHAPTER I

INTRODUCTION

System dynamics facilitates the solution of complex management problems, making it a powerful tool for the regional planner. This thesis addresses its application to an important regional planning problem: man's interrelationship with water. How will land development and population growth affect water pollution? In turn, how will water pollution affect further land development and population growth? A computer model answering these questions would have value.

Obviously, in order to answer the second question, the first should be answered as comprehensively as possible -- all significant consequences of land-use development and population growth should be assessed. This means consideration for all important pollutants and for each of the following situations:

1. pollutant concentrations during low flow events

2. pollutant concentrations during runoff events

3. long-term buildup of pollutants in aquatic sediments with subsequent leaching into the water column

4. long-term, physical alteration of the stream due to changes in the sediment load

In previous, basin-wide, water-quality-planning models, the first two have been addressed; the latter two have not. The objectives of this study were 1) to develop a system dynamics model to simulate the long-term effects of land use development, population growth, and water-pollution-control policies on each of these four situations, and 2) to develop it so that it has the capability to consider all pertinent pollutants. In other words, it was to be comprehensive.

The model was applied to the Occoquan basin in Northern Virginia. By dividing this basin into fifteen subbasins, water quality can be determined at fifteen stream stations, thereby allowing the testing of scenarios that are geographically oriented (e.g. development of a subdivision within a subbasin). Further, the subbasins allow consideration of the dilution and self-purification potential of each stream channel, and the buildup of pollutants in upland soils and stream sediments.

The model simulates input, transport, and transformation of three pollutants: dissolved oxygen (DO), phosphorus compounds, and sediment. In addition, eutrophication is modeled. Calibration and sensitivity analysis were performed for lake DO for 1979 using water quality data from the Occoquan Monitoring Laboratory in Manassas, Virginia, and input data from a variety of sources. The methodolgy is workable, and the large amount of input data available for other pollutants makes further model development appear worthwhile.

CHAPTER II

LITERATURE REVIEW

The Occoquan Basin

The Occoquan Basin, which drains 570 square miles of Northern Virginia near Washington, D.C., is one of the most rapidly growing urban areas in the United States (Figure 1). It is located in the northern Piedmont region of Virginia, with land slopes varying from flat to hilly, and with silt loam the predominant soil type. At present, most of the land is either forest or used for agriculture; only twenty percent is urban, mostly in the northeastern part. A important feature is the Occoquan Reservoir, located near the outlet of the basin, which serves for recreation and as a water supply for 650,000 people in Northern Virginia.

The reservoir has been cause for concern; there have been problems with eutrophication, and resulting algal blooms have threatened the water supply. (The water utility has had to resort to adding copper sulfate to the lake.) Metcalf and Eddy (1), among the first to study the problem, concluded that sewage discharges were the major cause, and a highly

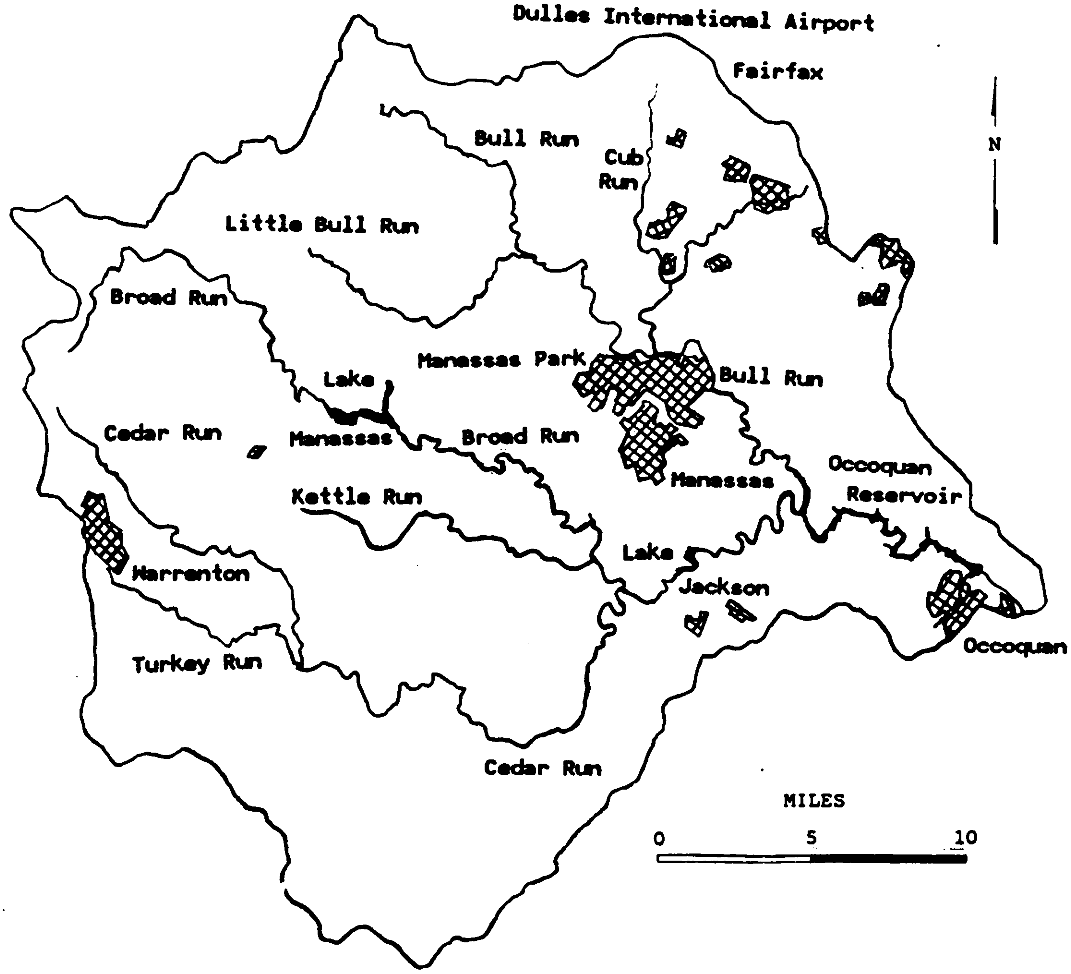

Figure 1. The Occoquan Basin. Taken from 1:250000 scale USGS mapping, revised 1979.

sophisticated, advanced wastewater treatment plant was built to alleviate that aspect of the problem. Later researchers showed that sewage discharges were not the only problem; urban runoff was shown to be a significant contributer of nutrients to the lake. In addition, observations made during the operation of the advanced wastewater treatment plant, completed in 1978 and serving the entire basin, have supported this contention. The urgency of the problem has resulted in the creation of the Occoquan Monitoring Laboratory in Manassas, Virginia, which has been monitoring stream quality and urban and agricultural runoff since 1972. At present, phosphorus, rather than nitrogen, is the limiting nutrient.

Previous Studies of Phosphorus in the Occoquan Basin

As far as river basins are concerned, the Occoquan basin is an exception, for a considerable amount of phosphorus data is available for it, including concentrations in water columns, concentrations in lake and stream sediments, rates of adsorption and release from sediments, and mass loadings due to runoff events. The water column data are from reports given by the Monitoring Program, while the sediment data are in the form of masters and doctoral theses at the Virginia Polytechnic Institute and State University.

To (2) is one of the first to have studied the effects of phosphorus in the basin. In a literature review, he cited other researchers as concluding that anaerobic conditions cause release of phosphorus from sediments, that 40 percent of dead algal biomass has a degradation rate of only a few percent per year, and that only a fraction of the phosphorus adsorbed to sediment is ever available again for release back into the water. From his laboratory experiments, he made five conclusions:

1. Phosphate releases from Occoquan reservoir sediments were enhanced by lower DO concentrations, higher rates of biological activity in the sediments, lower dissolved solids concentrations, higher concentrations of phosphates adsorbed to the sediment, and higher temperatures.

2. Phosphate releases from Occoquan Reservoir sediments were unaffected by pH changes within the normal range, depth of sediment, and depth of overlying water.

3. Rates of release decreased at a constant ratio as the experimental microcosms were flushed.

4. Sediments may act as a source or sink for phosphorus, depending on the concentrations in the sediment and in overlying water -- a critical water concentration exists,

below which release begins. (This is true for both aerobic and anaerobic systems.)

5. During phosphate release, an interstitial water layer in the sediment containing high phosphorus concentrations prevents higher rates of transfer.

In addition, To found that higher phosphorus concentrations in sediment exist in the Bull Run arm of the reservoir, which drains the majority of the urban area in the basin, and he listed these concentrations along with his experimental rates of release.

Chaney (3) is the next to have studied the effects of phosphorus in the reservoir, in particular, the availability of sediment phosphate for algal growth. In a literature review, she found the following:

1. At DO concentrations above 1 mg/L, a layer of ferric hydroxide forms on the sediment surface, preventing phosphate transfer.

2. The exchange layer at the top of the sediment is approximately 1 to 4 four mm thick

3. Algae have a "luxury uptake" mechanism for phosphorus.

From her experiments, she made the following conclusions:

1. The Occoquan Reservoir sediments can release enough phosphate to stimulate algal growth, and with mixing, release can occur under both anaerobic and aerobic conditions. However, release occurs much faster and to a greater extent under anaerobic conditions.

2. Alkalinity and pH may have important effects on release (To (2) disagreed.)

3. Sediments should not be a source of phosphate if nutrient inputs are reduced significantly.

4. Algal blooms should be expected after mixing events such as storms or lake turnover.

In 1976, Shugart (4) presented another thesis relating to the problem. He elected to study the readsorption of phosphates rather than the release; for, due to the irregular circulation of the reservoir and the frequency of turnovers, there are frequent mixings and opportunities for released phosphorus to readsorb to suspended sediment. From his experiments, in which he employed mixed microcosms, he concluded that readsorption did occur, and that it occurred in a two-step reaction: a rapid and a slow phase. In addition, he pointed out the following:

1. Readsorption was generally insufficient to prevent algae blooms.

2. Measured amounts of phosphates released were highly variable, even with samples collected at similar sites and at similar times.

3. Sediments from the Bull Run arm of the reservoir contained much more phosphorus than sediments from the Occoquan River arm.

4. Sediments low in phosphate removed greater amounts of phosphate in a shorter period of time.

5. Bull-Run-arm sediments contained only orthophosphate.

Also in 1976, Markley (5) presented a thesis in which the chemical natures of adsorption and release were studied. He found that the chemical interactions between phosphates and other ions may be complex, indeed. However, he also found that phosphate concentrations correlated strongly with iron concentrations throughout the reservoir and concluded that the major forms of bound phosphorus were ferric phosphate and complexes with other ferric compounds. In addition, he stated that leaf litter was a major source of iron into the reservoir.

McLaughlin (6) presented the most informative thesis on the subject yet, a study of unmixed lake microcosms. He agreed with Markley (5) in his statement that phosphate adsorption and release are complex chemical processes, and he cited Grizzard (7) as stating that the bottom exchange layer in the surface sediments of the reservoir is no more than 2 mm. From his microcosm experiments, he made the following conclusions:

1. Releases of phosphate during anaerobic conditions were sufficient to support heavy algal growth.

2. An enriched condition will extend for a considerable period of time after stoppage of phosphorus influx.

3. Such factors as station location, sediment characteristics, and sediment nutrient content exerted no statistically-significant influence on rates of uptake and release.

4. Iron and manganese concentrations did correlate with rates of uptake and release, suggesting that these species play an important role.

5. Reactive depths involved in the release of total phosphate to the water columns were estimated to be between 0.19 and 0.58 mm.

He recommended that nonpoint sources of phosphorus be curtailed because, at that time, even under aerobic conditions, phosphate levels were high enough to support algae blooms.

Sherman (8) studied another potential means of alleviating the problem: the use of nitrate in the hypolimnion to poise the oxidation-reduction potential (ORP) so that anaerobic release is retarded (or prevented). She concluded that as long as as the nitrate concentration remained above 0.2 mg/l as N, the ORP remained sufficiently high to prevent release of phosphates from the sediment. Of course, much nitrate is lost to denitrification when the oxygen concentration is low, but enough remains to significantly help. The AWT plant has heeded this need and presently releases a nitrified effluent with approximately 20 ml/L nitrate as N.

These studies are informative, but the important thing is that they give pertinent data which may be used for calibration and verification. Sediment phosphate concentrations and rates of adsorption and release from sediments are summarized in Tables B-1 and B-2, respectively.

In summary, it is generally accepted that the Occoquan Reservoir has a problem with phosphorus, And, at present, phosphorus is produced to the reservoir mainly from urban and agricultural runoff. (The AWT has virtually eliminated point discharge sources.) Algae utilize the dissolved orthophosphate, grow, die, settle, and rot, thereby releasing phosphorus into the water column and bottom sediments. When the lake stratifies in the summer, bacteria utilize the available organic substrate and create anaerobic conditions in the hypolimnion, thereby causing re-release of phosphates from the sediment into the water column. Thus, the feedback cycle is complete. The trouble is that there is more phosphorus entering the lake than is leaving; the means of export, which include outflow from the tailwaters, biological removal, and burial under incoming deposition, are insufficient to keep up with import. The problem is complicated, intractable, and no one knows the exact mechanisms by which the transformations are carried out.

Water-Quality Models

Water-quality models simulate pollutant concentrations in natural bodies of water. How and where will pollutants be transported? What effects will they have? What will be their fate? The answers to these questions depend on both the means of hydraulic transport in the water body and the rates of pollutant transformation or decay.

Hydraulic transport may be affected by three general processes: advection, dispersion, or diffusion. Advection is "gravity flow"; dispersion is the transport of pollutants due to differing velocity gradients; and diffusion is the process bringing about equilibrium concentrations of dissolved solids. All means of hydraulic transport, whether in rivers, lakes, reservoirs, or oceans, depend on these three processes.

Rates of decay, on the other hand, depend on both the specific pollutant itself and the environment it is in. There are many processes by which it may be brought about, including chemical speciation, hydrolysis, photolysis, volatilization, ion exchange, biodegradation, bioaccumulation, adsorption, etc. Not all pollutants decay; some, called conservative pollutants, are resistant. (Dissolved solids immediately comes to mind.) However, the majority of pollutants, including most of those causing the worst problems, are nonconservative, or degradable. And of the means of decay, adsorption is often the most important: many pollutants are strongly adsorbed to soil particles, some being transported to water bodies only with the soil.

Water-quality models start with the classic Streeter Phelps equation (9), published in 1922. It simulates the variables dissolved oxygen (DO) and biochemical oxygen demand (BOD) and is based on the assumption that a river can be divided into a number of reaches such that all pertinent environmental factors affecting these variables, including concentration and rates of flow and decay, are uniform (i.e. completely mixed) throughout the reach and are "steady state", or constant. In addition, no consideration is given to settling of suspended BOD, to longitudinal dispersion, to photosynthesis, or to oxygen demands exerted by nitrification, respiration, and the benthos, all of which are important.

From the time of publication of this equation until the late 1950's, almost no advances were made in the field, but with the subsequent passage of a series of federal water pollution control laws and the development of the digital computer, growth has been explosive. This fact is evident from Figure 2., as given by Thomann (10). The ordinate of the graph refers to additions to four areas: modeling of additional pollutants, refinement of descriptions of pollutant transport and transformation, advancement of methods of verification and sensitivity analysis, and development of cost-benefit-type models.

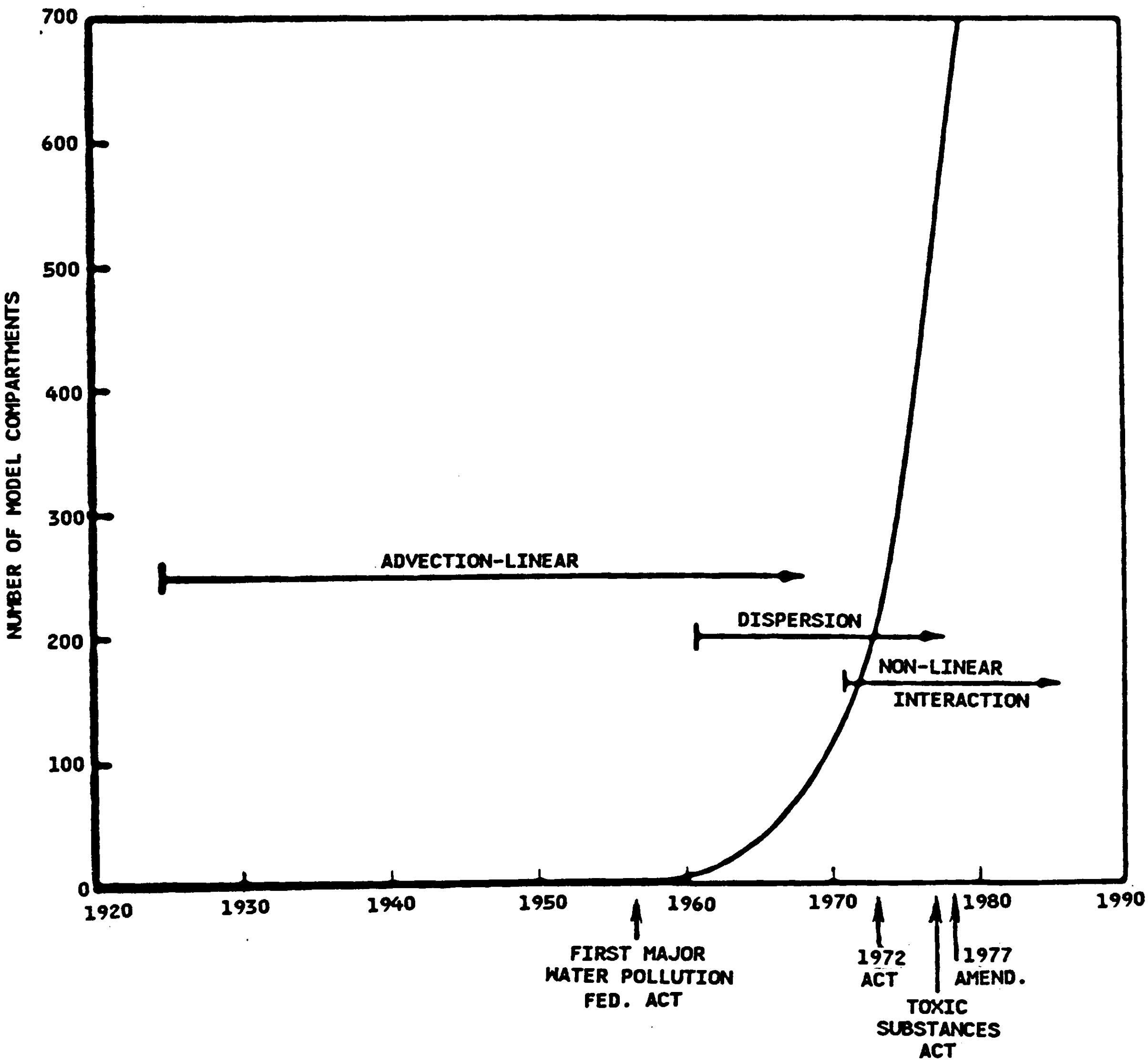

Figure 2. Increase of Numbers of Model Components with Time. From Thomann (10).

Such a wealth of new models requires a means of differentiation and, thus, the following nomenclature:

1. Static versus Dynamic. Static models are based on the assumption of steady-state conditions, while dynamic models are designed to reflect varying or transient phenomena (e.g. storm flows or diurnal variations in temperature, light, etc.)

2. One-Dimensional versus Two- and Three-Dimensional. This differentiation is based on the number of simulated dimensions of hydraulic transport.

3. Deterministic versus Stochastic. Deterministic models are based on the laws of classical physics, such as mass and momentum conservation, and on empirical formulas; they are frequently regarded as expected-mean-value models. On the other hand, stochastic models take into account the randomness of many phenomena.

4. Descriptive versus Black Box. Descriptive models are developed to simulate the internal mechanisms of a problem. Conversely, black box models are "input-output"; internal mechanisms are mostly ignored.

5. Stream versus Estuary versus Lake/Reservoir. These models differ in the simulation of hydraulic transport. Stream models commonly include only advection (plug flow), but may include one-dimensional, longitudinal dispersion. Estuary models, on the other hand, may include tidal effects, wind, stratified flow, diffusion, and more dimensions of flow, and emphasize longitudinal dispersion rather than advection. Lake models often include wind effects, dispersion, diffusion, density currents, summer stratification, and up to three dimensions of flow. Thus, estuary and lake models generally have more complicated hydraulics than stream models.

Stream Models

One of the first of the expanded stream models to see wide use has been DOSAG1, as developed by the Texas Water development board in the late 1960's (11). It is a steady-state, deterministic, one-dimensional, Streeter-Phelps DO model that considers nitrification and changes in temperature. Only advection is included, not longitudinal dispersion. Deoxygenation and nitrification coefficients in each reach are computed for the temperature entered into the program, and the model computes the streamflow required to maintain a specific DO concentration at each stream station. A modification of this program, SNOSCI (12), allows simulation of many more pollutants: total coliforms, fecal coliforms, algae, ammonia, nitrate, nitrite, orthophosphates, copper, lead, temperature, and four conservative substances. Transformations between the forms of nitrate are computed and each pollutant is given a source and sink term.

At approximately the same time, in 1969 and 1970, the Texas Development Board (13) developed a more accurate and precise deterministic, one-dimensional, stream model: QUAL I. Longitudinal dispersion is included as well as advection; a numerical integration of the one-dimensional advection-dispersion equation is accomplished. Additionally, the diurnal effect of temperature is considered, making this a "quasi-dynamic" model. (Only temperatures are dynamic -- the solutions have steady-state hydraulics, but dynamic water quality.) In addition, as many as three conservative substances may be modeled. Like DOSAG-I, this program has also been modified to simulate more pollutants; the modification, called QUAL-II (14), simulates ammonia, nitrate, nitrite, algae (chlorophyl A), phosphate phosphorus, benthic oxygen demand and radioactive materials. Multiple-limited Monod kinetics are used for simulation of algal growth; terms are included for limiting growth due to nitrogen, phosphorus, and available light.

According to Grimsrud (15), SNOSCI, QUAL I, and QUAL II have been extensively used, but only two published reports were been found in recent literature. White and Dracup (16) successfully applied SNOSCI to a mountain stream, and Bingham et al. (17) used QUAL-II to determine the wasteload allocation for a municipal wastewater treatment plant on the Great Miami River.

Other recent developments are the stochastic models, which consider the randomnesss of natural phenomena such as flow, temperature, etc., and the probabilistic models, which compute the expected frequency of exceeding pollutant standards. Stochastic models are invariably probabilistic models, but the reverse is not true. (Stochastic models are a special type of probabilistic model.) Beck (18) cited Loucks and Lynn (19), Thayer and Krutchkoff (20), Padgett et al. (21), Tiwari et al. (22), and Finney et al. (23) as good references for these types of models. From a planning viewpoint, the advantage of employing them is obvious.

Considerable effort has also been given to simulation of heavy metals, a type of pollutant typically strongly affected by adsorption. Somlyody (24) has studied the effects of a concentrated point discharge of cadmium in a river in Hungary and made four conclusions:

1. Metal content of the sediment decreases exponentially downstream from the source.

2. Under low flow, the longitudinal change in water column concentration is similar to that of the sediment pollution.

3. At high stream flows, the role of resuspension becomes apparent, sometimes causing increases in concentration in the flow direction.

4. Floods disrupt the exponentially decreasing pattern and bring about considerable changes in the concentration profile.

Fontaine (25) proposed a model for toxic-metal speciation in acidic, aquatic ecosystems in which he considered rates of adsorption and ion exchange, rates of sediment settling, resuspension, and transport, and differences between types of sediment. The model was tested with four metals, and it was shown that differing pH and differing types of sediment cause wide variations in rates of adsorption and ion exchange, but the model was not calibrated or verified with field data. Kuwabara _et al._ (26) developed and calibrated a one-dimensional, descriptive, deterministic model for copper transport in streams. By including expressions for periphyton uptake-release and adsorption-desorption, observed data were been duplicated well, and corresponding rate constants are are within the range of published values.

Other models have been developed to consider certain special situations, such as spills of toxic pollutants, natural systems which differ from the normal, etc. Gundelach and Castillo (27) proposed a BOD/DO model for an anaerobic stream. Bartell *et al.* (28) proposed a model for aromatic hydrocarbons in streams, which includes rates of chemical dissolution, volatilization, photolytic degradation, adsorption, and bioaccumulation. Chen and Wells (29) developed an ecological model for the Boise River in Idaho. Along with the normal water quality parameters, it simulates two types of floating algae, two types of benthal algae, zooplankton, insects, detritus, organic sediment benthos, and three types of fish: cold-water game, warm-water game, and benthic feeders. The model was calibrated with available data, and all derived rate constants are included in the paper.

Runoff Models

In the field of water pollution control, the significance of nonpoint source pollution has been well accepted. BOD, dissolved solids, suspended solids, coliforms, nitrogen, phosphorus, and toxic heavy metals are produced in great quantities by urban rainfall. Agricultural rainfall commonly produces pesticides, BOD, dissolved solids, suspended solids, coliforms, nitrogen and phosphorus. Randall et al. (30), from a study of urban runoff from the Occoquan basin, concluded that this source of pollution should be evaluated in all watershed pollution abatement programs. Krenkel and Novotny (31) stated that "Almost four billion tons of soil materials are washed into receiving waters of the United States every year.", and that "Approximately 75 percent of this material originates from forested and agricultural lands." Adsorbed pollutants travel along with this soil. Further, Sliter (32) estimated that, for 1976, after all the 1977 point-source effluent standards under P.L. 92-500 are met, 92 percent of the solids, 79 percent of the nitrogen, 53 percent of the phosphorus, and 43 percent of the zinc loads that existed before upgrading would still be reaching the nation's streams. Most of this is due to urban and agricultural runoff.

This new-found awareness of nonpoint pollution, along with the landmark provisions for its control in Section 208 of the Water Pollution Control Act Amendments of 1972 (P.L. 92-500) has stimulated development of mathematical modeling. Urban runoff models, agricultural runoff models, groundwater models, and acid rain models have all been developed since 1972.

The EPA's Stormwater Management Model, SWMM (33), is the first of the urban runoff models, and it has been widely used since being published in 1971. Its purpose is to determine the best means of stormwater pollution control and to help design abatement facilities. It has the following capabilities:

1. Accepts any rainfall hyetograph or multiple hyetographs and produces a runoff hydrograph for each modeled watershed. In doing this, it considers infiltration, depression storage, and velocities of overland flow.

2. Computes pollutographs on the basis of storm runoff and on antecedent conditions which include rainfall history, street sweeping data, land use, and related data.

3. Computes hydrographs and pollutographs for combined sewer systems for dry weather flows with daily and hourly variations and for infiltration into the sewer systems.

4. Hydraulically routes flow through sewer systems; variations in conduit sizes, lengths, slopes, and cross section configurations are considered, along with locations and design parameters of nonconduits. Pollutographs are also routed and combined.

5. Considers all types of storage facilities.

6. Provides the following treatment options: mechanically cleaned bar racks, fine screens, sedimentation, dissolved air floatation, microstainers, high rate filters, effluent screens, and chlorination.

7. Dynamically models receiving waters, whether they be rivers, lakes, or estuaries, and computes the effects of pollution.

8. Computes costs of various treatment measures so that approximate cost-effectiveness curves may be developed for decision making.

In applying and testing the original SWMM, three problems have been found (34):

1. SWMM is a "single event" model; continuous simulations cannot be performed. Thus, the randomness of runoff events cannot be considered and the frequency of water-quality violations cannot be easily estimated.

2. SWMM requires a large amount of data, more than is available for most watersheds.

3. In the original 1971 model, the only pollutants considered were five-day BOD, suspended solids, and coliforms.

Subsequently the EPA has recognized these shortcomings and has sponsored development of four levels of evaluation techniques (34):

Level I -- desktop calculator procedure for estimating quantity and quality of runoff and for preliminary screening. Data requirements are minimal.

Level II -- simplified, continuous-simulation model for planning and preliminary sizing of facilities; or a computerized optimization version.

Level III -- a refined, continuous-simulation model.

Level IV -- a sophisticated, single-event model.

These newer versions also simulate changes in total nitrogen and total phosphorus concentrations.

Following release of the original version of SWMM, several simplified, statistical runoff models have been developed that relate the mass flux of pollutants to selected, independent variables such as land-use, level of urbanization, meteorological characteristics, and topographic factors. Litwin and Donigian (35) cited the EPA (36,37) and Radzini (38) as giving examples of these models. However, Litwin and Donigian (35) felt these models are insufficient because they do not account for the processes involved and they represent average conditions which cannot describe nonpoint pollution.

In 1976, the Hydrologic Engineering Center (39) released STORM, a stormwater management model capable of continuous simulation. Its purpose is the same as that of SWMM: to aid in the sizing of treatment facilities. However, compared to SWMM, the original STORM model uses a simplified rainfall-runoff relationship, neglects the transport of water through the city, assumes a simple relationship between storage and treatment, and has no economic capabilites. On the other hand, input data requirements are considerably less than the original version of SWMM, and STORM calculates erosion using the Universal Soil Loss Equation. Later versions of STORM have been updated to include simulation of receiving waters, frequency analyses, and economic analyses, and the EPA has designated these updated versions of STORM as equivalent to level III of the evaluation techniques of SWMM.

Neither STORM nor SWMM can simulate sediment-pollutant interactions. Adsorption and ion exchange strongly affect the fate of many pollutants, such as ammonium, inorganic phosphorus, heavy metals, and many pesticides. Consequently, the EPA has sponsored development of models simulating soil/pollutant interactions.

The first of these is the Pesticide Runoff Simulation (PRS) Model, published in 1973 (40), which is a dynamic, one-dimensional, and deterministic model that is capable of simulating runoff, snow accumulation-melt, sediment loss, and pesticide-soil interactions. The object is to determine loadings to streams during storm events and to do it on a continuous basis, thereby establishing the frequency of occurrence of pollutant loadings. Testing has shown that the model simulates sediment transport well, and that the fate and transport of pesticides strongly adsorbed to sediment ,so that they are transported only with the sediment, are simulated well. However, simulation of the fate and transport of pesticides that move both in water and on sediment is fair to poor. The Agricultural Runoff Simulation Model (ARM), published in 1976 (41), is an updated version of PRS that is capable of using a first-order transformation approach to model nitrogen and phosphorus.

A simplified agricultural model designed to provide rough estimates of the nutrient runoff from cropland, the Simulation Model for Agricultural Non-Point-Source Pollution

(42), was published in 1981. It is similar to the simplified, urban runoff models in that no calibration is required, and therefore it has the same drawback: is an oversimplification.

Another runoff model, the Nonpoint Source Model (35), NPS, considers both urban and agricultural runoff, making its application suitable for any type of watershed. It has the same object as PRS and ARM: to compute pollutant loadings to streams. It is continuous, is designed to be universal in application, and is simple to use. As a result, it too is an oversimplified representation of nonpoint pollution, and special care is required for calibration.

A descriptive runoff model for phosphorus fate and transport was proposed by Novotny et al. (43) in 1978. Unlike previous runoff models, this model treats phosphorus as a nonconservative substance; terms are included for adsorption-desorption and uptake by microorganisms and plants. In addition, the model is capable of routing flow, sediment, and phosphorus through stream channels, a technique which requires consideration of sediment transport and deposition. The hydrologic portion is similar to SWMM and STORM, for it includes snowmelt, infiltration, excess rain, and runoff routing by the unit hydrograph method. Based on results of continuous-simulation tests performed on small watersheds in the Menomonee River basin, Wisconsin, the authors claimed that transport and transformation of phosphorus was simulated well.

A basin-wide runoff model written specifically for the Occoquan basin was developed by Hydrocomp Inc. (44). It combines the features of the NPS model along with HSP QUALITY, a sediment-routing routine. As with other runoff models, it is dynamic. The sediment-routing routine estimates scour and deposition, with several simplifying assumptions:

1. Sediment is divided into two categories: washload, composed of silt and clay, and sandload.

2. The supply of sand in channel reaches is assumed to be unlimited.

3. Scour and deposition have no effects on the geometry or hydraulic characteristics of the channel.

Calibration and verification have been performed with 1978 and 1979 data from the Occoquan Monitoring Program. The authors stated that these two years were ideal for verification because the advanced wastewater treatment plant had begun operation during this period and flows during 1978 were low, while those for 1979 were high. Because their results agreed well with observed data, the authors stated that their model has value.

For the more descriptive of the runoff models described in the preceding paragraphs, how does one acquire the necessary input data relating to pollutant buildup on land surfaces? Several papers have been written on this subject. Jewell and Adrian (45) claimed that it is impossible to derive general pollutant-washoff functions applicable to any area, that storm data must first be gathered for the basin in question, and that statistical procedures, such as hypothesis testing, should be used to develop washoff functions. However, other researchers have developed and studied generalized washoff functions based on such factors as land use, curb length per area, percentage impervious cover, average catchment slope, net dwelling unit density, rooftop area, street area, fertilized lawn area, ans off-street parking areas. Interest in such relationships has helped fuel stormwater monitoring studies across the country, including those reported by Randall _et al._ (30) and Bedient _et al._ (46).

Groundwater Models

Although groundwater modeling is not included within the scope of this paper, two models appear to be worth mentioning. A mathematical model describing the interaction between an ephemeral stream and its unconfined aquifer has been proposed by Dillon and Liggitt (47). It predicts the inflow and outflow from the stream during fluctuating water levels, and its authors claim it is sufficiently accurate; such a model may have value in predicting the ultimate fate of pollutants. Another groundwater model, given by Christopherson _et al._ (48), concerns acid rain and determines the impact of increasing or reducing sulfur emmissions. Insufficient testing has been performed to determine whether it is reasonably accurate.

Estuary Models

With estuary models, as with stream models, either steady-state or dynamic conditions may be assumed. In both cases, of course, steady-state models are simpler and easier to apply. However, steady-state, estuary models are also much more of an oversimplification than steady-state stream models because of the diurnal effect of tides.

Thus, steady-state estuary models, several of which are available, represent only net flow or tidally-averaged effects. An example is ES001 (49), useful for a rapid evaluation of the effects of varying wasteload conditions on DO. The Simplified Estuary Model, SEM (50), another example, is designed for hand-held calculators.

However, the dynamic estuary models offer a much more realistic representation of the hydraulics of estuaries. The Dynamic Estuary Model, DEM, as developed by the U.S. Department of the Interior in 1970 (51), is capable of simulating the diurnal tidal cycle at each point along the estuary and of simulating the first-order decay of five pollutants, any of which may be conservative or nonconservative. Another model, RECEIV (34), is similar to DEM, but has the added capabilities of dynamically modeling influent river flows and waste discharges and of computing the change in channel cross-section with tides. As mentioned previously, this model is designed to interface with SWMM. Both DEM and RECEIV simulate longitudinal dispersion, but not lateral or vertical dispersion. Neither is capable of simulation strongly-stratified estuaries, those typical of large river systems. For these estuaries a two-dimensional box model, such as that given by Pritchard (52), is often appropriate.

Lake Models

Lake models begin with the one-box, phosphorus model given by Vollenweider (53), a classic example of a black-box model. In it, the change in phosphorus concentration is related only to the rate of inflow, the rate of flushing, and the rate of internal removal. (All internal removal mechanisms are lumped into one parameter.) Complete mixing is assumed. For some lakes, this model is an adequate representation.

In order to simulate summer stratification, Bella (54) has proposed a two-box, lake-DO model with a completely-mixed box representing both the epilimnion and the hypolimnion. Exchange between the two layers is determined for both dispersion and water movement across the thermocline. thermocline. Snodgrass and O'Melia (55) have applied this two-box concept to a phosphorus model and have included settling of particulate phosphorus. These models also adequately represent some lakes, but in a comparison of one-box and two-box phosphorus models, Snodgrass and Dillon (56) claimed that there is no obvious advantage to either type of model when they are applied to shallow lakes of relatively high hydraulic loading.

Other researchers have applied the one-box and two-box concepts to toxic pollutants. Bierman and Swain (57) developed a one-box DDT model for Lakes Michigan and Superior, and verified it enough times to be able to make conclusions through a sensitivity analysis. They found that adsorption and settling are the major means of removal and have estimated the expected half-life of the pollutant. Schwarzenbach and Imboden (58) have proposed a two-box model for a lake in Switzerland for a variety of toxic pollutants. The model includes all expected rates of transformation of the pollutants, but it was not verified so that conclusions could be drawn.

Other lakes, especially large ones, cannot be adequately represented by one-box or two-box models; they are too complicated hydraulically. Therefore two- and three-dimensional lake models have been proposed, models accounting for density currents, wind, the earth's rotation, upwelling-downwelling, multiple withdrawals, etc. The LARM model (59) is a two-dimensional grid network and is capable of dynamically simulating temperature and multi-level withdrawals. Gordon (59) modified it for DO and used it to evaluate various releases for control of tailwater DO. Three-dimensional models, such as that developed by Halfon (60), are based on the three-dimensional advection-diffusion equation. There are two methods of solving them: the multiple-box method and the finite-difference method. These models are difficult to calibrate and verify.

Basin-Wide Planning Models

These models are another result of the heightened awareness of both point source and nonpoint source water pollution in the past twenty years, an awareness which has developed in both the United States and Europe. Basin-wide planning models have the purpose of maximizing the benefits and minimizing the costs of maintaining a water resource in the face of mounting population and land development; therefore they usually include some means of economic analysis.

The earliest of these models consider only point discharges and their resulting effects on DO; they involve linear optimizations of treatment levels, flow augmentation, and discharge locations to achieve minimum DO concentrations at each point in a river. The linear models, using the cost curves they are given, determine the least-cost management policies. Models such as those given by Revelle *et al.* (61) and Loucks *et al.* (62), in 1967, use the Streeter Phelps analysis to determine critical DO deficits. In later models, DO modeling was refined. The effect of temperature on BOD decay rates was included by Marsden *et al.* (63). Bayer (64) included feedback from thermal wastes along with second-order BOD exertion. Sedimentation of suspended BOD, photosynthesis, respiration, and benthal demand were included by Young and Beck (65). The model of the Saint John River, Canada, by Biswas (66), has a unique feature: it contains both an optimization model and a simulation model. The optimization model selects the best group of alternatives for maintaining at least 5 mg/L DO, while the simulation model further analyzes the best alternatives and determines operating policies.

The model of the Neckar River, Germany, by Hahn and Cembrowicz (67), is another DO optimization model. However, it is an in-depth optimization: such factors as water supply benefits, hydropower, fishing, and recreation are all accounted for. Furthermore, the DO model is detailed, with consideration of nitrification and ecological modeling of heterotrophs and autotrophs. Calibration has been performed, and scenarios have been tested, but no firm, basin-wide plan has been established.

Another comprehensive model, the model for the Seine-Normandy Basin, France (68), simulates no less than thirteen pollutants and includes a cost analysis of water treatment and needs. The modeling is relatively black-box, for pollutants are either considered conservative or are assigned a single first-order-decay term. In addition, nonpoint pollution is neglected. The model has the capability of setting limits on pollutant concentrations, based on need, and of summing all costs and benefits. The authors studied several management strategies and stated that their model has value.

Perhaps the most comprehensive and extensive, long-term planning model yet developed is the model of the Trent River System, England, published by Newsome (69). For a planning horizon of thirty years, almost all conceivable management options are included, such as desalinization of seawater, importation of water, water-quality-improvement lakes in rivers, storm detention basins, recharge of aquifers with stormwater, improved wastewater treatment, improved water treatment, water-supply reservoirs on clean streams, separate treatment for industrial use, and recreational benefits. The model can assess the costs of alternate strategies for meeting additional demands on water resources and can select combinations of least-cost policies. With regard to water quality modeling, it is a black box model; using existing data, pollutant-concentration "qual grams" are developed, depending on the quality in the preceding reach and the land-use and wastewater treatment practices in the intermediate reach. No firm management decisions have yet been made, but several scenarios have been evaluated, and the authors stated that the usefulness of the model has been shown.

One of the simplest, and yet most powerful, basin-wide planning model is the phosphorus-optimization model by Jeng *et al.* (70). It is designed specifically to prevent eutrophication of a lake in a small watershed. Cost curves relating total annual cost to percent phosphorus removal were developed for three types of abatements: street cleaning, stormwater retention basins, and advanced wastewater treatment. The allowable, yearly, phosphorus loading, which is used as a constraint in the linear optimization model, is determined from the stream and lake models. The stream model is plug flow with sink and source terms. The lake model can be any suitable one, with Vollenweider's model (53) being suggested. The optimization model determines the least-cost means of attaining the loading constraint. In this excellent paper, the authors stated that the model has been successfully applied to a small watershed in New Jersey.

The runoff model proposed by Hydrocomp (44) is also a basin-wide model capable of simulating many pollutants, and it is similar to the model proposed in this thesis in that it includes a rudimentary analysis of sediment transport and deposition. However, because it is based on the NPS model previously described, it simulates all pollutants as conservative substances, an aspect which greatly limits its descriptiveness. In addition, it neglects stream dynamics, and the maximum simulation interval is one hour, making it unsuitable for long-term simulation.

The Need for the Proposed Model

Basin-wide planning models, thus far developed, are oversimplifications of the overall problem, especially with regard to water quality modeling. The DO optimization models, however descriptive they are, fail to account for other important pollutants. The models which do account for other pollutants are black box, failing to adequately represent such factors as adsorption and sediment transport, often the most important factors affecting the fate of pollutants. The dynamic runoff simulation models, such as SWMM and STORM, can also be applied on a basin-wide, but they too simulate transformation of pollutants in a black-box manner and are not designed for long-term simulation. In order to really represent the available, long-term planning options, these models must become much more descriptive with regard to water-quality modeling.

System dynamics methodology may offer a means for overcoming this problem; descriptive and entailed models for simuating the long-term future may be developed. With the large data base available for the Occoquan basin, the possibilty exists for creating a powerful tool for developing management policies and for sensitivity analysis.

CHAPTER III

MODEL FORMULATION

This chapter begins with a description of basic ideas behind model development, along with a description of each significant group of pollutants. Following this, a brief introduction of system dynamics methodology and its application through the DYNAMO computer program is given, and the proposed model is described in DYNAMO terminology.

Basic Model Development

Before beginning, and keeping in mind that one of the objectives is that the model be as comprehensive as possible, it is necessary to answer four questions. Each question, with its corresponding answer, is stated in the following paragraphs:

1) *What pollutants should be simulated?* In general, there are seven pollutants, or groups of pollutants, that may cause problems and that are liable to be present in any given watershed. These are oxygen-demanding materials, pathogens, nitrogen compounds, phosphorus compounds, heavy metals, pes-

ticides, and sediment. In a comprehensive model, all of these should be simulated; however, in the proposed model it has been impossible to include them all. Dissolved oxygen, phosphorus compounds, and sediment are simulated in the current model. In addition, a eutrophication model is also included because of the effects of living organisms on water quality and because of their potential to serve as an indices of water quality.

2) What situations are critical? As mentioned in the introduction, there are four critical situations: concentrations in the water column during runoff events and during base flow events, buildup of concentrations in bottom sediments, and alterations of the physical nature of the channel due to changes in the sediment load. These four situations, inclusively, represent all problems which can occur. Therefore, the model is designed so that all four may be included into the steady state analysis.

3) How can the geography of the basin be taken into account? (i.e. zoning policies and the relative location of land development with respect to the stream and the water supply.), and 4) How can the dilution and self-purification potential of each segment of polluted stream, along with the buildup of pollutants in soils and stream sediments, be realistically modeled? To questions 3. and 4. there is only one answer:

the basin must be divided into a series of subbasins with associated stream reaches. This is the generally-accepted method for modeling basin-wide water pollution. It results in a tradeoff: the more subbasins, the higher the accuracy and, on the other hand, the higher the difficulty in developing and running the model. The fifteen Occoquan watershed subbasins, along with the fifteen stream stations located at each subbasin outlet, are shown in Figure 3. Descriptions of stream stations and stream channels are given in Table A-3, including Occoquan Monitoring Program designations for each stream station.

For the period of simulation, a period of one month was chosen because environmental conditions are relatively constant during each month, and yet the monthly period is long enough to permit long-term simulations without using too much computer time. During each month, all variables and rates of change, including such important variables as flow rates, are assumed constant, an assumption of fundamental importance.

A flow rate for simulation was also needed. In the proposed model, as will be seen later, all pollutant concentrations are dependent upon the rates of inflow to the channel from upstream as well as the rates of outflow downstream. Because these rates are written in terms of mass per month, only one flow is applicable: the monthly-average flow. Therefore,

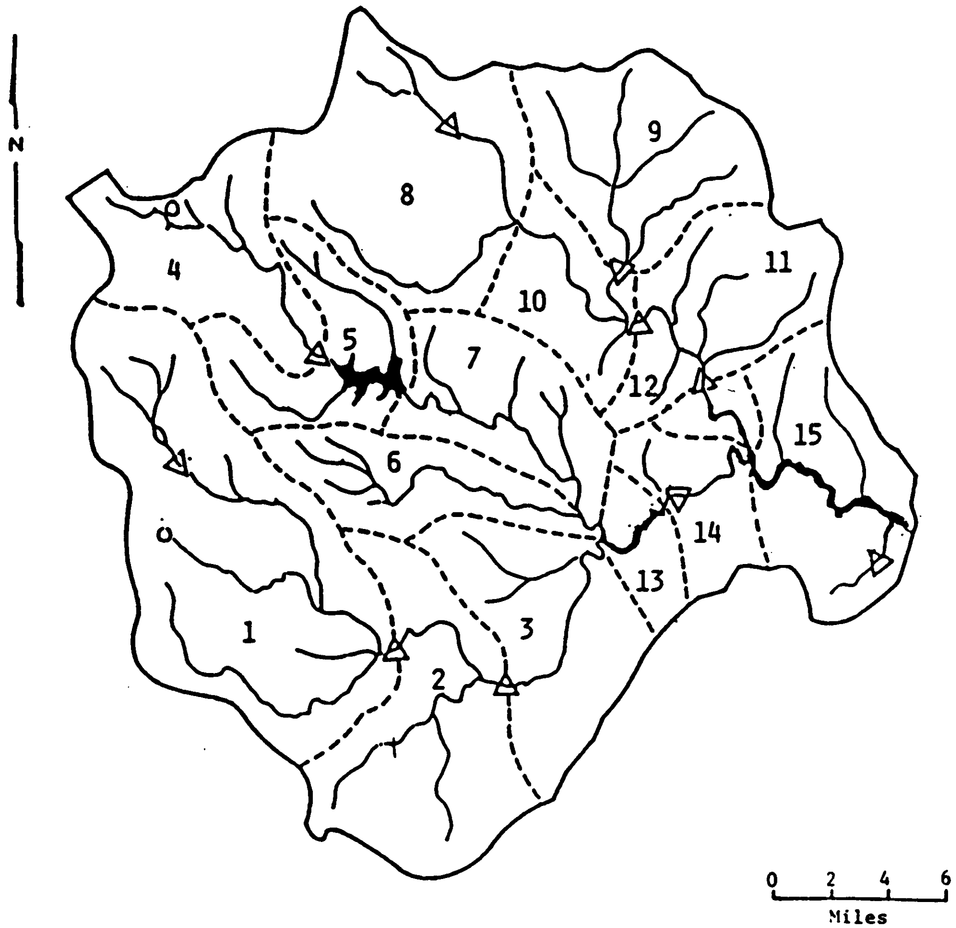

Figure 3. Subbasins for the Proposed Model.

in the original conceptualization, the monthly average flow was chosen for simulation, with the provision that simulation of pollutant concentrations during low-flow and runoff conditions may be added later.

Description of Pollutants to be Modeled

Descriptions of each group of pollutants to be modeled, including the reasons why it is significant, the factors governing its input to streams, the procedures normally used to model it, and the factors governing its transformation and fate, are presented in the following paragraphs.

DO

Dissolved Oxygen. Dissolved oxygen is important because many aquatic organisms require it for respiration, and yet it is easily depleted by the introduction of oxygen-demanding materials, especially organic matter and the ammonium ion, NH_4^+. Organic matter is oxygen-demanding because it serves as food for aerobic microorganisms, which in turn require oxygen for utilizing it. The ammonium ion serves as food for two genera of microorganisms, *Nitrosomonas* and *Nitrobacter*, which oxidize it for energy. These oxygen demands are expressed in terms of carbonaceous biochemical oxygen demand, CBOD, and nitrogenous oxygen demand, NBOD, both of which represent the equivalent mass of oxygen required per volume of polluted water.

Carbonaceous biochemical oxygen demand, which may be either dissolved or suspended, is added to streams through sanitary sewage, industrial wastes, and urban and agricultural runoff. Other, less defineable sources are excretion of aquatic organisms, death of aquatic organisms, and fallen leaves.

Exertion of CBOD is generally accepted as a first-order process, as defined by Streeter and Phelps in 1922 (9):

1. $$\frac{dL}{dt} = -K_1 L$$

where:

L is the BOD concentration (M/L^3)

K_1 is the first order rate constant

The corresponding equation for consumption of DO includes the effect of atmospheric reaeration, as the following equation shows:

2. $$\frac{dD}{dt} = K_1 L - K_a D$$

D is the oxygen deficit (M/L^3)

K_A is the first-order reaeration coefficient (T^{-1})

These equations are easily integrated and solved. As mentioned before, researchers have added many other significant factors in developing the expanded equations in use today.

The differential equation used in QUAL-II to describe the rate of change in dissolved oxygen is

$$3. \quad \frac{d}{dt}DO(X) = K_A\{DO_{SAT}(X) - DO(X)\} + (\alpha_3\mu_A - \alpha_4\mu_A)A - K_1 BOD - \frac{\sigma_B}{A_X} - \alpha_5\beta_1 NH_3 - \alpha_6\beta_2 NO_2$$

where:

$DO(X)$	is the dissolved oxygen concentration at location x (M/L^3)
K_A	is the reaeration coefficient (T^{-1})
$DO_{SAT}(X)$	is the temperature-dependent dissolved oxygen saturation at location x (M/L^3)
α_3	is the rate of oxygen production through photosynthesis per unit of algal biomass (M/M)
μ_A	is the algae growth rate $(M/L^3\text{-}T)$
α_4	is the rate of oxygen uptake from respiration per unit of algal biomass (M/M)
A	is the algal biomass concentration (M/L^3)

K_1 is the deoxygenation rate constant for CBOD (T^{-1})

BOD is the CBOD concentration (M/L^3)

σ_B is the benthal demand rate for DO (M/T-L)

A_X is the cross-sectional area of the stream (L^2)

α_5 is the rate of oxygen uptake per unit nitrification (M/M)

β_1 is the rate of oxidation of NH_4^+ to NO_2^- (T^{-1})

NH_4^+ is the ammonium ion concentration (M/L^3)

α_6 is the rate of oxygen uptake per unit of nitrite-nitrogen oxidation (M/M)

β_2 is the rate of oxidation of NO_2^- to NO_3^- (T^{-1})

NO_2 is the NO_2^- concentration (M/L^3)

Concerning their fate, CBOD and NBOD are nonconservative pollutants; they are completely removed from streams through biodegradation. Therefore, there is no long-term buildup.

PATHOGENS. Because pathogens are important regarding human health, and because many are spread through fecal matter, they have long been given high priority by environmental engineers. That the field was previously called Sanitary Engineering testifies to this fact. Fecal coliforms, being present in large numbers in fecal matter of all higher animals, and being relatively easy to test for, have been widely used as an indicator of possible pathenogenic contamination.

This wide use has resulted in coliform standards, both ambient and discharge, in many states. The purpose of modeling coliforms is to ensure that ambient standards are not violated.

For modeling coliforms in natural waters, QUAL II uses a first order analysis, the classic Chick's Law:

4. $$\frac{dC}{dt} = -K_C C$$

where:

C is the coliform concentration (number of organisms/L^3)

K_C is the first order death-rate constant (T^{-1})

Thus, like BOD, coliforms are nonconservative, and there is no concern about a long-term buildup.

Sanitary sewage is only one of several sources of coliforms in streams; like BOD, they are also contributed by diffuse sources. Runoff from cattle feedlots and pastures invariably contains high numbers of organisms, and urban runoff contains surprisingly large numbers. Thus, contrary to the general perception, coliforms are nonpoint-source pollutants as well as point source pollutants.

Sediment. Sediment, when produced in large quantities from erosion, has a strong impact on aquatic life. Excessive sedimentation gives the more-tolerant species an advantage, and when it occurs in quantities sufficient to change the nature of the stream bottom, it can disrupt the entire food chain through its effect on the primary producers and consumers.

As a pollutant, it is also important due to its adsorptive capacity for other pollutants, particularly ammonia, phosphorus, heavy metals, and pesticides. As mentioned before, these pollutants may be carried in runoff primarily with the soil. So concerning nonpoint source pollution, the importance of erosion cannot be overstated.

In addition, changing the sediment load to a stream can change the entire physical nature of the stream itself. The study of this phenomenon, called stream dynamics or geomorphology, concerns, among other things, changes in channel length, width, and meandering wavelength due to changes in the sediment load. Within a decade, significant changes may occur.

Besides its importance to water pollution, erosion adversely affects agriculture; it removes valuable topsoil which cannot be replaced easily. Thus, it may be an even worse problem in agriculture than in water pollution, concerning economic development and livelihood.

The generally-accepted and most widely-used means of modeling erosion due to storm runoff is the Modified Universal Soil Loss Equation, MUSLE:

5. $A = (M)(R)(K)(LS)(C)(P)$

where:

A is the annual yield of sediment to a first- or higher-order stream (tons/acre-year)

M is the sediment delivery ratio

R is the rainfall factor

K is the soil erodibility factor

LS is the length-slope factor

C is the vegetal cover factor

P is the conservation practice factor

This equation is a modification of the original Universal Soil Loss Equation (USLE) because it includes the sediment delivery ratio, M, which is used for estimating the deposition of sediment as it is transported from an upland field to a first-order stream. Thus, the USLE estimates erosion from an upland field, while the MUSLE estimates the yield of sediment to a first- or higher-order stream. These equations have later been modified to predict both monthly erosion and erosion due to a specific storm event.

Erosion occurs in the greatest amounts from denuded land, as expressed by the vegetal cover factor, C. In agricultural lands, conventional-tillaged land is a major source, while construction sites are critical in urban lands. Sediment loads from both urban and agricultural land are tremendous.

<ins>Phosphorus.</ins> Phosphorus is important because it is often the limiting nutrient for algal growth, not because it is toxic to humans or aquatic life. Profuse algal growth, such as that which has occurred in the Occoquan Reservoir, causes several problems:

1. Algae photosynthesize and respire during the day, producing more oxygen than they consume, but only respire at night, consuming DO. A large diurnal fluctuation in DO concentrations harmful to aquatic life can result.

2. The "collapse" of an algal bloom, which occurs when the algal concentrations get so large that the organisms die in large numbers, can cause a massive BOD loading and total utilization of DO.

3. Algal blooms are unsightly and sometimes odorous; they are detrimental to the recreational benefits of reservoirs.

4. Algae are difficult to remove at water treatment plants; they can clog sand filters, increasing the necessity for frequent backwashing. In addition, algae excrete organic compounds which cause taste-and-odor problems in water supplies.

Phosphorus exists in natural waters primarily in three forms: orthophosphate, polyphosphates, and organic phosphorus. Orthophosphate, composed of a phosphorus atom bonded to four oxygen atoms, is the most elemental dissolved form and is the most available biologically. Polyphosphates, the other predominant dissolved form, are essentially chains of orthophosphate bonded together. Depending on the pH of the ambient water, differing numbers of hydrogen atoms are bonded to the outer oxygen atoms in both dissolved forms. Organic phosphorus, on the other hand, exists in the form of phosphorus atoms within organic matter, either dissolved or suspended. It is released due to bacterial decay primarily in the form of orthophosphate.

In QUAL II, the two forms of dissolved phosphate are modeled together, and only the interaction of phosphorus and algae, plus a sink term, are considered. The equation is:

6. $$\frac{dP}{dt} = \alpha_2 A(\rho_A - \mu_A) + \frac{\sigma_2}{A_X}$$

where:

P	is the phosphate concentration (M/L^3)
α_2	is the fraction of algal biomass that is phosphorus
A	is the algae concentration (M/L^3)
ρ_A	is the loss rate of algae (T^{-1})
μ_A	is the growth rate of algae (T^{-1})
σ_2	is the benthal source rate for phosphorus $(M/T\text{-}L)$
A_X	is the cross-sectional stream area (L^2)

Phosphorus is contributed to streams from both point and nonpoint sources. Domestic sewage is a large source, typically containing all three forms. In addition, industrial wastes can sometimes contain phosphorus, and urban and agricultural runoff contains phosphorus originating from fertilizers, organic matter, feces, and automotive exhausts.

Nitrogen. Nitrogen, another essential inorganic nutrient for all life, exists in natural waters in the form of ammonia (NH_3), ammonium ion (NH_4^+), nitrite (NO_2-), nitrate (NO_3-), and organic nitrogen. It can cause the following problems:

1. It can be the limiting nutrient for algal growth.

2. The ammonium ion and free ammonia are toxic to fish.

3. The ammonium ion and free ammonia can exert an oxygen demand when nitrification occurs.

4. Nitrate can cause infantile methemoglobinemia, or "blue baby" syndrome.

As seen in the representation of the nitrogen cycle shown in Figure 4, nitrogen is subject to more transformations in natural waters than is phosphorus. As a consequence, modeling it is more involved; nitrification, dissimilatory denitrification, algal uptake, excretion and deamination (the process by which organic nitrogen is decomposed ammonia), must all be considered.

Nitrification is a process in which two genera of bacteria, Nitrosomaonas and Nitrobacter, gain energy by oxidizing ammonium ion to nitrite, then nitrite to nitrate, respec-

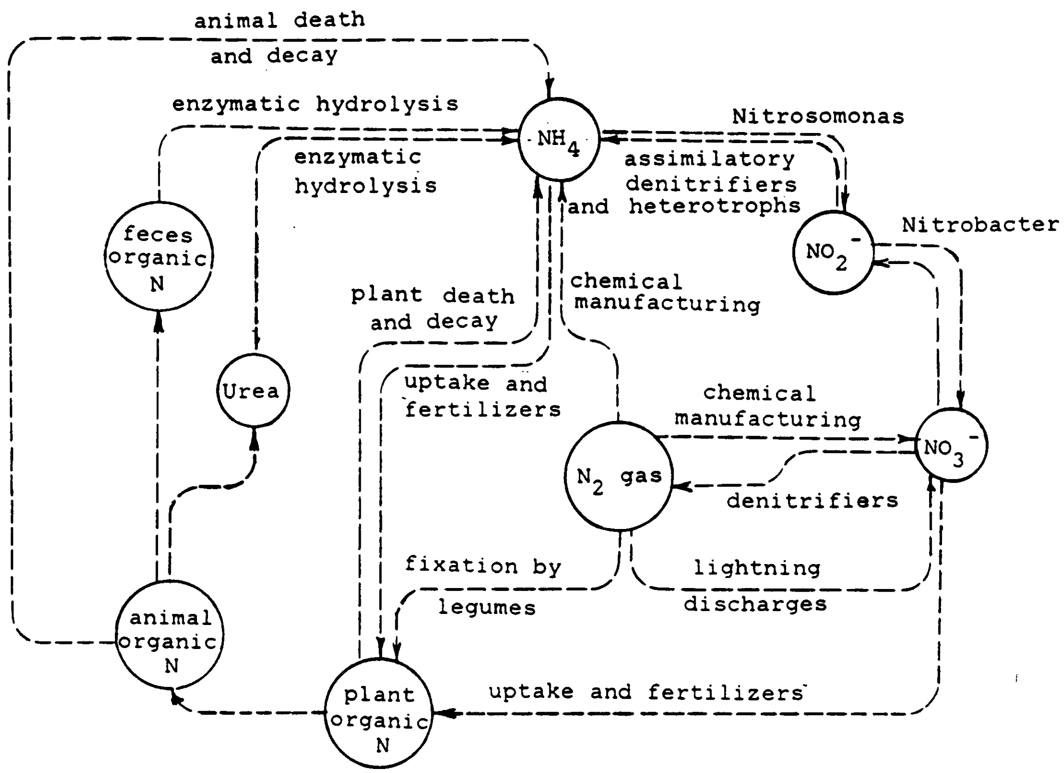

Figure 4. Nitrogen Cycle.

tively. On a stoichiometric basis, much more oxygen is required to do this than to oxidize an equivalent mass of organic matter. Although nitrification has often been considered a first-order process in natural waters, Krenkel and Novotny (71) and Tuffey *et al.* (72) disagreed: they claimed that it is more dependent on suitable habitat for the nitrifiers rather than the available concentration of ammonium ion. (Nitrifiers, being relatively slow-growing, generally require a longer time to multiply than many other bacteria.) Therefore, shallow streams with gravel and boulder substrate, which supply attached-growth sites, and slow-moving waters, such as lakes and estuaries, provide the best habitat. Thus, a zero order expression is presently considered to be the best representation. It is:

7. $$\frac{dNH_4^+}{dt} = -K_N$$

where:

K_N is the zero-order nitrification coefficient (M/L^3-T)

The zero-order nitrification rate coefficient is highly dependent on the stream in question and is best determined through field measurements.

However, QUAL II uses first order expressions For all nitrogen interactions. For deamination:

8. $$\frac{dNH_3}{dt} = \alpha_1 \rho_A A - \beta_1 NH_3 + \frac{\sigma_3}{A_X}$$

where:

NH_3	is the concentration of ammonia-nitrogen (M/L^{-3})
α_1	is the fraction of nonliving algal biomass resolubilized as ammonia-nitrogen by bacteria.
ρ_A	is the temperature-dependent specific-loss rate (T^{-1})
A	is the algal biomass concentration (M/L^3)
β_1	is the temperature-dependent rate of biological oxidation of NH_3 (T^{-1})
σ_3	is the benthic source rate for NH_3 (M/T-L)
A_X	is the average stream cross-sectional area at location x (L^2)

For nitrite-nitrogen, NO_2^-:

9. $$\frac{dNO_2^-}{dt} = \beta_1 NH_3 - \beta_2 NO_2^-$$

where:

NO_2^- is the concentration of nitrite-nitrogen (M/L^3)

β_1 is the rate of oxidation of NH_3 to NO_2^- (T^{-1})

β_2 is the rate of oxidation of NO_2^- to NO_3^- (T^{-1})

For nitrate-nitrogen, NO_3^-:

10. $$\frac{dNO_3^-}{dt} = \beta_2 NO_2^- - \alpha_1 \mu_A A$$

Denitrification is a process in which nitrate, instead of oxygen, is used by certain heterotrophic bacteria as an external electron acceptor. An anaerobic environment is required; thus, denitrification in natural waters generally occurs within stream bottom sediments or at the bottom of stratified lakes. Like nitrification, it is therefore dependent on the stream in question, and is generally considered a zero-order process.

Similarly to phosphorus, nitrogen is contributed to natural waters through domestic sewage, industrial wastes, and urban and agricultural runoff. Both nitrogen and phosphorus may be almost completely removed from domestic and industrial wastes through advanced wastewater treatment.

Heavy Metals. These are defined as all metals with a greater atomic weight than sodium, with the more prevalent water pollutants being iron, lead, zinc, copper, chromium, mercury, cadmium, and nickle. A variable group, they differ with respect to toxicity, transformation, and fate. Some, such as lead, mercury, cadmium, copper and chromium are highly toxic; others, such as iron and magnesium, are known to play important roles in natural chemical reactions. Obviously, in a comprehensive model, each should be simulated separately; however, modeling only one would allow some observation of trends significant to them all.

Heavy metal pollution comes primarily from nonpoint sources; although heavy metals are present in many industrial wastes, these are subject to National Pollution Discharge Elimination System (NPDES) permits and are mostly removed through wastewater treatment. Of the nonpoint sources, automobiles are considered a major cause, contributing lead, zinc and copper, and to a lesser extent, chromium, mercury, and nickle. In addition, many pesticides contain heavy metals, which are later introduced in streams through agricultural runoff.

Adsorption is the predominant mechanism of removal from the water column. One exception is mercury, which is known to bioaccumulate in aquatic organisms such as fish, making it a threat to humans. On the other hand, most of the others adsorb so strongly onto soil particles that they are never released again. If it were not for adsorption, there would indeed be trouble.

One equation simulating adsorption is the Freundlich isotherm:

11a. $$\frac{X}{M} = K(C)^{1/N}$$

where:

X/M is the equilibrium adsorbed concentration on solids (M/M)

K,N are dimensionless constants

C is the concentration in the water column (M/L^3)

As this expression estimates only the equilibrium concentrations, an expression for the kinetics of adsorption is needed. Krenkel and Novotny (73) have presented the following equation as an adequate representation:

11b. $$\frac{dS}{dt} = K(S_E - S)$$

where:

K is the adsorption kinetics coefficient (T^{-1})

S_E is the equilibrium adsorbed concentration on solids (M/M)

S is the actual adsorbed concentration (M/M)

Pesticides. Resulting primarily from the spraying of agricultural lands, pesticides -- and there are many of them -- are produced to streams in agricultural runoff. Highly toxic, some may exist in the environment for years, and many bioaccumulate through the food chain. Although many are similar to heavy metals in that they are strongly adsorbed to soil particles, there are also other means by which they are removed from the water column, including hydrolysis, photolysis, volatilization, biodegradation, and chemical degradation. Most often, the rates of these processes have been assumed to be first order, often with long half-lives.

In order to adequately simulate pesticide movement, one must consider several factors. Among these are buildup within the soil, transport into the soil by infiltration (this, by the way, is presently considered a permanent sink), rates of degradation, erosion, sediment transport, and rates of desorption. As previously mentioned, these models invariably are dynamic, hydrologic-simulation models, estimating the production to a stream by storm events from an upland field.

System dynamics and DYNAMO

The word "system" is difficult to define; rather, its meaning is better described by its attributes. A system is large, complex, and has hierarchial structure; it contains subsystems, components, and elements. It may be acted upon by extermal or internal inputs, and any resulting output depends on the "state" of the system and the "rules of transformation" within the system. In addition, a system must exist within an "environment" which gives the system its characteristics.

For the civil engineer, examples of important systems are towns, cities, states, river basins, etc. In system dynamics terminology, these are STEP systems: systems with social, technological, economic, and political interactions.

System dynamics, developed by Forrester (74), is a method for analyzing the behavior of dynamic STEP systems. It is to be used as a planning tool, to evaluate the effects of policy decisions on the system. It consists of three steps: 1)the formulation of a mental model in a verbal description, 2)the expression of this verbal description in a flow diagram, and 3)the conversion of this flow diagram in a set of simultaneous difference equations.

In many cases the resultant set of equations is too large for manual solution to be practical; a digital computer is necessary, and for this, the DYNAMO (DYNAmic MOdels) computer program was developed. Through the finite difference method, this program solves integral and differential equations. Through the continuous simulation, it solves systems of linear and nonlinear equations and allows inclusion of feedback relationships. Thus, it serves as a powerful tool for simulating the future.

The basis of DYNAMO is three simple types of equations: the level equation, which performs the function of the integral; the rate equation, which performs the function of the derivative; and the auxiliary equation, which performs intermediate calculations. Each variable -- whether it be a level, rate, or auxiliary -- is given a timescript denoting past, present, or future time, and each is held constant during every simulation time interval. In order to simulate into the future, each present or future value is calculated from past or present values of other variables respectively, and, thus, the model "churns" into the future.

In order to clarify this, and in order to enable the reader to understand the ideas behind equations presented later in this chapter, a description of each of the three types of equations is now given. The level equation takes the following form:

12a. L LEVEL.K=LEVEL.J+(DT)(RATE.JK)

where:

L	indicates a level equation
LEVEL.K	is the value of the level variable "LEVEL" at present time K
LEVEL.J	is the value of the level variable "LEVEL" at past time J
DT	is the magnitude of the time interval for simulation, as chosen by the modeler
RATE.JK	is the value of the rate variable "RATE" during the time interval from past time J to present time K

In more conventional, mathematical terms, the function of the level equation is expressed in the following equation:

12b. $$L_T = L_{T-1} + \frac{d}{dt}(R)$$

where:

L_T is the value of the level at present time T

L is the value of the level at past time T-1

R is the rate of change during the time interval dt

Thus, a "level" expresses a quantity, any quantity, whether it be mass, length, volume, or any other. Rates in DYNAMO, on the other hand, perform the function of R in Equation 12; they indicate the rate of change of the level over time. However, in DYNAMO, dt is a constant of finite length, and all rates are assumed constant during this time interval.

Rates may be equal to any function of other variables in the model, using the standard arithmetic operations: addition (+), subtraction (-), multiplication (*), exponentiation (**), and division (/). A typical rate equation follows:

13. R RATE.KL=(((LEVEL.K/AUX.K)-RATE1.JK)*RATE2.JK

where:

R	indicates a rate equation
RATE.KL	is the value of rate variable "RATE" during the time interval from present time K to future time L
AUX.K	is the value of the auxiliary variable "AUX" at present time K

RATE1.JK, RATE2.JK are the values of rate variables "RATE1" and "RATE2" during the previous time interval JK

Auxiliary equations, which perform intermediate computations, may also be any simple mathematical function of other variables. An example follows:

14. AUX.K=(AUX1.K/LEVEL.K)+RATE.JK

DYNAMO uses the following computation sequence: 1) levels at present time K are calculated from rates through past time interval JK, 2) auxiliary variables at present time K are calculated from other auxiliaries at present time K, levels at present time K, and/or rates at past time interval JK, 3) rates for the future time interval KL are calculated from other rates at past time interval JK, levels at present time K, and/or auxiliaries at present time K, 4) the time interval is shifted forward, changing all KL time intervals for rates to JK time intervals, and 5) the procedure is repeated. Note that the level equation requires a standard form, but that auxiliaries and rates may be calculated from any combination of other variables. The simulation, by itself, estimates the solution of integral and differential equations and solves simultaneous equations, both linear and nonlinear.

Another important DYNAMO function, the TABLE function, deserves explanation. It allows any rate or auxiliary variable to be related to any combination of other variables through a graph-type function. An example follows:

```
15.  A AUX1.K=TABLE(TNAME,AUX2.K,1,4,1)
     T TNAME=6,8,8,10
```

This simply means that as AUX2 varies from 1.0 to 4.0 by an increment of 1.0, AUX2 varies from 6.0 to 10.0., a relationship that is shown in more detail in Figure 5.

Approach to System Dynamics Formulation

As stated previously, the first step in development of a system dynamics model is the formulation of a mental model in a verbal description. This has already been done, as the model has already been given the following stated purpose: to simulate the effects of population growth and land development on water pollution, including all critical situations and all important pollutants.

The next step, the expression of this verbal description in a flow diagram, is shown in Figure 6. This is a general description of the model, showing how development has a positive effect on pollutant concentrations. Higher levels of

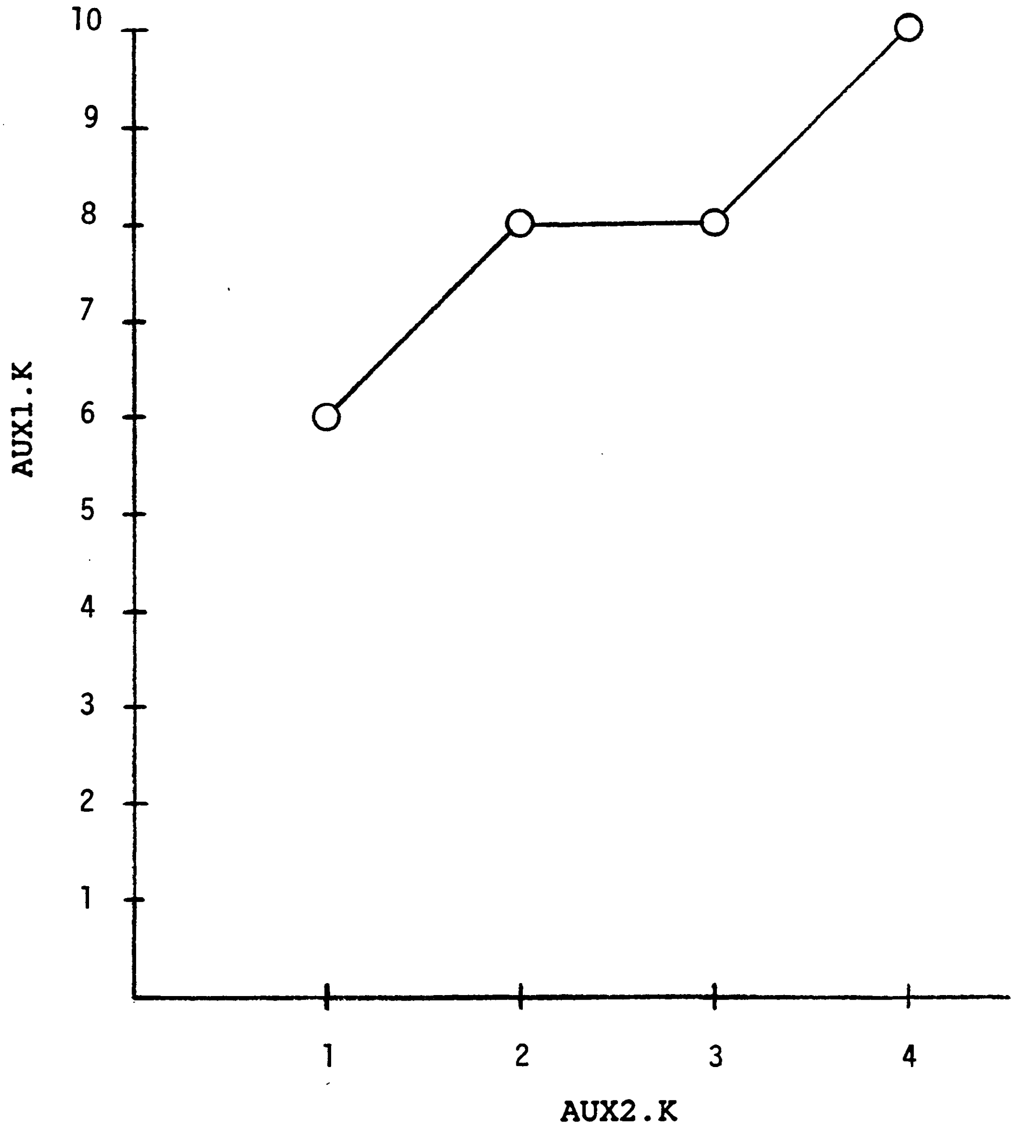

Figure 5. Illustration of the Table Function.

population, industries, and land use increase the rates of pollution generation, which in turn increase the pollutant levels in waterways.

However, this diagram leaves out many rates that affect pollutant concentrations, but that have no relation to population, industries, or land use. Examples are the rates of decay of each pollutant and the rates of inflow and outflow of pollutants from a stream channel. These are shown in the causal diagram in Figure 7, which is a representation of how the model simulates pollutant transport and transformation between the fifteen stream channels. Of course, the channels of headwater subbasins have no input from upstream, while those occurring below an intersection of major tributaries, such as subbasin 13 (Lake Jackson, 51ST10), have two or more rates of inflow from upstream.

Notice from Figure 7 that each pollutant level has a feedback relationship with its corresponding rates of decay and rate of outflow downstream. The level affects the rates, the rates affect the level. Because one effect is positive while the other is negative, these are called negative feedback loops: one variable acts to increase the other, which in turn acts to decrease the first. The result tends to produce an equilibrium.

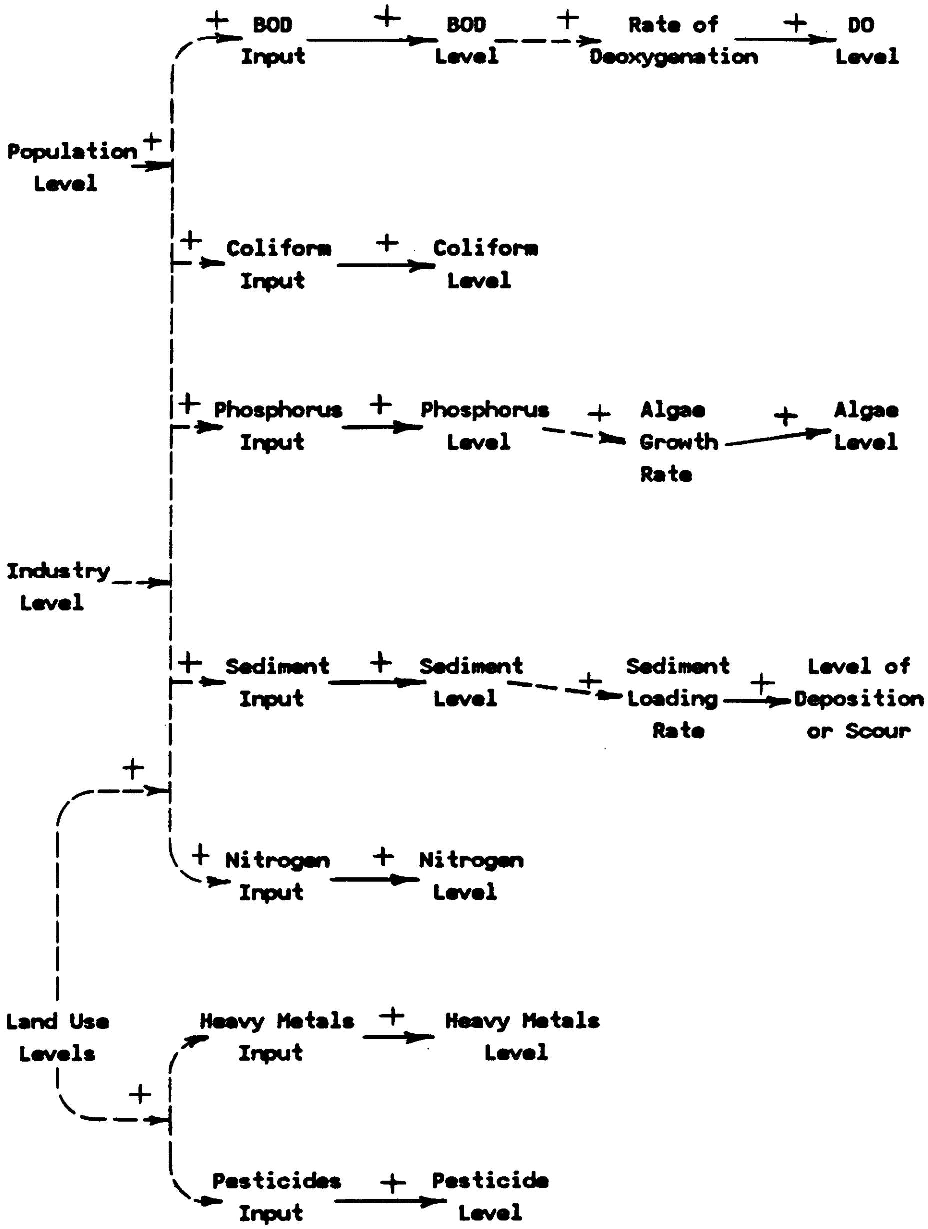

Figure 6. Causal Diagram Illustrating the Function of the Model. (A solid line indicates the effect of a level on a rate. A dashed line indicates all other effects.)

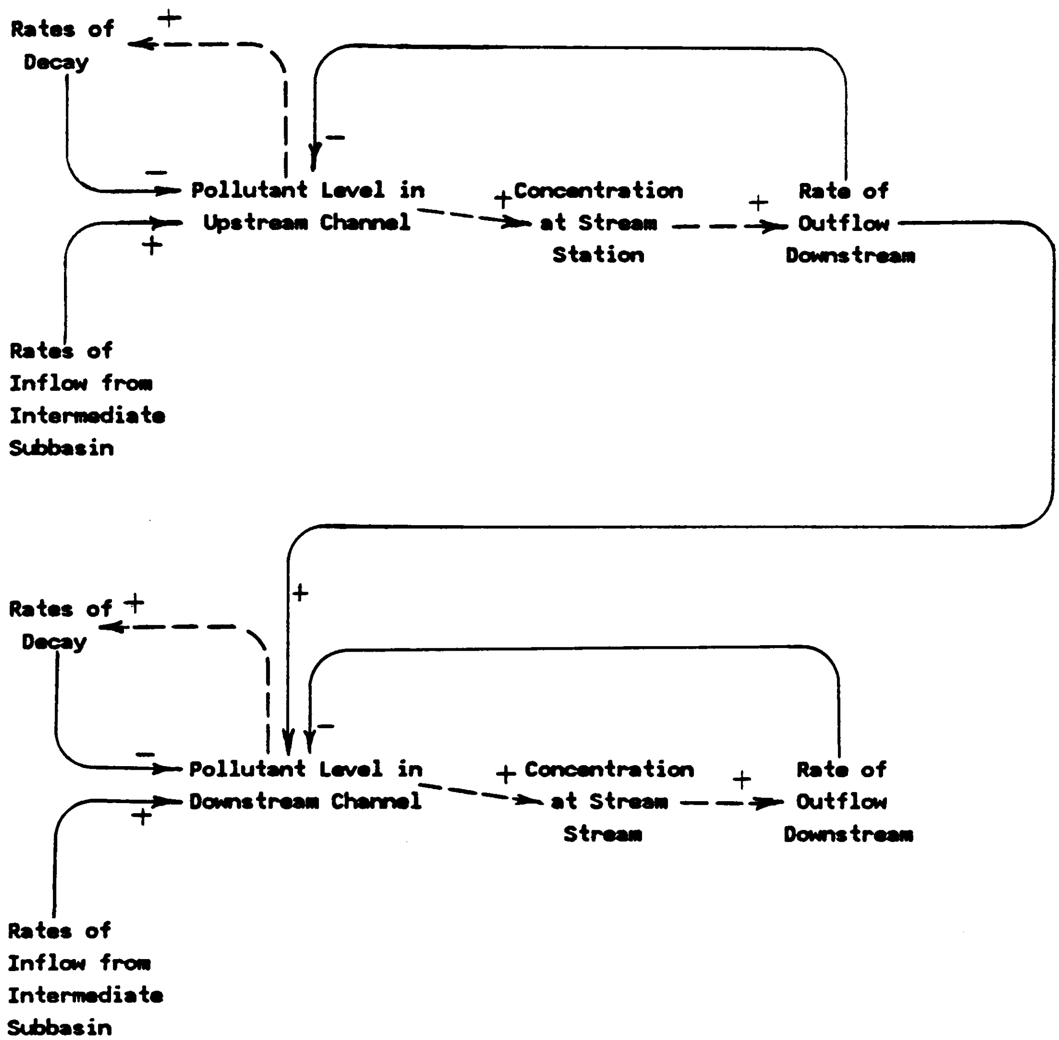

Figure 7. Illustration of Pollutant Transport and Transformation. (Solid line indicates the effect of a level on a rate. Dashed line indicates all other effects.)

The causal diagram in Figure 7 shows the modeling procedure used for each pollutant, whether it be in stream, channel, or lake. However, for stream channels it must be remembered that the entire system shown is valid for only one flow rate: either low flow, runoff flow, or average flow. In order to represent more than one flow, each level and rate must be duplicated. On the other hand, for lakes the only imporant flow rate is the monthly average flow, and no duplications are needed.

Development of System Dynamics Equations for Pollutant Modeling

Lake DO Submodel

This is the first submodel to be coded with DYNAMO. It is composed of two parts: a two-box stratification model and a one-box, winter-pool model. Stratification is assumed for eight months of the year, March through October, and winter pool is assumed for the remaining four months.

Stratified Lake DO Submodel: This part is based on the work of Bella (54), who is the first to have modeled the change in stratified lake DO with depth and time. Each lake is divided into two, completely-mixed, horizontal slices: one for the epilimnion and one for the hypolimnion. Within each slice the total rate of change of DO equals the sum of all DO import and removal rates for that slice.

Bella (54) expressed this concept in the following partial differential equation:

16. $$\frac{\delta(AC)}{\delta t}dz = F_I - F_0 + S$$

where:

A is the horizontal area of the lake slice (L^2)

C is the DO concentration within the slice (M/L^3)

F_I is the DO flux into the slice (M/T)

F_O is the DO flux out of the slice (M/T)

S is the sum of all DO sources and sinks acting on the slice (M/T)

Combining this equation with expressions for the flux of DO due to net water movement and the flux of DO due to velocity variations across horizontal areas and turbulent motions, Bella (54) came up with the following mass balance:

17. $$\frac{\delta(AC)}{\delta t}dz = \frac{\delta(D_V A\frac{\delta C}{\delta z})}{\delta z} - \frac{\delta(UAC)}{\delta z} + S$$

where:

D_V is the vertical dispersion coefficient (L^2/T) (Which is similar in concept to the longitudinal dispersion coefficient, D_L, which is often used in one-dimensional, stream models.)

U is the average flow velocity across the thermocline (L/T)

The DO sources and sinks term, S, was taken as:

18. $S = A(P - R)dz - Q_E C dz + Q_I C_I dz$

where:

P is the rate of DO change within the slice due to photosynthesis $(M/L^3\text{-}T)$

R is the rate of DO change within the slice due to respiration $(M/L^3\text{-}T)$

Q_E is the rate of water exported per unit of depth $(L^3/L\text{-}T)$

Q_I is the rate of water imported per unit of depth $(L^3/L\text{-}T)$

C_I is the DO concentration in imported water.

Reaeration is modeled as a boundary condition:

19. $F_H = A_H K_L (C_S - C_H)$

where:

F_H is the DO flux at the surface (M/T)

A_H is the area of the lake surface (L^2)

K_L is the surface-transfer coefficient (L/T)

C_S is the saturated DO concentration (M/L^3)

C_H is the DO concentration immediately below the lake surface (M/L7u.3)

Deoxygenation due to consumption of CBOD and NBOD were neglected.

From applying the model to Lake Sammamish, Washington, Bella (54) found that both vertical dispersion and hypolimnetic respiration have a greater influence on the hypolimnetic DO in the summer months than does either photosynthetic oxygenation or reaeration.

Simulating Bella's (54) concepts in DYNAMO equations results in much simpler mathematics. For Lake Manassas, subbasin 5, the mass of DO in the epilimnion is simulated in the following DYNAMO level equation:

```
20.  L MDOE.K(5)=MDOE.J(5)+(DT)(RTDOEP.JK(5)-IODEF.JK(5)
                                 +IDEP.JK(5)-RRDORE.JK(5)
                                 +RIDOLI.JK(5)+RODOEP.JK(5)
                                 +RREAEL.JK(5)-ODDCE.JK(5)
                                 -ODDSCE.JK(5)+ODDNE.JK(5))
```

where:

MDOE.K(5)	is the mass of DO in the epilimnion of lake 5 (M)
RTDOEP.JK(5)	is the rate of vertical transfer of DO across the thermocline of lake 5 due to diffusion (M/T)
IODEF.JK(5)	is the rate of vertical transfer of DO across the thermocline of lake 5 due to water movement (M/T)
IDEP.JK(5)	is the rate of production of DO in the epilimnion of lake 5 by photosynthesis (M/T)
RRDORE.JK(5)	is the rate of consumption of DO in the epilimnion of lake 5 by respiration (M/T)
RIDOLU.JK(5)	is the rate of inflow of dissolved oxygen to the epilimnion of lake 5 from upstream (M/T)
RODOEP.JK(5)	is the rate of outflow of dissolved oxygen from outlet structure from the epilimnion of lake 5 (M/T)
RREAEL.JK(5)	is the rate of increase in DO in the epilimnion of lake 5 due to atmospheric reaeration (M/T)
ODDCE.JK(5)	is the rate of consumption of DO in the epilinion of lake 5 due to decay of carbonaceous BOD (M/T)

ODDSCE.JK(5) is the rate of consumption of DO in the epilimnion of lake 5 due to decay of suspended organic matter (M/T)

ODDNE.JK(5) is the rate of consumption of DO in the epilimnion of lake 5 due to nitrification (M/T)

The number "5" within parenthesis after each variable indicates that this level equation uses the subscripting features of DYNAMO III. The model was developed using this subscripting feature, which considerably reduces the number of equations required. An example of the value of subscripting is the level equation for the masses of DO in the other lakes, lakes 12, 13, 14, and 15. Because there is no discontinuity in the ascending numbers of these lakes, and because, for each, the level equation for the mass of DO is similar, one level equation is all that is needed:

```
14.  L MDOE.K(R)=MDOE.J(R)+(DT)(RTDOEP.JK(R)-IODEF.JK(R)
                                  +IDEP.JK(R)-RRDORE.JK(R)
                                  +RIDOLI.JK(R)+RODOEP.JK(R)
                                  +RREAEL.JK(R)-ODDCE.JK(R)
                                  -ODDSCE.JK(R)+ODDNE.JK(R))
```

where:

R is a subscript that indicates 12, 13, 14, and 15

This equation simultaneously computes the mass of DO in lakes 12,13,14,and 15. (See subbasin map in Figure 3 and key for stream stations in Table A-3.)

The DO concentration in the epilimnion, as opposed to the mass, is computed by using an auxiliary equation to divide the mass by the volume of the epilimnion.

22. A CDOEP.K(5)=MDOE.K(5)/VOLE(5)

where:

CDOEP.K(5)	is the concentration of DO in the epilimnion of lake 5 (M/L^3)
MDOE.K(5)	is the mass of DO in the epilimnion of lake 5 (M)
VOLE(5)	is the volume of the epilimnion of lake 5 (L^3)

Each of the ten rates in the level equation for the mass of DO in the epilimnion is defined in DYNAMO as follows:

```
23.  R RTDOEP.KL(5)=VDCO.K(5)*ARTH.K(5)*(DOEP.K(5)
                    -DOHY.K(5))/THTH.K(5)
```

where:

RTDOEP.KL(5) is the rate of vertical transfer of DO across the thermocline of lake 5 due to diffusion (M/T)

VDCO.K(5) is the vertical dispersion coefficient for the thermocline of lake 5 (L^2/T)

ARTH.K(5) is the horizontal area of the thermocline of lake 5 (L^2)

DOEP.K(5) is the concentration of DO in the epilimnion of lake 5 (M/L^3)

DOHY.K(5) is the concentration of DO in the hypolimnion of lake 5 (M/L^3)

THTH.K(5) is the depth of the thermocline of lake 5 (L)

24. R IODEF.KL(5)=AVAT.K(5)*ARTH.K(5)*DOEP.(5)

where:

IODEF.JK(5) is the rate of vertical transfer of DO across the thermocline of lake 5 due to water movement (M/T)

AVAT.K(5) flow velocity across the thermocline of lake 5 (L/T)

25. R IDEP.KL(5)=GRAE.JK(5)*UDPAG

where:

IDEP.JK(5) is the rate of production of DO in the epilimnion of lake 5 by photosynthesis (M/T)

GRAE.JK(5) is the growth rate of algae in the epilimnion of lake 5 (M/T)

UDPAG is the ratio of DO produced per algal biomass produced (M/M)

26. R RRDORE.KL(5)=ALGE.K(5)*URALR.K+HZEP.K(5)*URHZR.K
+CZEP.K(5)*URCZR.K+HTEP.K(5)*URHTR.K

where:

RRDORE.JK(5) is the rate of consumption of DO in the epilimnion of lake 5 by respiration (M/T)

ALGE.K(5),HZEP.K(5),CZEP.K(5),HTEP.K(5)
are the biomasses of algae, herbivorous zooplankton, carnivorous zooplankton, and higher trophs, respectively, in the epilimnion of lake 5. (M)

URALR.K,URHZR.K,URCZR.K,URHTR.K
are the unit seasonal respiration rates of algae, herbivorous zooplankton, carnivorous zooplankton, and higher trophs, respectively.

27. R RIDOLI.KL(5)=(MFVO.K(5)-MFVO.K(4))*DOTR.K

where:

MFVO.K(5), MFVO.K(4) are monthly flow volumes at stream stations 4 and 5, respectively (L^3)

DOTR.K is the typical, seasonal DO concentration in small tributary streams (M/L^3)

28. R RODOEP.KL(5)=DOEP.K(5)*MFVO.K(5)*RRZM.K(5)

where:

RODOEP.KL(5) is the rate of outflow of dissolved oxygen from outlet structure from the epilimnion of lake 5 (M/T)

MFVO.K(5) is the monthly flow volume at stream station 5 (L^3)

RRZM.K(5) is the reservoir release zone multiplier for lake 5

(Note: All three reservoirs have the capacity for varying the level of withdrawal. A value of 1.0 for RRZM means complete withdrawal from the epilimnion. If the value is between 0.0 and 1.0, the subtracted fraction denotes the fraction of release from the hypolimnion.)

29. R RREAEL.KL(5)=ARLS(5)*LRCO.K(5)*(OSAT.K-DOEP.K(5))

where:

RREAEL.JK(5)	is the rate of increase in DO in the epilimnion of lake 5 due to atmospheric reaeration (M/T)
ARLS(5)	is the surface area of lake 5 (L^2)
LRCO.K(5)	is the seasonal surface aeration coefficient for lake 5 (L^2)
OSAT.K	is the saturation oxygen concentration (M/L^3)
DOEP.K(5)	is the DO concentration in the epilimnion of lake 5 (M/L^3)

30. R ODDCE.KL(5)=KDEP.K*BODE.K(5)

where:

ODDCE.JK(5)	is the rate of consumption of DO in the epilimnion of lake 5 due to decay of carbonaceous BOD (M/T)
KDEP.K	is the seasonal (temperature dependent) deoxygenation coefficient in upper lake waters (1/T)
BODE.K(5)	is the mass of dissolved BOD in the epilimnion of lake 5 (M)

31. R ODDSCE.KL(5)=DORGE.K(5)*KDSEP.K*BDGBR

where:

ODDSCE.JK(5)	is the rate of consumption of DO in the epilimnion of lake 5 due to decay of suspended dead organic matter(trypton)(M/T)
DORGE.K(5)	is the mass of trypton suspended in the epilimnion of lake 5 (M)
KDSEP.K	is the temperature-dependent deoxygenation rate constant for trypton in upper lake waters (1/T)
BDGBR	is the ratio of DO consumed per mass of trypton degraded (M/M)

32. R ODDNE.KL(5)=KN.K*NBODE.K(5)*VOLE.K(5)

where:

ODDNE.JK(5)	is the rate of consumption of DO in the epilimnion of lake 5 due to nitrification (M/T)
KN.K	is the seasonal (temperature dependent) nitrification coefficient in upper lake waters (1/T)

NBODE.K(5) is the nitrogenous BOD concentration in the epilimnion of lake 5 (M/L^3)

VOLE.K(5) is the volume of the epilimnion of lake 5 (L^3)

BOD in the epilimnion is also determined by a level equation:

```
33.  L BODE.K(5)=BODE.J(5)+(DT)(RICBI.JK(5)-ROCBE.JK(5)
                                -RBCBE.JK(5)+RVTTB.JK(5)
                                +RVDCB.JK(5))
```

where:

BODE.K(5) is the mass of dissolved BOD in the epilimnion of lake 5 (M)

RICBI.JK(5) is the rate of inflow of dissolved BOD into the epilimnion of lake 5 from runoff from intermediate subbasin 5 (M/T)

ROCBE.JK(5) is the rate of outflow of dissolved BOD from the epilimnion of lake 5 (M/T)

RBCBE.JK(5) is the rate of removal of dissolved BOD from the epilimnion of lake 5 due to biodegradation (M/T)

RVTTB.JK(5) is the rate of vertical transport of dissolved BOD across the thermocline of lake 5 due to water movement (M/T)

RVDCB.JK(5) is the rate of vertical transport of dissolved BOD across the thermocline of lake 5 due to dispersion (M/T)

For the hypolimnion, the level and rate equations are similar to those for the epilimnion; however, there are some differences. In the hypolimnion, there are no rates of reaeration, photosynthesis, respiration, or inflow of BOD from the intermediate subbasin. In addition, the temperature-dependent rate constants for the hypolimnion, in which colder temperatures prevail, are lower. And incoming BOD from upstream channels is assumed to enter the hypolimnion directly, bypassing the epilimnion.

Winter Pool Lake DO Submodel. Again, the level and rate equations are similar to those for the epilimnion. However, there is only one box, not two, so there is no stratification and no rates of transfer across a thermocline; the entire lake is assumed to be one completely-mixed reactor.

The assumption of complete-mix brings up an important point: Grizzard (75) stated that transport in the Occoquan Reservoir is plug flow rather than complete mix. However, this problem is partially solved through the choice of subbasins; the upper arms of Occoquan Reservoir, subbasins 12 and 14, account for a certain amount of plug-flow effect. (The more numerous the completely-mixed segments for modeling the lake, and the smaller they are, the more the model simulates plug flow.) Complete mix was assumed because it is the most convenient and it is not thought to affect the results significantly.

Modeling of BOD Input to Waterways

Significant sources of BOD to waterways are many, including domestic sewage, industrial waste, urban runoff, fallen leaves, death of autochthonous organisms, excretion by autochthonous organisms, and excretion by waterfowl. However, for modeling purposes, there exist little or no data on the latter four mechanisms. All are included in the model, but values for the latter four are to be found only through calibration.

The model simulates two types of BOD: dissolved and suspended. Of course, rate constants for degradation of dissolved BOD are much higher than those for suspended BOD. However, suspended BOD exerts significant effects, especially in lakes, because of the enormous quantity produced and the tendency for it to settle to the bottom of lakes.

Input of dissolved BOD from an intermediate subbasin to a channel, either stream or lake, is simulated by the following rate equation:

34. R RIDBS.KL(I)=SIDBS.K(I)+SIDBI.K(I)+SIDBUR.K(I)

where:

I	is a subscript indicating all subbasins, numbers 1 through 15
RIDBS.KL(I)	is the rate of inflow of dissolved BOD to channel I from intermediate subbasin I (M/T)
SIDBS.K(I)	is the unit rate of inflow of dissolved BOD to channel I from treated sewage discharges into subbasin I(M/T)
SIDBI.K(I)	is the unit rate of inflow of dissolved BOD to channel I from industrial discharges into subbasin I (M/T)
SIDBUR.K(I)	is the unit rate of inflow of dissolved BOD to channel I from urban runoff from intermediate subbasin I (M/T)

Each of these three unit rates is mathematically defined below:

35. A SIDBS.K(I)=POP.K(I)*LPCD*MEBS(I)*LOF

where:

POP.K(I)	is the population of subbasin I
LPCD	is the sewage input per person (L/person-T)
MEBS(I)	is the BOD concentration in treated domestic effluent from subbasin I (M/L)
LOF	is the location of outfall multiplier

36. A SIDBI.K(I)=NIND.K(I)*LPID*IEBS(I)

where:

NIND.K(I)	is the number of discharging industries in subbasin I
LPID	is the unit industrial discharge (L^3/industry-T)
IEBS(I)	is the BOD concentration in treated industrial effluent from subbasin I (M/L^3)

```
37.  A SIDUR.K(I)=FEST.K(I)*SDBRES.K+FIND.K(I)*SBDRID.K
                 +FLLR.K(I)*SDBRLR.K+FMDR.K(I)*SDBRMD.K
                 +FTH.K(I)*SDBRTH.K+FCOM.K(I)*SDBRCM.K
                 +FFOR.K(I)*SDBRFO.K+FPAS.K(I)*SDBRPS.K
                 +FINS.K(I)*SDBRIN.K+FCTG.K(I)*SDBRCT.K
```

where:

FEST.K(I)	is the fraction of estate land in subbasin I
FIND.K(I)	is the fraction of industrial land in subbasin I
FLLR.K(I)	is the fraction of large lot residential land in subbasin I
FMDR.K(I)	is the fraction of medium density residential land in subbasin I
FTH.K(I)	is the fraction of town house land in subbasin I
FCOM.K(I)	is the fraction of commercial land in subbasin I
FFOR.K(I)	is the fraction of forest land in subbasin I
FPAS.K(I)	is the fraction of pasture land in subbasin I
FINS.K(I)	is the fraction of institutional land in subbasin I
FCTG.K(I)	is the fraction of conventional-tillaged land in subbasin I
FMTG.K(I)	is the fraction of minimum-tillaged land in subbasin I
SDBR"LAND USE".K	is the monthly production of dissolved BOD in runoff from "land use" (M/L^2-T)

AREA(I) is the area of subbasin I (L^2)

The monthly unit rates of production of dissolved BOD for each type of land use, the "SDBR" variables, are taken from published stormwater monitoring data. (See Table A-27) They are written as TABLE equations, in which a monthly loading is assigned to each land use for each month of the year. The expression for estate land is as follows:

```
38.  A SDBRES.K=TABLE(TSDBES,MOD.K,0,11,1)
       T TSDBES=6.6,8.8,4,1.8,1.3,3.1,.4,1.8,5.7,7.9,2.2,.9
```

where:

SDBRES.K is the monthly dissolved BOD loading due to runoff from estate land (M/L^2-T)

MOD.K is the variable denoting the month of the year, 0 being January, 11 being December

Suspended BOD, on the other hand, is simulated through the separate level variables DORG, DORGE, DORGH, and DORGW, for the water column, epilimnion, hypolimnion, and winter pool, respectively. The DORG variables are defined as masses of dead organic matter (tripton), so a conversion factor is later used to convert them to terms of BOD for the DO model. The equation for DORGE is:

```
39.  L DORGE.K(R)=DORGE.J(R)+(DT)(RISDS.JK(R)+DRAE.JK(R)
                                  +DRHZE.JK(R)+DCZE.JK(R)
                                  +DRHTE.JK(R)-RWDDE.JK(R)
                                  -RBDDEP.JK(R)+RIDOU.JK(R)
                                  -RSDOE.JK(R)+RIDOGC.JK(R)
                                  +REXCWF.JK(R))
```

where:

DORGE.K(R) is the mass of trypton suspended in the epilimnion of lake R (M)

RISDS.JK(R) is the rate of inflow of trypton to lake R from intermediate subbasin R (M/T)

DRAE.JK(R),DRHZE.JK(R),DCZE.JK(R),DRHTE.JK(R) are the death rates of algae, herbivorous zooplankton, carnivorous zooplankton, and higher trophs, respectively, in the epilimnion of lake R (M/T)

RWDDE.JK(R) is the rate of outflow of trypton from the epilimnion of lake R (M/T)

RBDDEP.JK(R) is the rate of biodegradation of trypton in the epilimnion of lake R (M/T)

RIDOU.JK(R) is the rate of inflow of trypton to the epilimnion of lake R from upstream (M/T)

RSDOE.JK(R) is the rate of settling of trypton from the epilimnion of lake R (M/T)

RIDOGC.JK(R) is the rate of increase in trypton in channel R due to falling leaves from intermediate subbasin R (M/T)

REXCWF.JK(R) is the rate of increase in trypton in channel R due to excretion in subbasin R (M/T)

The expression for the utilization of DO due to the degradation of suspended trypton in the epilimnion takes the following form:

40. R ODDSCE.KL(R)=DORGE.K(R)*KDSEP.K*BDGBR

where:

ODDSCE.KL(R) is the rate of reduction of DO in the epilimnion of lake R due to the degradation of suspended trypton (M/T)

KDSEP.K is the temperature-dependent, deoxygenation coefficient for suspended BOD in epilimnions (1/T)

BDGBR is a conversion factor relating organic biomass to BOD (M/M)

Sediment and Stream Dynamics Submodel

This submodel is crucial for modeling the fate and transport of the adsorbable pollutants phosphorus, nitrogen, heavy metals, and pesticides, for it allows estimation of the buildup of these pollutants in aquatic sediments. As this is a significant process, any basin-wide, planning model which does not include it is an oversimplification.

What will be the net result of sedimentation? What fraction of the sediment particles, along with the pollutants adsorbed to them, will become deposited in the floodplain? What fractions will become buried under deposition in the streambed? In what sections of the stream will deposition occur? How will this deposition, or lack of it , affect the geometry and character of stream channels? How long will it take for reservoirs to fill in? The Sediment and Stream Dynamics Submodel is an attempt to answer these questions.

In order to answer them, the model must be capable of simulating two basic processes: the yield of eroded sediment to streams and, once the sediment arrives, its transport within streams. The proposed model is designed to accomplish both of these objectives.

The first process, the yield of sediment to streams, is simulated by the Modified Universal Soil Loss Equation (MUSLE), which is represented by several DYNAMO equations, the first of which follows:

```
41.  A SEDL.K(I)=SLEST.K(I)+SLLLR.K(I)+SLMDR.K(I)+SLTH.K(I)
                 +SLCOM.K(I)+SLIND.K(I)+SLINS.K(I)+SLFOR.K(I)
                 +SLPAS.K(I)+SLCTG.K(I)+SLMTG.K(I)
```

where:

SEDL.K(I)	is the monthly sediment yield to channel I from intermediate subbasin I (M)
SL"LAND USE".K(I)	is the monthly sediment yield to channel I from particular "land use" in subbasin I (M)

Each of these "SL" variables is defined similarly to the following equation, which is an MUSLE equation for estate land in each subbasin.

```
42.  A SLEST.K(I)=SDDR(I)*SEDP(I)*SEDE.K*SEDK(I)*SDLS(I)
                  *SCFEST*SSLM.K*FEST.K(I)*AREA(I)*FESTP(I)
```

where:

SDDR(I)	is the sediment delivery ratio typical of subbasin I
SEDP(I)	is the conservation practice factor for subbasin I
SEDE.K	is the rainfall factor for the Occoquan basin
SEDK(I)	is the soil erodibility factor for subbasin I
SDLS(I)	is the length slope factor for subbasin I
SCFEST	is the vegetal cover factor for estate land
SSLM.K	is the monthly sediment loss multiplier, which accounts for the seasonal variation in erosion
FEST.K(I)	is the fraction of land in subbasin I which is estate land
AREA(I)	is the area of subbasin I
FESTP(I)	is the typical fraction of estate land which is pervious (not paved or in buildings)

The second process, sediment transport within streams, has been more difficult to model. For one thing, it necessitates separating sediment into size categories; that is, sand, silt, clay, gravel, and boulders. (This is necessary anyway, because particle size has a great effect on adsorptive capacity, with smaller particles typically having much greater capacities.) Development of sediment transport and stream dynamics equations has been based on concepts and speculations given by West (76) and Schumm(77).

The underlying ideas are simple. In a "short term" geological time period, the three controls on stream behavior -- average discharge, average sediment load, and valley slope -- remain constant, and an equilibrium is in effect. When a control is changed, the equilibrium is disrupted, and the stream attempts to compensate for it. For example, if the bed load (load of heavier sediment particles) is increased, deposition occurs, the channel length is shortened, the channel slope is increased, and the bed load carrying capacity is increased until a new equilibrium condition exists. Decreasing the sediment load can cause scour instead of deposition, and the opposite effect results. A causal diagram illustrating how the model simulates stream dynamics is shown in Figure 8. As noted by Schumm(77) and Lyons and Beschta (78), significant changes in a stream channel may occur within ten years.

The submodel starts with the level variable SUMD, which represents the cumulative deposition into each stream channel:

```
43.  L SUMD.K(I)=SUMD.J(I)+(DT)(DPSA.JK(I)-RSSA.JK(I)
                                +DPGR.JK(I)-RSGR.JK(I)
                                +DPBL.JK(I)+RSBL.JK(I)
                                +DPC.JK(I)+RSCL.JK(I)
                                +DPSI.JK(I)-RSSI.JK(I))
```

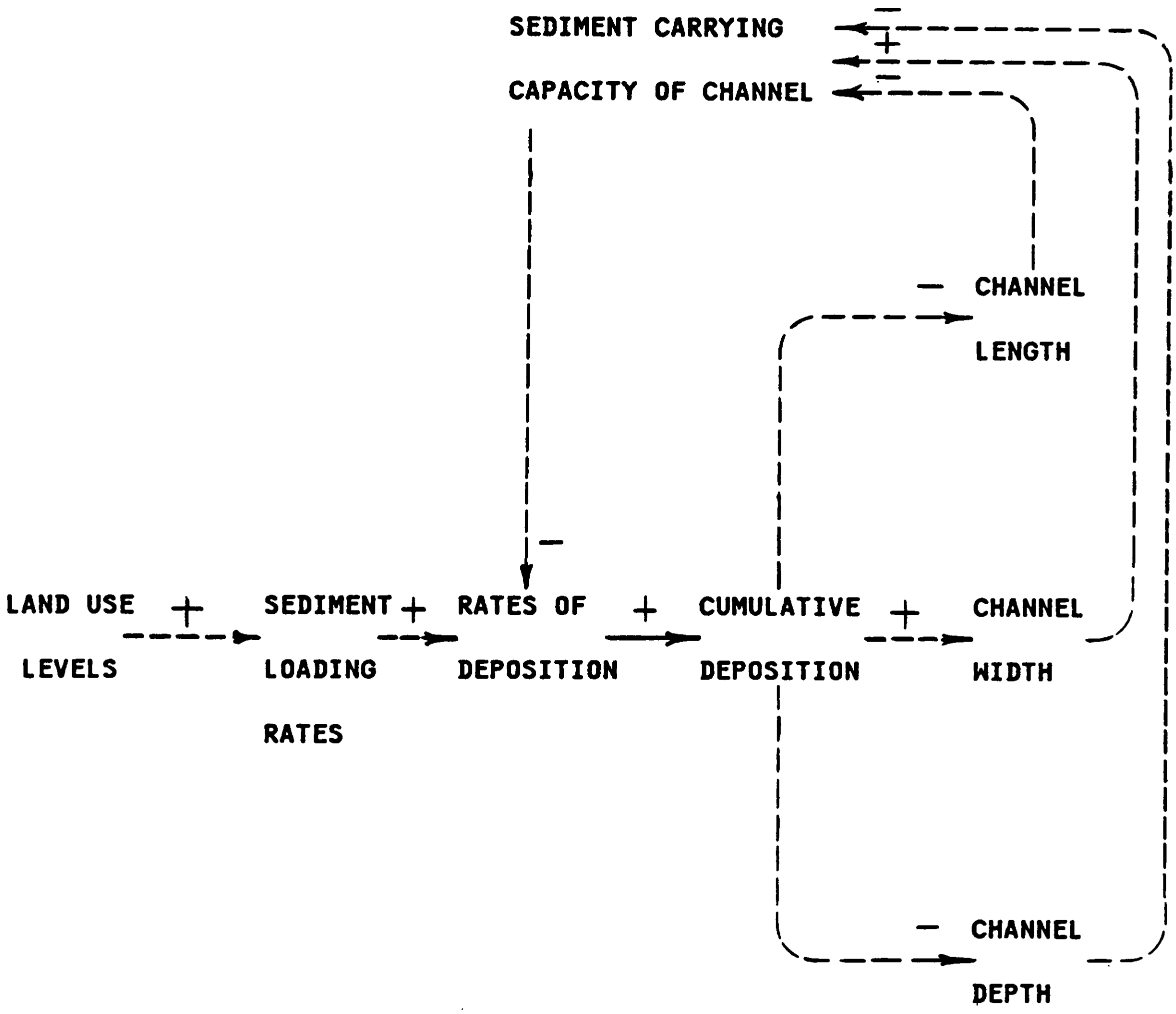

Figure 8. Illustration of the Stream Dynamics Submodel.

DPSA.JK(I),DPGR.JK(I),DPBL.JK(I),DPC.JK(I),DPSI.JK(I)
: are the rates of deposition of sand, gravel, boulders, clay, and silt, respectively, into channel I (M/T)

RSSA.JK(I),RSGR.JK(I),RSBL.JK(I),RSCL.JK(I),RSSI.JK(I)
: are the rates of scour of sand, gravel, boulders, clay, and silt, respectively, from channel I (M/T)

A typical equation for the rate of deposition of sand, DPSA, which is written in the same manner as the equations for deposition of gravel and boulders, but not the same as for clay and silt, is as follows:

```
44.  R DPSA.KL(2)=MAX(0,SALEI.K(2)+SALBE.K(2)-SATR.JK(2)
                 +SATR.JK(1)-SADV.JK(2)+RDSAGR.JK(2)
                 +RDSABL.JK(2))
```

where:

MAX — is a DYNAMO macro which chooses the higher of the values inside the parentheses, those separated by a comma

SALEI.K(2) — is the monthly sand load to channel 2 due to erosion from intermediate subbasin 2 (M)

SALBE.K(2) is the monthly sand load to channel 2 due to bank erosion from channel 2 (M)

SATR.JK(2),SATR.JK(1) are the monthly rates of transport of sand through channels 2 and 1, respectively (M/T)

SADV.JK(2) is the rate of deposition of sand to the floodplain of channel 2 (M/T)

RDSAGR.JK(2) is the rate of deposition of sand in channel 2 due to deposition of gravel in channel 2 (M/T)

RDSABL.JK(2) is the rate of deposition of sand in channel 2 due to deposition of boulders into channel 2 (M/T)

Silt and clay, being considerably smaller and lighter than sand, are not ordinarily deposited into stream channels. However, if there is any deposition of the larger bed load material, sand and clay are deposited too, and sand and clay are deposited in reservoirs. These phenomena are expressed in the following two equations for the rate of deposition of clay. For stream channels:

45. R DPC.KL(1)=DPSA.JK(1)*FCWS+DPGR.JK(1)*FCWGR+DPBL.JK(1)
*FCWBL

where:

DPC.KL(1) is the rate of deposition of clay in stream channel 1 (M/T)

DPSA.JK(1),DPGR.JK(1),DPBL.JK(1)

are the rates of deposition of sand, gravel, and boulders, respectively, in channel 1 (M/T)

FCWS is the ratio of clay deposited to sand deposited

FCWGR is the ratio of clay deposited to gravel deposited

FCWBL is the ratio of clay deposited to boulders deposited

For lakes:

46. R DPC.KL(5)=CLAY.K(5)-LCLTR.K(5)

where:

DPC.KL(5) is the rate of deposition of clay into lake 5 (M/T)

CLAY.K(5) is the total monthly clay loading to lake 5 (M)

LCLTR.K(5) is the monthly mass of clay transported through lake 5 (M)

The next variable to be described is SALEI.K(I), the monthly sand loading to a channel due to erosion from the intermediate subbasin. The equation for it is given below.

47. A SALEI.K(I)=SALEST.K(I)+SALLLR.K(I)+SALMDR.K(I)
+SALTH.K(I)+SALCOM.K(I)+SALIND.K(I)
+SALINS.K(I)+SALFOR.K(I)+SALPAS.K(I)
+SALCTG.K(I)+SALMTG.K(I)

where:

SAL"LAND USE".K(I) is the sand loading to channel I from "land use" land in intermediate subbasin I (M)

These "SAL" variables are all defined similarly to that for estate land, SALEST, which is given below:

48. A SALEST.K(I)=SLEST.K(I)*(FSANDA(I)*FESSHA.K+FSANDB(I)
*FESSHB.K+FSANDC(I)*FMTSHC.K)

where:

SLEST.K(I) is the monthly mass of sediment yielded to channel I due to erosion from estate land in subbasin I (M)

FSANDA(I),FSANDB(I),FSANDC(I)
are the fractions of sand, by weight, in soil of

the A,B, and C horizons, respectively, of soil of subbasin I.

FESSHA.K,FESSHB.K,FESSHC.K

are the fractions of estate-land soil erosion occuring from the A, B, and C horizons, respectively

The separation of erosion into that which occurs from different soil horizons is quite necessary for water quality modeling, as Ryden et al.(79) pointed out. They stated that essentially all the extractable phosphorus in soil occurs in the A horizon, being deposited there by fertilizers, and that eroded soil from the lower horizons can actually remove large amounts of dissolved phosphates through adsorption. In addition, Baker (80), in reviewing data on extractable soil phosphate in the Occoquan basin, agreed with the assessment that essentially all extractable phosphorus occurs in A horizons. Thus, from a water quality standpoint, all erosion is not bad. Ryden et al. (79) further pointed out that erosion from the various horizons occurs in differing proportions due to land use. For instance, in urban land a higher portion of erosion occurs from soils of the lower horizons, due partially to the action of bulldozers in mixing and overturning the soil.

The next variable in the equation for deposition of sand, SALBE.K(2), the monthly sand load to channel 2 due to bank erosion from channel 2, is defined in another auxiliary equation:

```
49.  A SALBE.K(I)=LCHA.K(I)*FSAV(I)*DEGB.JK(I)
```

where:

LCHA.K(2) is the length of channel 2 (L)

FSAV(2) is the fraction of sand in the floodplain soil of channel 2

DEGB.K(2) is the unit rate of bank erosion occurring from channel 2 (M/L-T)

DEGB.K(2) is defined by a TABLE equation:

```
51.  A DEGB.K(2)=TABLE(TDEGB2,SPOW.K(2),0,250,25)
       T TDEGB2=0/.1/.2/.3/.6/1/1.4/1.8/2.5/3.5/5
```

where:

SPOW.K(2) is the power of stream 2 (M/T)

The next variable is the rate of transport of sand through channel i, SATR.KL(I), another fundamental variable, which is defined as follows:

```
51.  R SATR.KL(I)=MIN(SAND.K(I)+CDSA.K(I),SACC.K(I))
```

where:

MIN	is a DYNAMO macro which chooses the lower of the values inside the parentheses, those separated by a comma
SAND.K(I)	is the total monthly sand loading to channel I (M)
CDSA.K(I)	is the cumulative deposition of sand into channel I (M)
SACC.K(I)	is the monthly sand carrying capacity of channel I (M/T)

SACC.K(I) is another variable dependent on the power of the stream, and it too is defined in a TABLE equation:

```
52.  A SACC.K(2)=TABLE(TSAC2,SPOW.K(2),0,200,25)
     T TSAC2=1510,1510,1510,1520,1530,1560,1540,2000,13500
```

where:

SPOW.K(2) is the power of stream 2 (M/T)

SPOW.K(2) as defined by West (76), is

53. A SPOW.K(2)=MMAF.K(2)*STSL.K(2)

where:

MMAF.K(2) is the monthly average flow (L^3/T)

STSL.K(2) is the slope of channel 2 (L/L)

The next variable to be defined in the sand deposition equation is SADV.KL(I), the rate of deposition of sand to the floodplain of channel I. As this variable is dependent on flooding, it is seasonal, and it is defined in a TABLE function as being dependent on the month of the year:

54. R SADV.KL(2)=TABLE(TSAD2,MOD.K,0,11,1)
T TSAD2=0,0,0,0,.2,.3,.4,.6,.8,1,1.2,3,4

where:

MOD.K is a variable denoting the current month of the year, 0 being January, 11 being December

To account for the deposition of sand along with deposition of gravel and boulders, the variables RDSAGR.JK(I) and RDSABL.JK(I) are included as the last variables in the equation for deposition of sand. They are defined in DYNAMO as follows:

```
55.  R RDSAGR.KL(I)=DPGR.JK(I)*FSAGR
```

and

```
56.  R RDSABL.KL(I)=DPBL.JK(I)*FSABL
```

where:

DPGR.JK(I),DPBL.JK(I)
: are the rates of deposition of gravel and boulders, respectively, in channel I

FSAGR,FSABL
: are the ratios of sand deposited to gravel and boulders deposited, respectively

The rate of scour of sand from subbasin I, RSSA.JK(I), is the opposite of the rate of deposition. It occurs only when deposition is zero, as expressed in the following equation:

```
57.  R RSSA.KL(I)=CLIP(0,DEGC.JK(I)*FSACB.K(I),TMDE.K(I),1)
```

where:

CLIP	is a DYNAMO macro which chooses the first value if the third is greater than the fourth, and chooses the second otherwise
DEGC.JK(I)	is the rate of scour of the bottom of channel I (M/T)
FSACB(I)	is the fraction of sand in the bottom layer of channel I
TMDE.K(I)	is the total monthly mass of deposition in channel I (M)

The scour of the channel bottom is another variable dependent on the power of the stream, as expressed in the following relationships:

```
58.  R DEGC.KL(2)=CLIP(0,UDEGC.K(2)*LCHA.K(2)*WIDC.K(2),
                    TMDE.K(2),10)
```

and

```
59.  A UDEGC.K(2)=TABLE(TDEGC,SPOW.K(2),0,250,25)
```

where:

DEGC.KL(2) is the rate of scour of the channel bottom (M/T)

UDEGC.K(2) is the unit rate of degradation of the bottom of channel 2 ($M/T-L^2$)

LCHA.K(2) is the length of clannel 2 (L)

WIDC.K(2) is the width of channel 2 (L)

TMDE.K(2) is the total monthly mass of deposition into channel 2 (M)

SPOW.K(2) is the power of stream 2 (M/T)

This concludes the feedback system of the rates of deposition and scour of sand.

The rates of deposition and scour are used to estimate, among other things, the change in physical dimensions of stream channels. Length, width, and depth are simulated as levels, as in the following equation:

60. L LCHA.K(I)=LCHA.J(I)+(DT)(RCCL.JK(I))

where:

LCHA.K(I) is the length of channel I (L)

RCCL.JK(I) is the rate of change of length of channel I (L/T)

RCCL.JK(I) is modeled as a TABLE function dependent on the rate of deposition or scour in the channel.

These channel dimensions are used to estimate the average velocity of flow in each stream channel, which is accomplished by Manning's equation. Each channel is assigned a Manning's roughness coefficient (n) for each month of the year, and the channel dimensions are used to determine the channel slope and hydraulic radius used in the equation.

Eutrophication Submodel

Even though they offer completely different environments, streams and lakes harbor somewhat similar biological communities. In both, the primary producers are algae, including diatoms, and aquatic macrophytes, and fish occupy one of the higher steps in the food chain.

However, there are also considerable differences. In streams, algae and diatoms colonize only the periphyten, the community attached to rocks; in lakes, they grow primarily suspended in the water, though they can colonize the bottom of the littoral zone (shallows where light penetrates to the bottom) as periphyton. Streams and lakes also harbor differing groups of primary consumers: macroinverebrates, or benthos, in streams and zooplankton in lakes. In addition, differing species of algae and fish are predominant in streams as opposed to lakes. In the proposed model, these differences are taken into account, as shown in Figure 9.

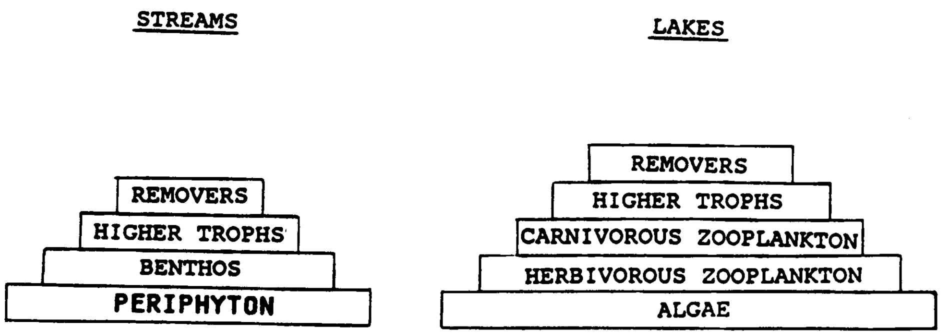

Figure 9. Trophic Levels Included in the Proposed Model.

Each trophic level is modeled as a level, as in the case of lake algae:

```
61.  L ALGE.K(5)=ALGE.K(5)+(DT)(GRAE.JK(5)-DRAE.JK(5)
                                      -RAWR.JK(5)-GHZE.JK(5))
```

where:

ALGE.K(5) is the biomass of algae in the epilimnion of lake 5 (M)

GRAE.JK(5) is the growth rate of algae in the epilimnion of lake 5 (M/T)

DRAE.JK(5) is the death rate of algae in the epilimnion of lake 5 (M/T)

RAWR.JK(5) is the rate of outflow of algae from the outlet structure of lake 5 (M/T)

GHZE.JK(5) is the rate of grazing of algae by herbivorous zooplankton in the epilimnion of lake 5 (M/T)

Monod kinetics are used to estimate growth rates of each trophic level, rates which are dependent on maximum seasonal growth rates and the amounts of food available. For algae in the epilimnion, the following applies:

```
62.  R GRAE.KL(5)=ALGE.K(5)*MUMA.K*(COHE.K(5)/AKSATP
                     +COHE.K(5))(LOGN((AKSATL+LIGHTI.K(5)
```

/((AKSATL+(LIGHTI.K(5)*EXP(-LEXTC
*AVSD.K(5))))))/(LEXTC*AVSD.K(5)))

where:

GRAE.JK(5)	is the growth rate of algae in the epilimnion of lake 5 (M/T)
ALGE.JK(5)	is the mass of algae suspended in the epilimnion of lake 5 (M)
MUMA.K	is the seasonal, maximum algae growth rate (T^{-1})
COHE.K(5)	is the concentration of orthophosphate in the epilimnion of lake 5 (M/L^3)
AKSATP	is the half-saturation constant for algal growth influenced by phosphorus (M/L^3)
AKSATL	is the half-saturation concentration for algal growth influenced by light (Langleys/time)
LIGHTI.K(5)	is the monthly light intensity to channel 5 (Langleys/T)
LEXTC	is the light extinction coefficient (L^{-1})
AVSD.K(5)	is the average depth of stream 5 (L)

In the Monod growth expressions for the other trophic levels, only the trophic level immediately below the one being considered is expressed, as was suggested by Loucks _et al._ (81).

The other three rates in the equation for ALGE.K(5) take the following forms:

63. DRAE.KL(5)=ESVA(5)*ARTH.K(5)*ALGE.K(5)

where:

DRAE.KL(5) is the death rate of algae suspended in the epilimnion of lake 5 (M/T)

ESVA(5) is the effective settling velocity of algae suspended in the epilimnion of lake 5 (L/T)

ARTH.K(5) is the horizontal area of the thermocline of lake 5 (L^2)

64. R RAWR.KL(5)=ALGE.K(5)*MFVO.K(5)*RRZM.K(5)/VOLE(5)

where:

RAWR.KL(5) is the rate of outflow of algae from the control structure of reservoir 5 (M/T)

MFVO.K(5) is the monthly flow volume at station 5 (L^3)

RRZM.K(5) is the reservoir release zone multiplier for reservoir 5

VOLE.K(5) is the volume of the epilimnion of lake 5 (L^3)

65. A GRAE.K(5)=HZEP.K(5)*UGHZW.K

where:

GRHE.K(5)	is the grazing rate of herbivorous zooplankton in the epilimnion of lake 5 (M/T)
HZEP.K(5)	is the mass of herbivorous zooplankton suspended in the epilimnion of lake 5 (M)
UGHZW.K	is the seasonal unit grazing rate of herbivorous zooplankton (M/M-T)

Phosphorus Submodel

The phosphorus submodel is more descriptive than previous basin-wide phosphorus models because it accounts for uptake by algae, release from detritus and excreta, and adsorption and buildup in aquatic sediments. Such descriptiveness enhances its potential for management decision-making and for recommendations for future data collecting and research.

Another aspect of the phosphorus submodel is its utilization of a "two box" lake phosphorus model similar to that given by Snodgrass and O'Melia (55), a model that is used for each of the three reservoirs in the basin. In many ways, the lake and stream phosphorus models used in the proposed model are similar, and yet they also differ.

The stream model, which is described first, is centered around the three forms of phosphorus normally found in streams: orthophosphate, polyphosphates, and organic phosphorus. Orthophosphate, being the most elemental of the dissolved forms, is the most available biologically. The concentration in the water column of a stream channel, like the concentration of DO in the epilimnion, is computed through an auxiliary equation:

66. A OHWC.K(I)=MOPW.K(I)/VOLW.K(I)

where:

OHWC.K(I) is the orthophosphate concentration in the water column of channel I (M/L^3)

MOPW.K(I) is the mass of orthophosphate in the water column of channel I (M)

VOLW.K(I) is the volume of water in channel I (L^3)

In turn, the mass of orthophosphate in the water column is defined by a level equation:

```
67.  L MOPW.K(P)=MOPW.J(P)+(DT)(RIOI.JK(P)+RIOU.JK(P)
                                  -ROOWC.JK(P)+RACL.JK(P)
                                  +RASI.JK(P)+AOCLBR.JK(P)
                                  +AOSIBR.JK(P)+AOSABR.JK(P)
```

-RAUP.JK(P)+RHPP.JK(P)

+RROD.JK(P)+RROHEB.JK(P))

where:

P	is a subscript denoting channels 1, 2, 3, and 4
MOPW.K(P)	is the mass of dissolved orthophosphate in the water column of channel P (M)
RIOI.JK(P)	is the rate of input of orthophosphate to channel P from runoff from intermediate subbasin P (M/T)
RIOU.JK(P)	is the rate of inflow of orthophosphate to channel P from upstream (M/T)
ROOWC.JK(P)	is the rate of outflow of orthophosphate from channel P (M/T)
RACL.JK(P)	is the rate of adsorption/desorption of orthophosphate to/from clay suspended in channel P (M/T)
RASI.JK(P)	is the rate of adsorption/desorption of orthophosphate to/from silt suspended in channel P (M/T)
AOCLBR.JK(P)	is the rate of adsorption/desorption of orthophosphate to/from clay in the bottom exchange layer of channel P (M/T)

AOSIBR.JK(P) is the rate of adsorption/desorption of orthophosphate to/from silt in the bottom exchange layer of channel P (M/T)

AOSABR.JK(P) is the rate of adsorption/desorption of orthophosphate to/from sand in the bottom exchange layer of channel P (M/T)

RAUP.JK(P) is the rate of uptake of orthophosphate by algae in channel P (M/T)

RHPP.JK(P) is the rate of hydrolysis of polyphosphates to orthophosphate in channel P (M/T)

RROD.JK(P) is the rate of release of orthophosphate from suspended trypton in channel P (M/T)

RROHEB.JK(P) is the rate of input of orthophosphate due to excretion in channel P (M/T)

The rate of inflow of orthophosphate from the intermediate subbasin, RIOI.JK(P), is one of the more important of these rates, and as such, it is described in some detail. The equation takes the following form:

```
68.  R RIOI.KL(I)=OEST.K(I)+OLLR.K(I)+OMDR.K(I)+OTH.K(I)
                 +OCOM.K(I)+OIND.K(I)+OINS.K(I)+OMTG.K(I)
                 +OCTG.K(I)+OFOR.K(I)+OPAS.K(I)+OIRS.K(I)
                 +OITS.K(I)
```

where:

O"LAND USE".K(I) is the monthly production of orthophosphate from runoff from "land use" in subbasin I (M/T)

In turn, these variables are defined similarly to the following equation, that for estate land:

69. A OEST.K(I)=SOEST.K*FEST.K(I)*AREA(I)

where:

OEST.K(I)	is the monthly production of orthophosphate from runoff from estate land in subbasin I (M/T)
SOEST.K	is the seasonal unit production of orthophosphate from runoff from estate lands (M/L^2-T)
FEST.K(I)	is the fraction of estate land in subbasin I
AREA(I)	is the area of subbasin I (L^2)

The rates of adsorption/desorption to the different soil sizes also exert significant effects on orthophosphate concentrations in stream channels. The rates of adsorption/desorption to suspended clay, such as in the following, are one example.

70. R RACL.KL(P)=KACLO*(EQOC.K(P)-OACL.K(P))*CLWC.K(P)

where:

RACL.KL(P) is the rate of adsorption/desorption of orthophosphate to clay suspended in stream channel P (M/T)

KACLO is the adsorption kinetics coefficient for clay (T^{-1})

EQOC.K(P) is the equilibrium adsorbed concentration of orthophosphate to clay in channel P (M/M)

OACL.K(P) is the adsorbed concentration of orthophosphate to clay transported to stream channel P (M/M)

CLWC.K(P) is the mass of clay suspended in the water column of stream channel P (M)

Krenkel and Novotny (73) stated that this equation is a reasonable estimate of the kinetics of adsorption.

The equilibrium concentration on clay, EQOC.K(P), is defined by the Freundlich isotherm as follows:

71. A EQOC.K(P)=KOCLAY*OHWC.K(P)**(1/NFOCL)

where:

KOCLAY,NFOCL	are Freundlich isotherm constants
OHWC.K(P)	is the concentration of orthophosphate in the water column of channel P (M/L^2)

The actual adsorbed content, on the other hand, is defined as a weighted average of contents on all the clay yielded to the channel, as in the following example:

```
72.  A OACL.K(2)=(CLLEI.K(2)*WAOC.K(2)+CLTR.JK(1)*LFOCL.K(1))
                  /CLAY.K(2)
```

where:

OACL.K(2)	is the adsorbed concentration of orthophosphate to clay transported to stream channel 2 (M/M)
CLLEI.K(2)	is the mass of clay yielded to channel 2 due to erosion from intermediate subbasin 2 (M)
WAOC.K(2)	is the weighted-average, adsorbed orthophosphate concentration on clay eroded from intermediate subbasin 2 (M)
CLTR.JK(1)	is the rate of transport of clay through channel 1 (M/T)
LFOCL.K(1)	is the adsorbed concentration of orthophosphate on clay at stream station 1 (M/M)

CLAY.K(2) is the mass of clay yielded to channel 2 during the month (M)

To determine WAOC.K(I), one must have estimates of the extractable orthophosphate concentrations on soils in all types of land use in each subbasin, and weight them according to clay eroded from each land use in each subbasin. In the proposed model, this is accomplished through an auxiliary equation:

```
73.  A WAOC.K(I)=(CLLFOR.K(I)*COHCFO.K(I)+CLLCTG.K(I)
                 *COHCCT.K(I)+CLLMTG.K(I)*COHCMT.K(I)
                 +CLLEST.K(I)*COHCES.K(I)+CLLLLR.K(I)
                 *COHCLR.K(I)+CLLMDR.K(I)*COHCMD.K(I)
                 +CLLTH.K(I)*COHCTH.K(I)+CLLCOM.K(I)
                 *COHCCM.K(I)+CLLIND.K(I)*COHCID.K(I)
                 +CLLINS.K(I)*COHCIS.K(I))/CLLEI.K(I)
```

where:

CLL"LAND USE".K(I) is the mass of clay eroded during the month from A horizons of "land use" in subbasin i (M)

COHC"LAND USE".K(I) is the content of orthophosphate in soil of A horizons in "land use" in subbasin I (M/M)

CLLEI.K(I) is the monthly mass of clay yeilded to channel I erosion from intermediate subbasin I (M)

The adsorbed concentrations in upland soil of each land use are also variable, and they are simulated with level equations, as in the following example:

74. L OTES.K(I)=OTES.J(I)+(DT)(MRAOES.JK(I))

where:

OTES.K(I) is the adsorbed content of orthophosphate on A horizon soil in estate land in subbasin I (M/M)

MRAOES.K(I) is the rate of change of content normally expected in estate land (M/M-T)

As was shown in the level equation for the mass of orthophosphate in streams, equation 67, rates of adsorption/desorption to sediment in the bottom exchange layer are also computed. For this computation, some idea of the mass of bed exchange material in channels is needed. As before, this estimate is provided by level equations, such as the following:

```
75.  L MSAB.K(I)=MSAB.J(I)+(DT)(DPSA.JK(I)-RBSAD.JK(I)
                                -RSSA.JK(I)+RUSAS.JK(I)
                                +RCSACL.JK(I)+RCSACW.JK(I))
```

where:

MSAB.K(I)	is the mass of sand in the bed exchange layer of channel I (M)
DPSA.JK(I)	is the rate of deposition of sand into channel I (M/T)
RBSAD.JK(I)	is the rate of burial of sand in deposition in channel I (M/T)
RSSA.JK(I)	is the rate of scour of sand from channel I (M/T)
RUSAS.JK(I)	is the rate of uncovering of sand due to scour in channel I (M/T)
RCSACL.JK(I)	is the rate of change in sand in the bed exchange layer of channel I due to change in channel length (M/T)

RCSACW.JK(I) is the rate of change of sand in the bed exchange layer of channel I due to change in channel width (M/T)

Besides masses of sand, masses of each of the other sediment types -- silt, clay, gravel, and boulders -- are computed similarly, with some exceptions. As mentioned before, silt and clay are deposited in stream channels only along with heavier material, making the silt- and clay-carrying capacities of each channel large indeed. Gravel and boulders, on the other hand, are not deposited in floodplains as silt, clay, and sand are. Also, the silt and sand carrying capacity of each reservoir depends on the concentration of suspended silt and clay in the lake water, variables that are simulated by a level equation:

```
76.  L MCLEP.K(5)=MCLEP.J(5)+(DT)(RICLEU.JK(5)+RTCLTW.JK(5)
                                    -ROCLEP.JK(5)+RSCLE.JK(5))
```

where:

MCLEP.K(5) is the mass of clay suspended in the epilimnion of lake 5 (M)

RICLEU.JK(5) is the rate of inflow of clay to the epilimnion of lake 5 from upstream (M/T)

RTCLTW.JK(5) is the rate of transfer of clay across the thermocline of lake 5 due to water movement (M/T)

ROCLEP.JK(5) is the rate of outflow of clay from the epilimnion of lake 5 (M/T)

RSCLE.JK(5) is the rate of settling of clay from the epilimnion of lake 5 (M/T)

Polyphosphates, which constitute most of the rest of the dissolved phosphate in Occoquan basin waters, are also simulated through a level equation:

77. L MPPWR.K(P)=MPPWR.J(P)+(DT)(RIPP.JK(P)-RWPP.JK(P)
+RIPPU.JK(P)+RHPP.JK(P))

where:

MPPWR.K(P) is the mass of dissolved polyphosphates in the water column of channel P (M)

RIPP.JK(P) is the rate of inflow of polyphosphates to stream channel P from intermediate subbasin P (M/T)

RWPP.JK(P) is the rate of outflow of polyphosphates from stream channel P (M/T)

RIPPU.JK(P) is the rate of inflow of polyphosphates to channel P from upstream (M/T)

RHPP.JKJ(P) is the rate of hydrolysis of polyphosphates to orthophosphate in channel P (M/T)

Polyphosphates are used in large quantities as builders in detergents; therefore, their inflow is dependent on sewage flow, both treated and untreated, and on laws regulating the use of phosphate detergents.

One aspect of the proposed analysis is that one may estimate the accumulation of phosphorus in each stream channel due to deposition, as expressed in the following equation:

78. L CDEPO.K(I)=CDEPO.J(I)+(DT)(RDEPO.JK(I))

where:

CDEPO.K(I) is the cumulative deposition of adsorbed orthophosphate into channel I (M)

RDEPO.JK(I) is the rate of deposition of adsorbed orthophosphate into channel I (M/T)

RDEPO.KL(I) is defined as follows:

79. R RDEPO.KL(I)=DPSA.JK(I)*FOSA.K(I)+DPSI.JK(I)
*FOSI.JK(I)+DPC.K(I)*FOCL.K(I)

where:

DPSA.JK(I),DPSI.JK(I),DPC.K(I)
are the rates of deposition of sand, silt, and clay into channel I (M/T)

FOSA.K(I),FOSI.K(I),FOCL.K(I)
are the adsorbed contents of orthophosphate on sand, silt, and clay at stream station i (M/M)

Lake Phosphorus Submodel

As mentioned before, the lake phosphorus submodel is composed of a one-box, winter pool and a two-box, stratified, summer pool, just as the Lake DO Submodel is. Thus, it would be repetitious to describe it in detail. However, it seems justifiable to present the equation for orthophosphate in the epilimnion:

80. L MOHE.K(5)=MOHE.J(5)+(DT)(ROHI.JK(5)-ROHO.JK(5)
-RIPA.JK(5)+RHPPEP.JK(5)
+RDOT.JK(5)+RTWM.JK(5)
+RAOCLE.JK(5)+RAOSIE.JK(5))

where:

MOHE.K(5)	is the mass of dissolved orthophosphate in the epilimnion of lake 5 (M)
ROHI.JK(5)	is the rate of inflow of orthophosphate to the epilimnion of lake 5 from intermediate subbasin 5 (M/T)
ROHO.JK(5)	is the rate of outflow of orthophosphate from the epilimnion of lake 5 (M/T)
RIPA.JK(5)	is the rate of uptake of orthophosphate by algae in the epilimnion of lake I (M/T)
RHPPEP.JK(5)	is the rate of hydrolysis of polyphosphates into orthophosphate in the epilimnion of lake 5 (M/T)
RDOT.JK(5)	is the rate of diffusion of orthophosphate across the thermocline of lake 5 (M/T)
RTWM.JK(5)	is the rate of transfer of orthophosphate across the thermocline of lake 5 due to water movement (M/T)
RAOCLE.JK(5)	is the rate of adsorption/desorption of orthophosphate to clay suspended in the epilimnion of lake 5 (M/T)
RAOSIE.JK(5)	is the rate of adsorption/desorption of orthophosphate to silt suspended in the epilimnion of lake 5 (M/T)

The equation for orthophosphate in the hypolimnion is similar, but it has additional expressions for adsorption/desorption to the bottom exchange layer and inflow from upstream, and there is no algal uptake term. For the winter pool, all of these processes are combined, just as in the Lake DO Submodel.

Innovative Features of the Proposed Model

The proposed model, as it has been described in the previous sections, is innovative for several reasons:

1. It is the first application of system dynamics methodology to water-quality modeling, wherein the simulation incorporates integral equations, differential equations, and systems of linear and nonlinear equations.

2. Rather than including new equations for water-quality modeling, the model combines the work of a variety or researchers, merely converting them to system dynamics equations and adding them together. This combination has created a highly descriptive model for long term planning on a basin-wide scale.

3. This is the first basin-wide planning model that considers such factors as phosphorus contents and particle-size

distributions in upland soils, phosphorus contents in stream-bottom sediments, stream-bottom characteristics, periphyton densities, and channel and floodplain dimensions. It is also the first attempt to gather such information for use in a water-quality model.

4. The system dynamics submodel, designed for simulating changes in the physical dimensions of stream channels due to changes in sediment loads, written especially for this model, is an innovation.

5. The model is designed to fulfill the need for a "strategic" model, capable of analyzing zoning, abatement, and best management policies together, capable of aiding in the development of a strategy for watershed development.

CHAPTER IV

CALIBRATION

A necessary step in development of any model, calibration is the process of fitting output to match observed data. In order to calibrate a model, one must first gather input data, as required, and insert it into the model; then one can adjust parameters so that observed data are matched. Therefore this chapter is divided into two sections: Input Data and Calibration.

Input Data

Input data exist in a myriad of sources, and so far, certainly all have not been found and utilized. However, much of it was found, including measurements made in the Occoquan basin itself. Approximately two hundred pages of calculations were performed to process these data, as described in this section. The large amount of data available and the prospects of even more yet uncovered are exciting features of this project, because few modelers have this much data available for refinement of their models.

A brief description of the availibility of data follows:

1. Soil Particle Distributions. Information is available in County Soil Surveys developed jointly by the U.S. Department of Agriculture and the Virginia Agricultural Experiment Station (82). Using the maps provided in these documents, one can determine the predominant soil types in any piece of land in the county. This was done for each subbasin involved in the proposed model. However, the soil survey of Prince William County has not yet been published, and that for Fauquier County is somewhat lacking, so considerable guesswork was involved in the estimations for subbasins 1 through 7 and subbasin 13.

   Once the predominant soil types are known, one can determine the particle size distribution from keys such as shown in Figure 10. By weighting these values with respect to the percentage of soil type within each subbasin, one can compute the approximate particle size distribution of soil in each subbasin. This too has been done for each horizon, A, B, and C, as shown in Tables A-4, A-5, and A-6, respectively.

2. Phosphorus Contents in Soils. The soil-phosphorus data are from the Virginia Soil Test Summaries, as prepared

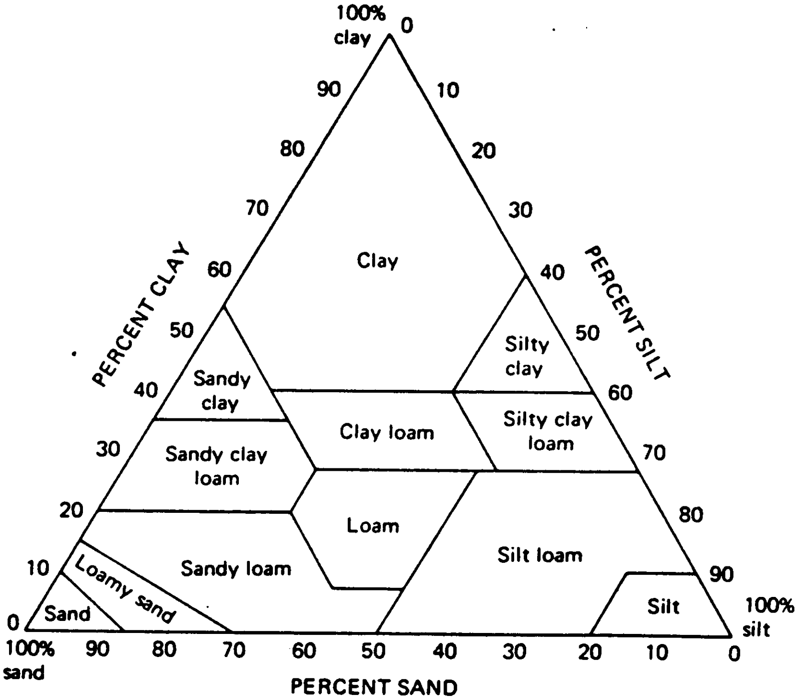

Figure 10. Soil Size Distribution Key. From Brady (96).

by Donohue (83). Included are tabulations of all phosphorus sampling performed in the state for a fiscal year; a State summary is given, along with breakdowns by region and county. The number of samples recorded for counties ranges from hundreds to thousands, with most samples being taken from various agricultural lands, but also from residential lawns, golf fairways, surface mines, and others.

The computation has involved combining the data into the land uses of the proposed model, by county, and estimating soil phosphorus contents for each subbasin by weighting the area which lies in separate counties. Results are shown in Table A-7. In all cases it was assumed that soil of lower horizons contains no extractable phosphorus. (An important note: there exists no differentiation with respect to particle size.)

3. Composition of the Bed Exchange Layers in Streams and Lakes. The available data are from two sources: published reports and a stream survey performed as a part of this study. Reports are by Bass (84), Dawson (85), To (2), Shugart (4), and Lorenz (86); a map of the data-collection stations used by these authors is shown in Figure 11. For the stream survey, sampling locations are shown in Figure 12, and results of the survey are

given in Table A-8. The fractions of channel covered by each type of bottom material have been estimated from these sources, and the masses of each have been computed (Table A-9).

4. Phosphorus Content of Stream Sediments. These data are from graduate theses written at the Virginia Polytechnic Institute and State University during the 1970's and early 1980's, with sampling stations shown in Figure 13. Based on a tabulation of these data, the phosphorus content in bottom sediment of each channel have been estimated, as shown in Table A-1. As with upland soil-phosphorus data, there exists no differentiation with respect to particle size. (An important point.)

5. Universal Soil Loss Equation. Using the methodology of Chen (87) and Meyer and Ports (88), estimations were made for each of the factors used in the equation. Chen (87) is an especially good reference for applying the MUSLE equation. The procedure used for each factor is given below:

   a. Rainfall factor, R. Chen (87) gave an annual average value of 200 for the Northern Piedmont Region of Virginia, while Meyer and Ports (88) gave 175. By chance, Chen also gave a monthly distribution of R

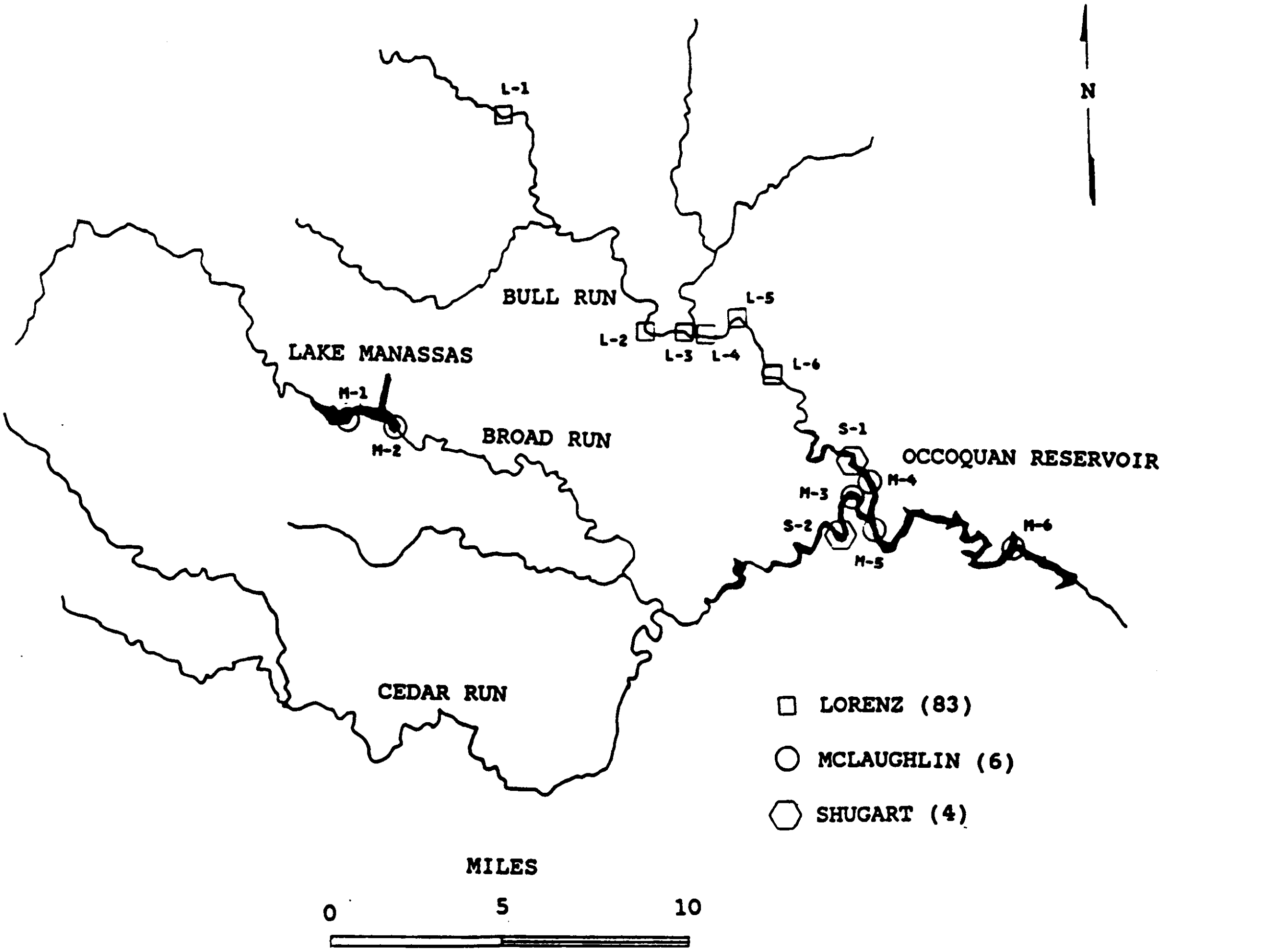

Figure 11. Bottom-Sediment Sampling Stations Used by Lorenz (86), McLaughlin (6), and Shugart (4).

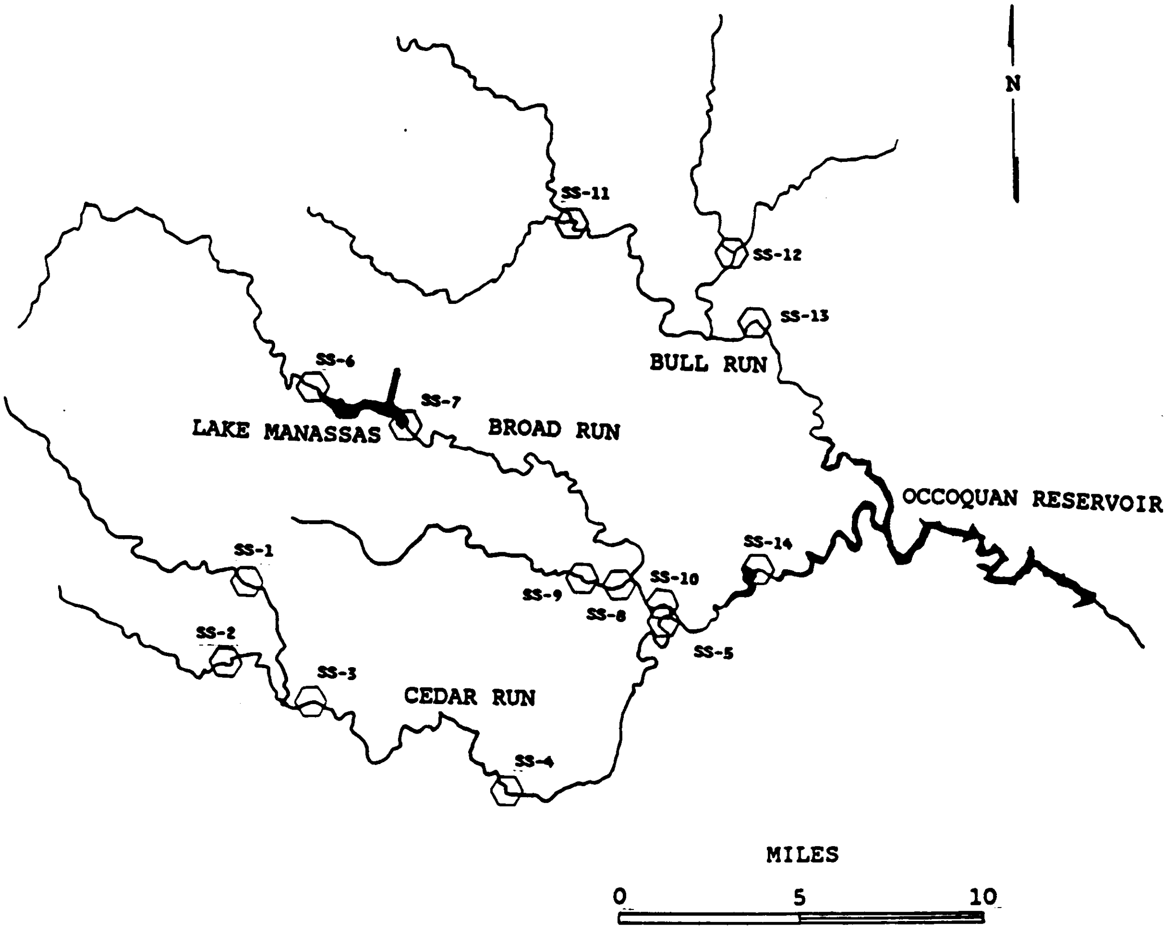

Figure 12. Sampling Stations for the Stream Survey Performed on 21 March 1985.

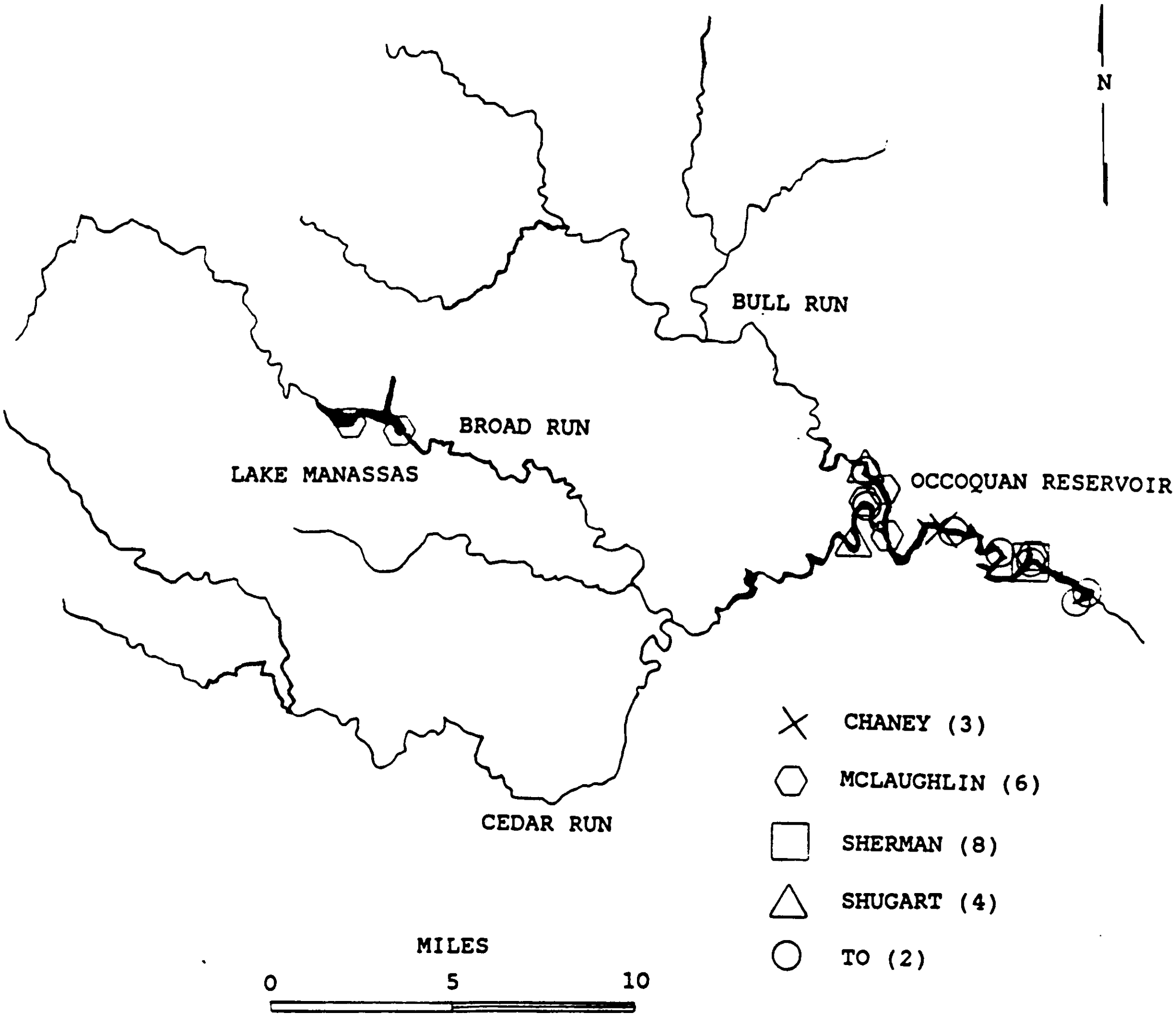

Figure 13. Sampling Stations for Phosphates in Bottom Sediments Used by Chaney (3), McLaughlin (6), Sherman (8), Shugart (4), and To (2).

for Fairfax County. An average annual value of 200 was used to calculate the monthly values (Table A-10).

b. Soil Erodibility Factor, K. Chen (87) also presented K values for the predominant soils of Fairfax County, many of which are also present in subbasins outside the county, but near it. These data, along with the predominant soil types in each subbasin already determined, were used to estimate K for subbasins 1 through 4, subbasins 8 through 11, and subbasin 15. For the others, the nomograph method of Chen (87), which is based on soil textures and permeability of soils of each subbasin given by Hydrocomp (44), was used. Results are shown in Table A-11.

c. Length Slope Factor (LS). In estimating this factor, the average land slopes of each subbasin, as given by Hydrocomp (44), were helpful indeed. With these data, the nomograph given by Chen (87) made the estimations easy. Results are shown in Table A-12.

d. Vegetal Cover Factor (C). The importance of this factor to the proposed model cannot be overstated; it is a major means by which land-uses exert their effects. For each land use, C was estimated from values given by Haan and Barfield (89) (Table A-13).

e. <u>Control Practice Factor (P).</u> As minimum tillage is the only control practice simulated by the model, a factor of 0.5 was used for these lands, with a value of 1.0 used for the others.

f. <u>Sediment Delivery Ratios.</u> This factor is used to account for deposition which occurs between the upland field and the stream channel; therefore it is highly dependent on the distance from the upland field to the stream channel in question. The first step in estimating this ratio was to determine a typical drainage area of first-order tributaries to each channel from 1:250000 scale USGS maps; next, the delivery ratios were estimated from a plot of delivery ratios versus drainage areas for Maryland watersheds given by Chen (87). Results are in Table A-14.

6. <u>Orthophosphate Release Rate Data from Stream Sediments.</u> The sources of these data were theses written at Virginia Polytechnic Institute and State University, all concerned with the Occoquan basin. In these studies lake microcosms containing bottom sediment and lake water,

both mixed and unmixed, both aerobic and anaerobic, were used. Sampling stations are shown in Figure 13. McLaughlin (6) derived most of the data; the data of To (2) and Sherman (8) have also been helpful. Invariably these data are in an unapplicable form -- many pages of calculations were required to derive unit rates of release in terms specified in the proposed model. In comparing the data, disparities are common, even between data given by the same author. The results seem to show that aerobic uptake and release are first order processes, dependent on the concentrations of both adsorbed and dissolved orthophosphates, and that anaerobic release is a zero order process, dependent only on the DO concentration in the water column. Although these samples were taken at different times throughout the year, the temperature in all experimental microcosms was 20 degrees Celsius, and thus no seasonal variations in uptake and release rates could be ascertained. As is shown in Table A-2, only a single value could be determined, and it was assumed to be valid year-around and for each sediment size.

7. <u>Channel Dimensions.</u> These were estimated through the stream survey performed as a part of this thesis and through USGS topographic maps of three scales: 1-to-24000, 1-to-62500, and 1-to-250000. The 1-to-62500

scale mapping is old, typically dated in the 1940's, while the other two scales are recent, being photorevised in the late 1970's and early 1980's. Potentially, the older mapping may be used for model verification.

From the 1-to-24000 scale mapping, or quad sheets, elevations of the water surface of the beginning and end of each channel were recorded, as were the lengths of channels and fooodplains as measured along their respective centerlines. Channel and valley slopes were computed from these values. Lengths and slopes are tabulated in Table A-15.

8. Flow Data. Because the basin, at one time or another, has had no less than eleven USGS gaging stations, and because stream stations were chosen to coincide with these gages where possible, the compilation of flow data was easy. At stream stations where there was no gage, flows were estimated from drainage area ratios.

The original plan was to simulate two flows for each channel for each month of the year: a low flow and a monthly average flow. Low flows were derived based on the log normal distribution, specifically, 7-day, 10-year low flows. Monthly average flows, even though they too seemed to be log normally distributed, were derived differently: from a list of ten years of data, the median flow was chosen. The reason for this was that the highest frequency event, rather than the mean, was desired. (In the log normal distribution, the median approximates the highest frequency event much closer than does the mean.) These data are shown in Tables A-16 and A-17.

9. Land Uses. The land-use fractions shown in Tables A-18 and A-19 were taken from a map prepared by the Northern Virginia District Planning Commission in December 1977, and revised in April 1979. The grid-counting method was employed in manually ascertaining these fractions.

10. DO Rate Constants. Typical values for initial input data have been found from the literature as follows.

   a. Deoxygenation Coefficient. Used in the proposed model purely for dissolved BOD, this variable serves interchangeably in estimating degradation of BOD and the consumption of DO. An initial value of 6 $mo.^{-1}$ has been chosen, as given by Chen and Wells (29). Highly dependent on temperature, this variable has been estimated for each month, and the results are shown in Table A-20.

b. <u>Nitrification Coefficient.</u> Krenkel and Novotny (90) stated that the first-order nitrification coefficient for streams varies from 0.1 to 15.8 day^{-1}. Because this constant is highly dependent on the abundance of suitable sites for attached growth, the estimations have included consideration of the available data on channel bottom material. Also highly dependent on temperature, seasonal estimations of this constant are given in Table A-20.

c. <u>Decay Rates for Suspended Organic Matter.</u> Chen and Wells (29) gave a value of 0.032 mo.$^{-1}$, presumably for summer. Again seasonal estimations, shown in Table 20, were made. In order to convert organic matter to terms of BOD, the theoretical demand of glucose was employed, assuming half is exerted.

11. <u>Biological Data.</u> For each trophic level, available data are given below.

a. <u>Periphyten</u> For the Occoquan basin, two sources of data are available: biomass data from Bass (84), and growth rate data from Dawson (85). Bass' study (84) concerned the Colonial Oil pipeline spill of March, 1980, in which large quantities of fuel oil and kerosene where discharged to the Rappahannock River system and to Bull Run. With the purpose of determining the extent of damage, Bass (84) measured biomass densities in both impacted and unimpacted areas, thus giving a general idea of the biomass to be expected per area of stream bottom in the Occoquan basin. These estimations, along with the area of gravel and boulder habitat in each stream channel, were used to estimate the ash-free dry biomasses shown in Table A-21.

Dawson (85), in studying the effects of urban runoff on the periphyton community of Bull Run, computed productivity rates for several locations for the months of July through August 1979. These are given in Table A-22.

b. Benthos. The available data concerning masses per unit stream area are in another report on the Colonial pipeline spill: that by Voshell (91). He sampled stream stations at locations similar to those used by Bass (84) and derived ash-free dry weights for benthos. From these data, a macroinvertebrate biomass was estimated for each stream channel (Table A-23).

In addition, Chen and Wells (29), in their study of the Boise River, published emergence rates for benthos by month (Table A-24). While no such data were available for the Occoquan, the Boise River data may serve as a first best-estimate for calibration.

c. Fish. Again the only data available on biomasses per stream area were from a study of the Colonial Pipeline spill, this time by McHugh (92). Because these measurements are taken at only two stations in the Occoquan Basin, in the Bull Run and Occoquan Creek arms of the reservoir, and because the measurements are recorded in terms of number of fish caught per 1000 seconds of electrofishing or number of fish caught per trap net night, the data are sketchy indeed. Nevertheless, estimates of dry weight biomasses for each channel were made (Table A-25).

d. Zooplankton. Buikema (93) stated that, to his knowledge, no data are available for the Occoquan basin. So, in order to keep values within reasonable ranges, seasonal concentrations of both herbivorous and carnivorous zooplankton in Lake Ontario, presented by Chen and Smith (94), were used for calibration. (Table A-26).

e. Detritivores. It appears that no data are available.

f. Lake Algae. An excellent source of algal data is available; Chlorophyl-A measurements are routinely taken as a part of the Occoquan Monitoring Program. In general, values are available for seven stations in the Occoquan Reservoir for each month of the year; however, values for Lake Manassas and Lake Jackson are not included.

12. Lake Volumes. Lake volumes were estimated, as best as reasonably possible, from values given by McLaughlin (6), Markley(5), and Dawson (85) and from contour maps. A 5-foot depth was assumed for all epilimnions, and estimated volumes are shown in Table A-27.

13. Pollutant Export in Runoff. From previous urban runoff monitoring studies, Randall and Grizzard (95) compiled tables of annual export rates from several types of urban land, and included such pollutants as BOD, orthophosphates, total phosphorus, and various forms of nitrogen. From these tables, annual values for dissolved BOD and orthophosphates for each land use in the proposed model have been estimated (Table A-28).

Calibration

Because the available data appear centered around 1979, within six years each way, and because the AWT became operational in June of 1978, 1979 was the year chosen for calibration. Initially, a calibration of the entire model was tried, but it was found that this is impossible; the DYNAMO model must first be broken into small segments, then the segments need to be reassembled after all portions have been calibrated. Although this requires duplicating many variables outside the calibrated submodel and inserting dummy values for many others, it is necessary.

During the initial attempt at calibration, when an attempt was made to calibrate the entire model, an important problem was found, one important to stream channels but not lakes. The assumption of a one-month period of constant flow is unrealistic; there exist two distinct periods during each month: base-flow meriods and runoff periods. Water quality is entirely different during each. Therefore, levels and rates applying to stream channels need to be duplicated and modified to simulate both periods. (Level and rate equations for lakes will not need to be modified because the differentiation between base flow and runoff conditions in lakes is not nearly as important.) Such work will first involve determing a typical fraction of each month in which base flow and runoff conditions exist, then determining typical base and runoff flows. Pollutant levels for each period will be modeled as separate levels, even though they are for the same month; rates will be modified to account for the change. Although this procedure appears workable, it will be time-consuming and will add to the complexity of the model.

For the initial try at smaller calibration, the Lake DO Sub-model submodel was chosen, as this submodel includes all basic types of pollutant transport and transformation processes simulated in the overall model, and yet it is small enough to ensure enough time for complete calibration. (In addition, because no stream channels are included, no simulation of base-flow and runoff conditions is required.) Seasonal rates of export of BOD in runoff were modified to account for the pattern of runoff events which occured in 1979.

At first, calibration was difficult, for a good calibration method was not initially known. At any change of input data, the model yielded unreasonable results, values for some variables ranging into the trillions and beyond. As a result, it was quickly ascertained that all levels and rates needed to be confined to certain limits. (Through the MAX and MIN macros available in DYNAMO, this is easily done.) Thus, the following plan was used for calibration:

1. Adjust each rate equation to yield expected values, keeping in mind values cited in the literature.

2. Set maximum and munimum limits to each rate, never letting a rate affect a level more than a specified amount.

3. Set maximum and minimum limits on each level. For example, the mass of DO in a channel or lake was limited so that the concentration never becomes less than 0.0 mg/L or becomes higher than 15.0 mg/L.

4. For each channel and lake, set limits on the difference between the rates of inflow of pollutants from upstream and rates of outflow downstream.

With this plan, calibration was accomplished, with results for DO in each lake given in Figures 14 through 18 and results for BOD given in Figures 19 through 23. From the plots of DO, one can see the typical variations that occur during a year: DO is highest in winter, decreasing to a minimum in summer or late summer. Further, DO in the hyplimnions decreases to much less than that in the epilimnions, falling to near zero in lakes 13, 14, and 15. On the other hand, one generally fails to see such trends in the BOD plots; for one thing, this indicates the unreliability of the BOD test. However, in all lakes a peak BOD occured in August and September, possibly indicating the occurrence of a simultaneous algal bloom.

One problem involves lake stratification in the spring and turnover in the fall. During 1979, these events appear to have occurred in the Occoquan Reservoir in March and November, respectively. At these times there is a difficulty with the model: under present constraints, there is no way the rates can operate through the change, so the new pollutant levels are either set equal to values for the previous month or are read into the program through multipliers rather than being computed by the simulation. In long-term simulations, this will obviously be a problem.

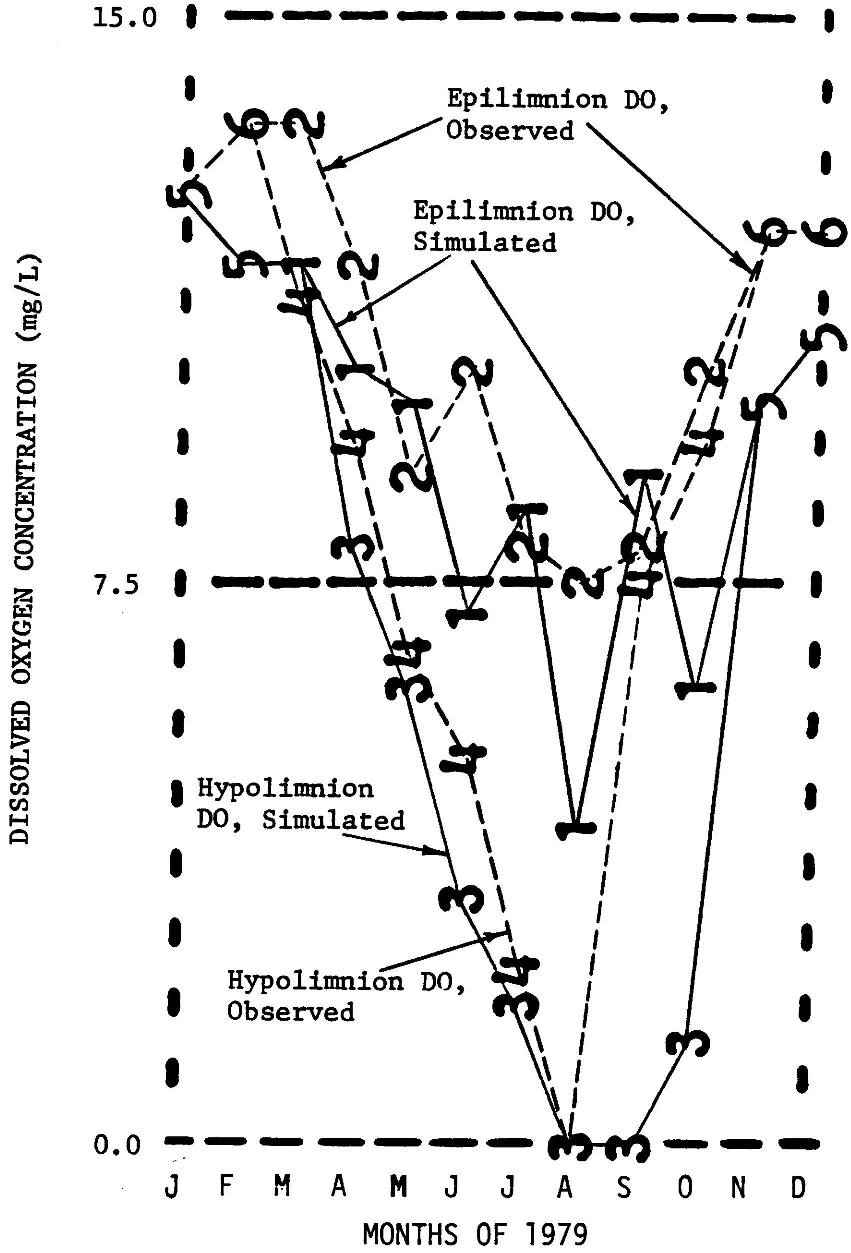

Figure 14. Dissolved Oxygen Calibration for Lake Manassas for 1979.

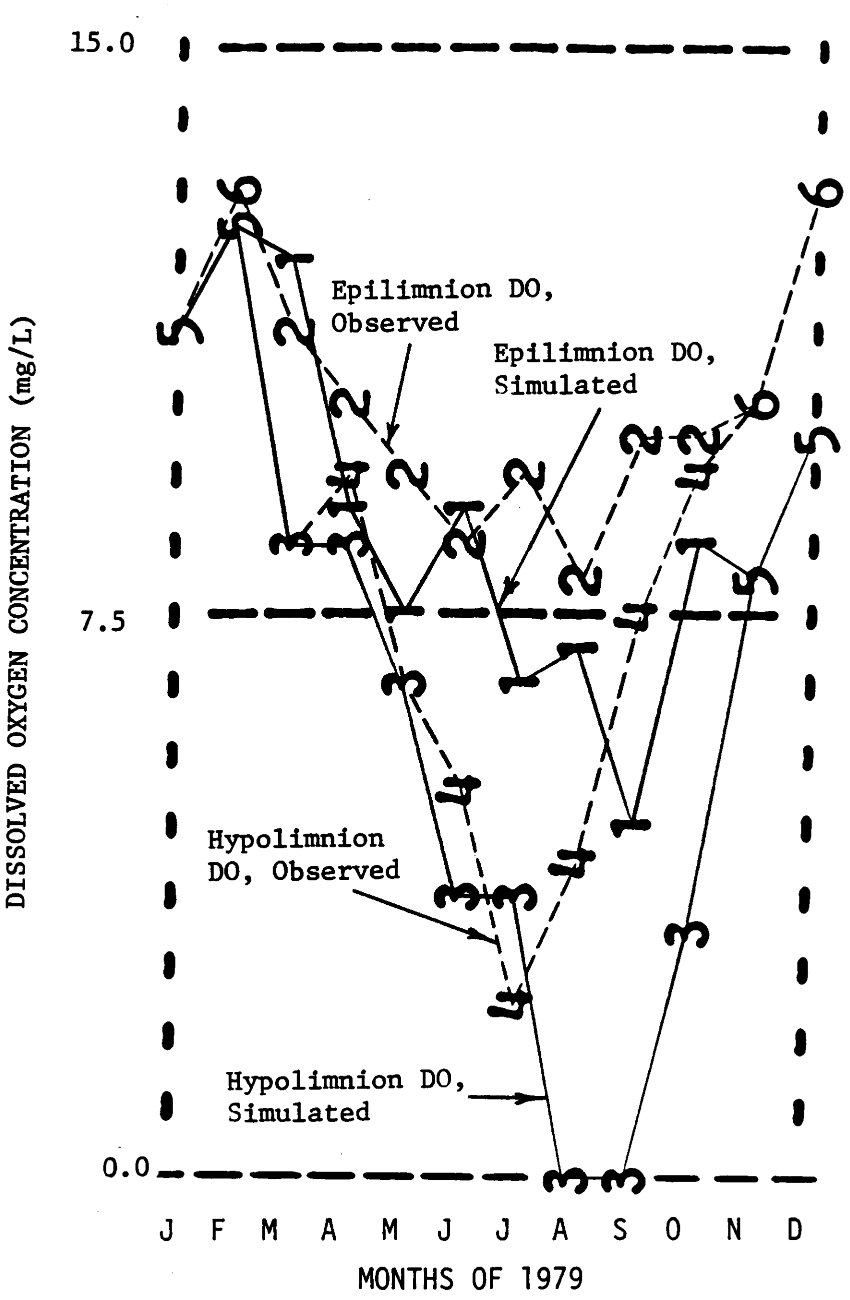

Figure 15. Dissolved Oxygen Calibration for the Bull Run Arm of the Occoquan Reservoir for 1979.

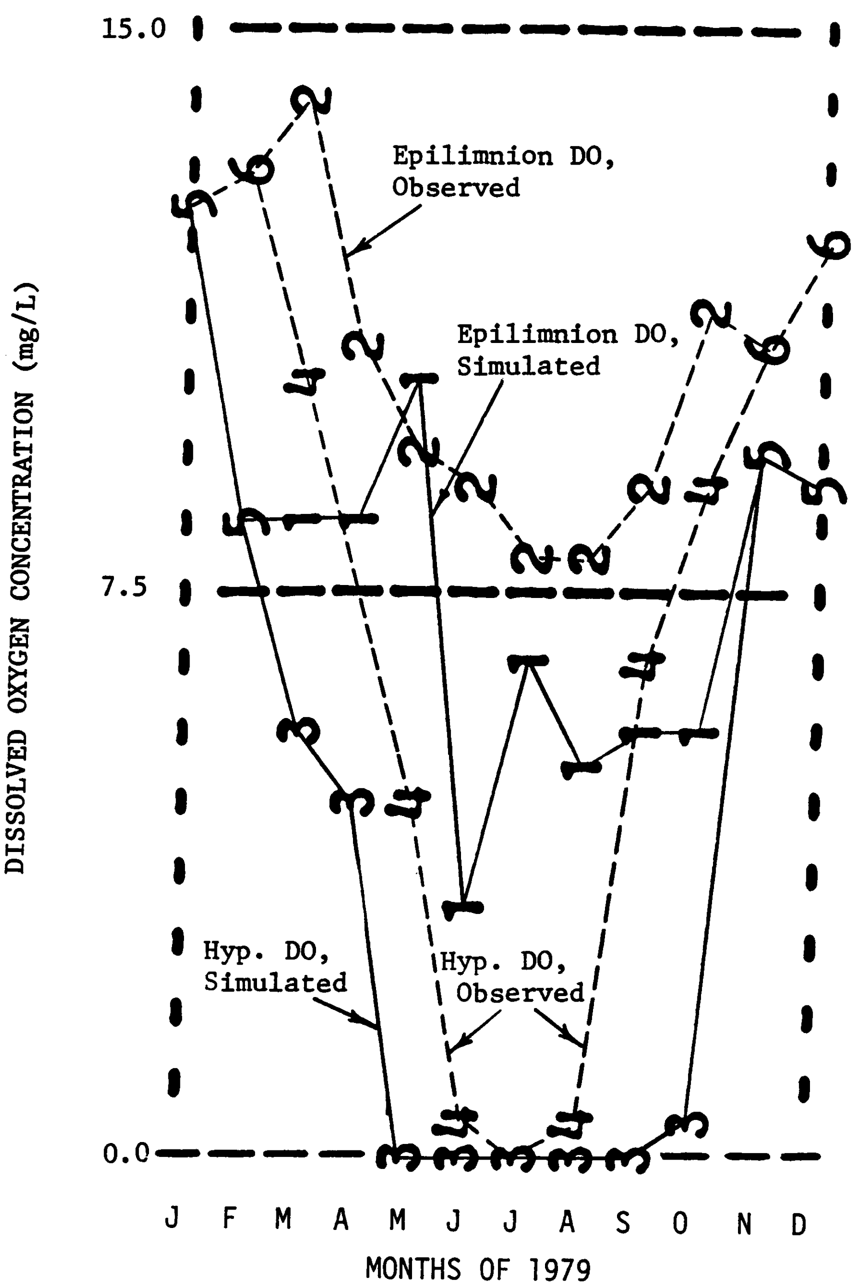

Figure 16. Dissolved Oxygen Calibration for Lake Jackson for 1979.

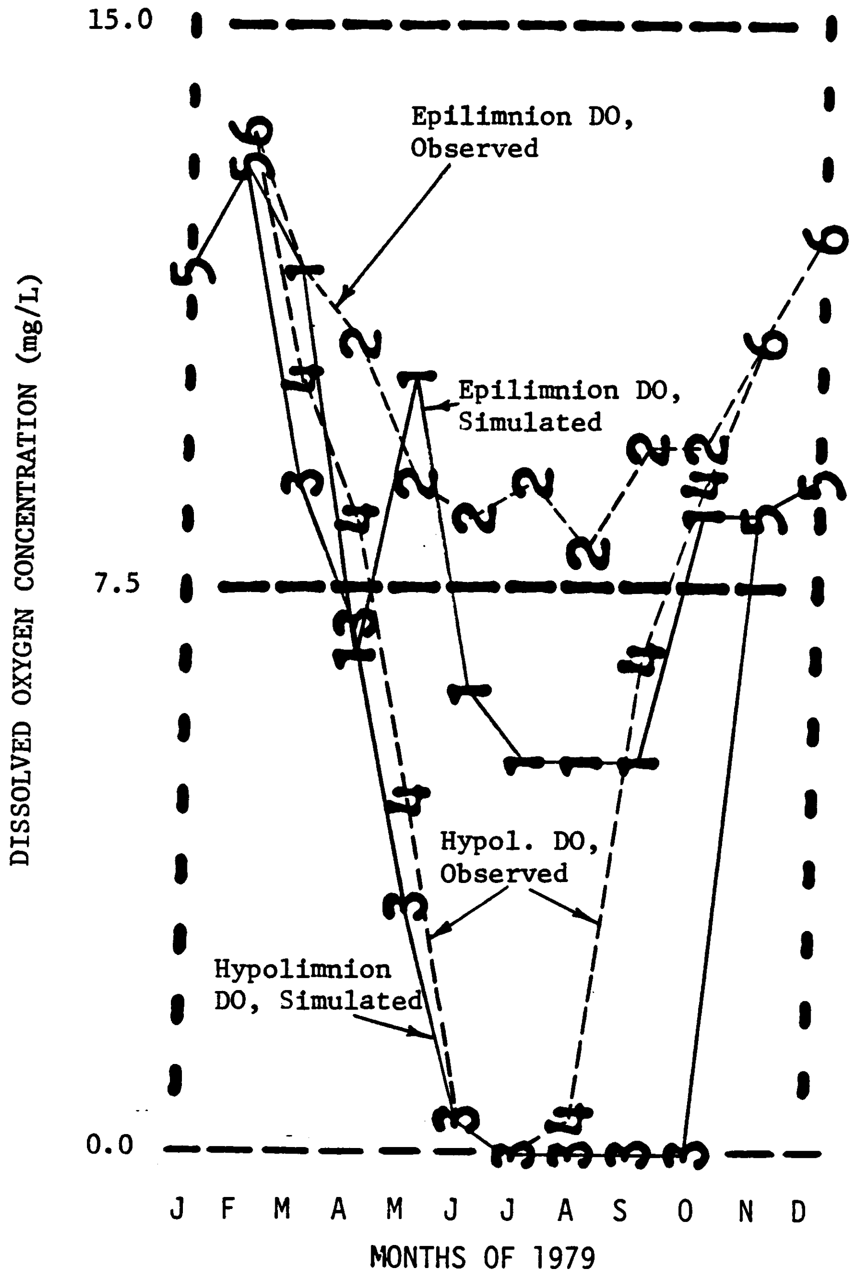

Figure 17. Dissolved Oxygen Calibration for the Occoquan Creek Arm of Occoquan Reservoir for 1979.

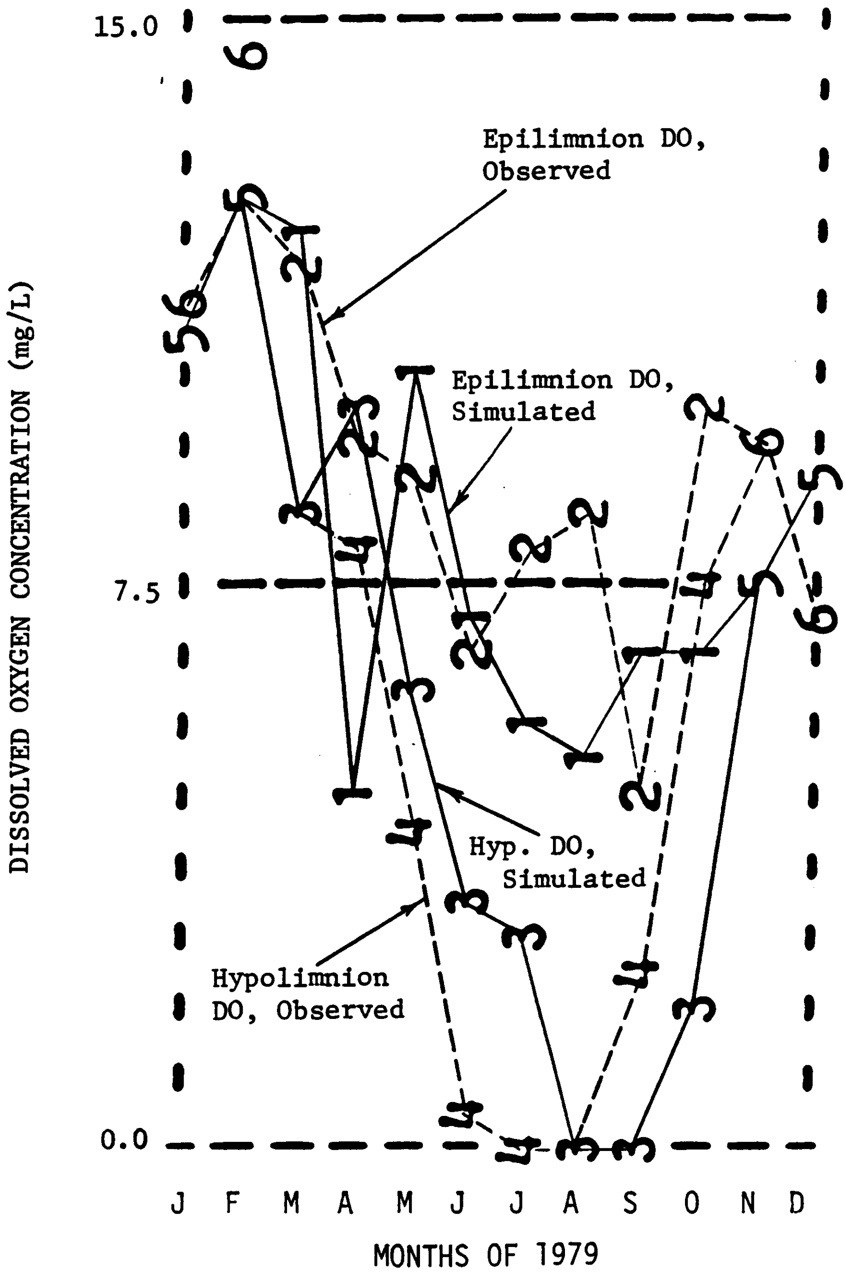

Figure 18. Dissolved Oxygen Calibration for the Main Stem of Occoquan Reservoir for 1979.

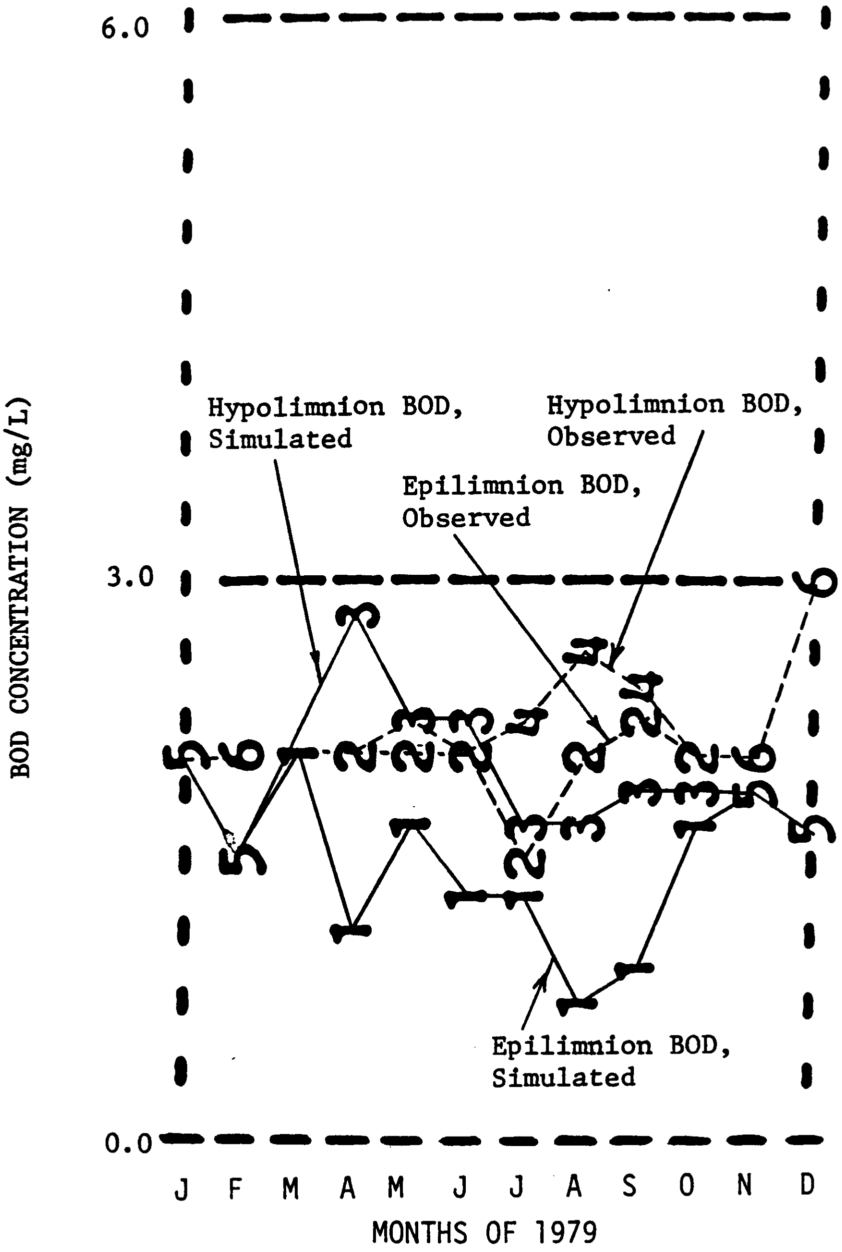

Figure 19. BOD Calibration for Lake Manassas for 1979.

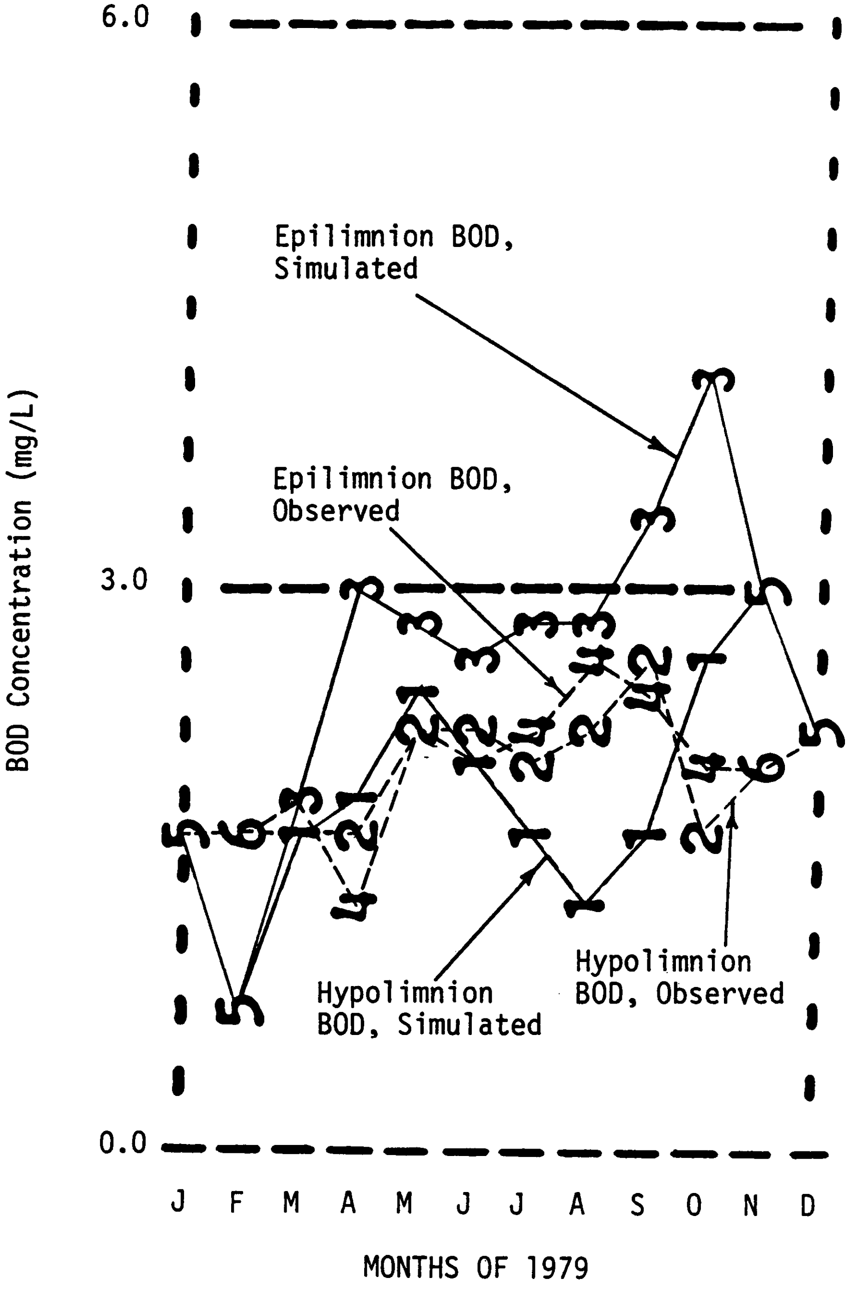

Figure 20. BOD Calibration for the Bull Run Arm of the Occoquan Reseroir for 1979.

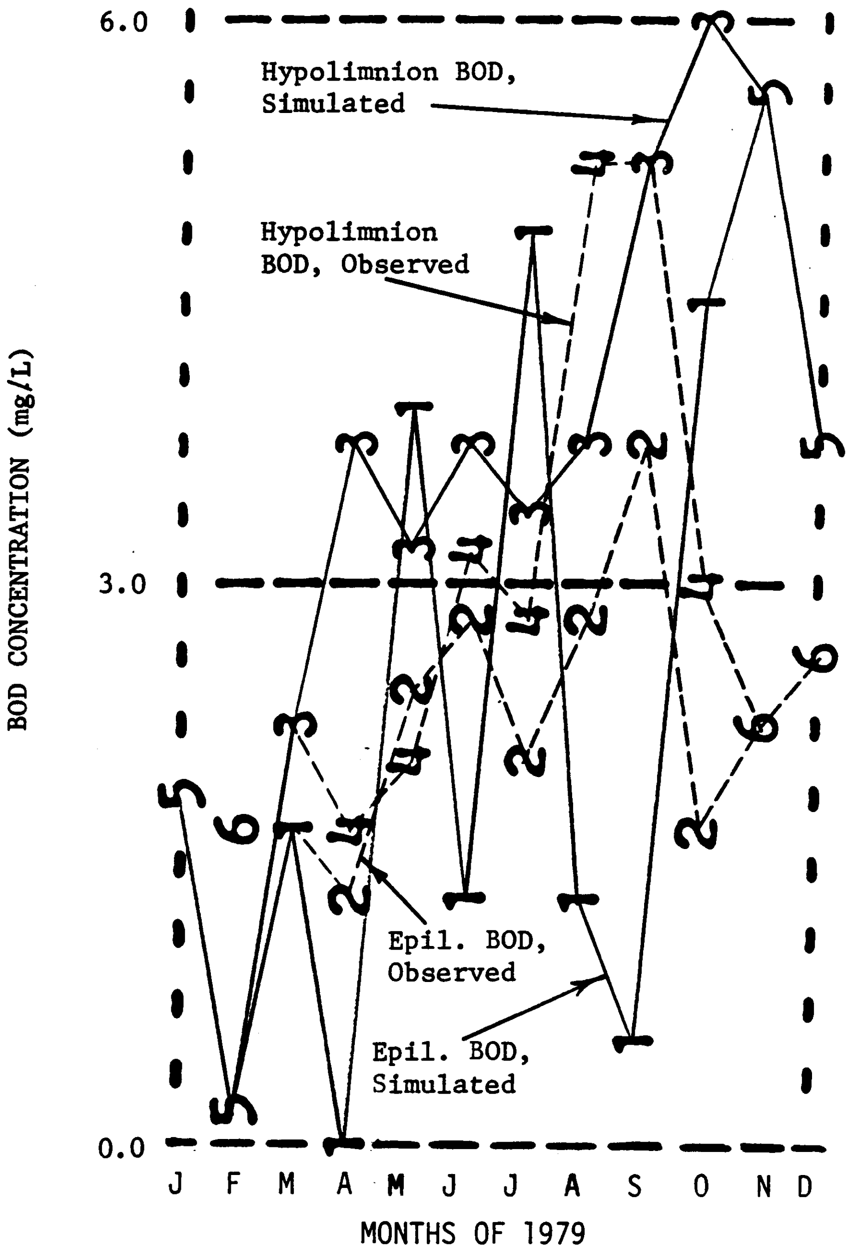

Figure 21. BOD Calibration for the Lake Jackson for 1979.

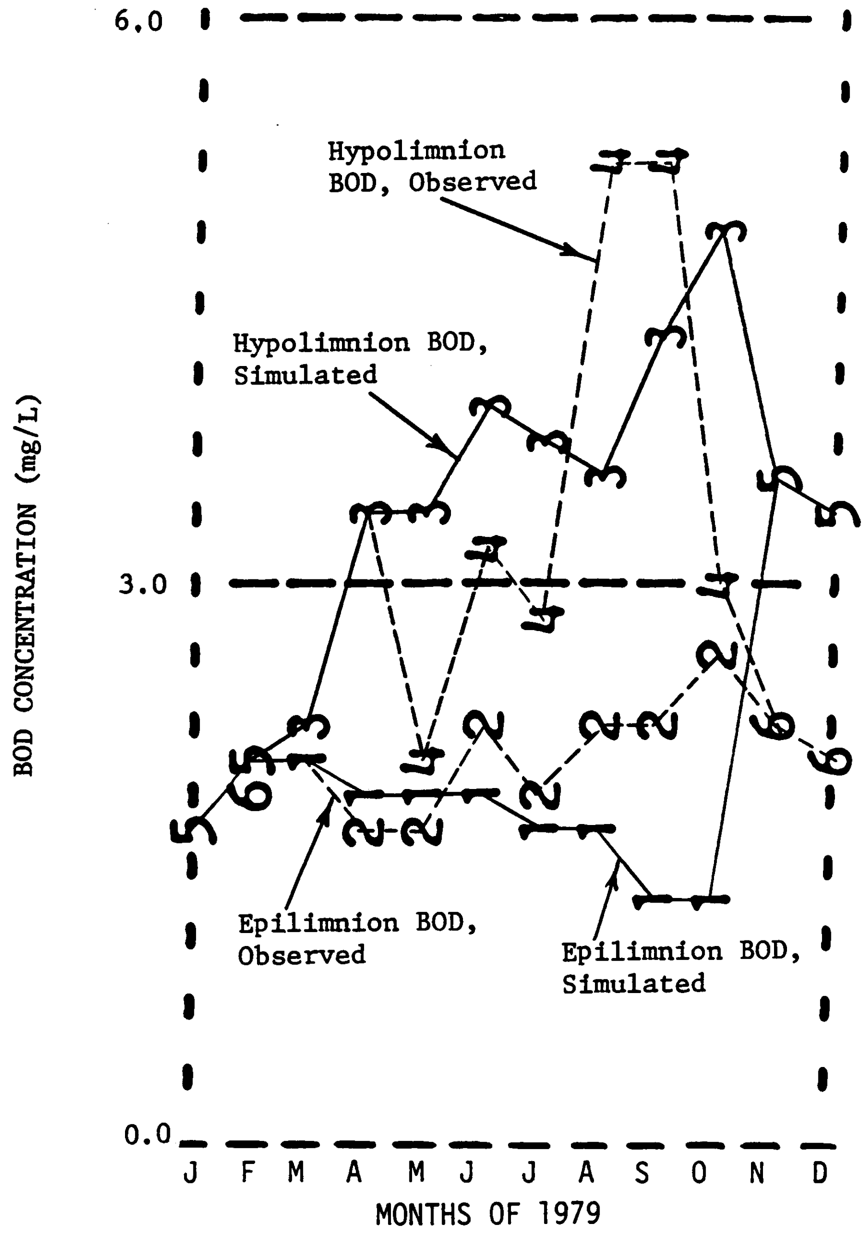

Figure 22. BOD Calibration for the Occoquan River Arm of the Occoquan Reseroir for 1979.

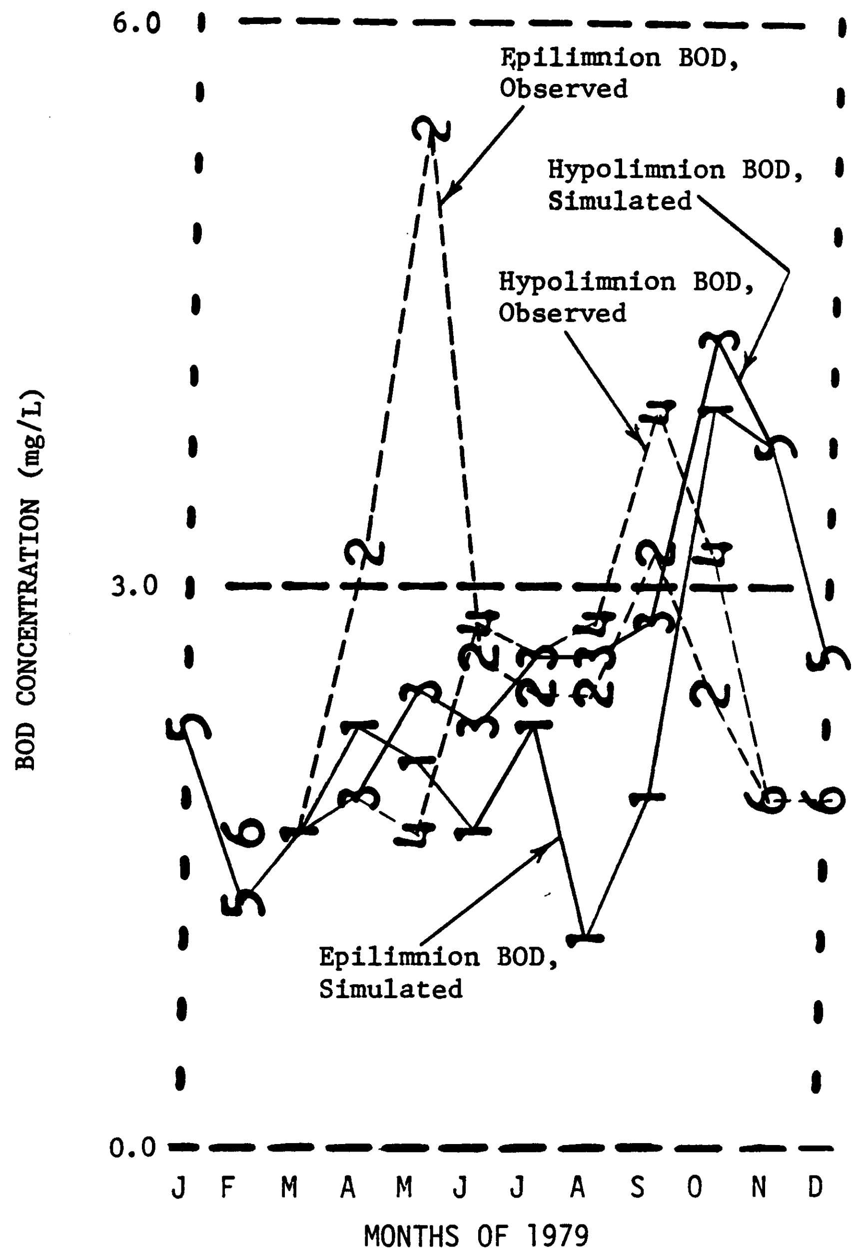

Figure 23. BOD Calibration for the Occoquan Reservoir for 1979.

CHAPTER V

SENSITIVITY ANALYSIS AND APPLICATION

Sensitivity Analysis

Sensitivity analysis is the process of observing and analyzing the effects of changes in input. It is important for evaluating the workability of a model and for helping to determine which parameters need to be studied more than others. With the calibrated model, the effects of changing the following coefficients were studied: the lake reaeration coefficient, K_a the diffusion coefficient for thermoclines, D_C, and the deoxygenation coefficient, K_d. Six sensitivity analyses were performed, and descriptions of each are given in the following paragraphs:

1. Sensitivity Analysis Number 1: Reaeration coefficients for each lake were multiplied by 1.1 for the entire year. As expected, this increased the DO concentration in both the epilimnion and hypolimnion of all five lakes; however, the increases were not as great as expected. Results for DO in lake 13 (Lake Jackson, 51ST10) are given in Figure 24.

2. <u>Sensitivity Analysis Number 2</u>: Reaeration coefficients for each lake were multiplied by 0.9 for the entire year. The results were again as expected; the DO concentrations in both the hypolimnion and epilimnion of each lake were decreased. However, as before, the decreases were somewhat small. Results for DO in lake 15 (Occoquan Reservoir, 51RE01) are given in Figure 25.

3. <u>Sensitivity Analysis Number 3</u>: Dispersion coefficients for the thermocline of each lake were multiplied by 1.2 for the entire year. Such a change would increase the tendency for exchange across the thermocline; the difference between epilimnion and hypolimnion DO concentrations would become less. (The epilimnion concentration would decrease, the hypolimnion concentration would increase.) The results for each lake were as expected and are similar to those for lake 14 (The Occoquan River Arm, 51RE25)(Figure 26).

4. <u>Sensitivity Analysis Number 4</u>: Dispersion coefficients for the thermocline of each lake were multiplied by 0.8 for the entire year. Again, the results were as expected; the DO concentrations in epilimnions were increased, while those for hypolimnions were decreased. Results for lake 5 (Lake Manassas) are shown in Figure 27.

5. <u>Sensitivity Analysis Number 5</u>: Deoxygenation coefficients for each lake were multiplied by 1.5 for the entire year. This change would increase rates of exertion of BOD, thereby decreasing both BOD concentrations and DO concentrations. This was exactly the case for each reservoir, and the results for DO and BOD for lake 5 (Lake Manassas) are given in Figures 28 and 29, respectively. As with the results of sensitivity analysis with the reaeration coefficients, the changes were less than expected.

6. <u>Sensitivity Analysis Number 6</u>: Deoxygenation coefficients for each lake were multiplied by 0.5 for the entire year. As expected, BOD and DO concentrations were increased, although the increases in DO concentrations were not as high as expected. Results for BOD and DO in lake 12 (the Bull Run Arm of Occoquan Reservoir, 51RE30) are given in Figures 30 and 31, respectively.

<u>Scenario Testing</u>

To observe the effects of a policy change, the next iteration involved changing the BOD input to one of the lakes. The fraction of commercial land in subbasin 13 was increased from 0.0 to 0.5 for the entire year, with a corresponding decrease in forest fraction from 0.789 to 0.289. This change in BOD loadings was enough to increase the DO concentration of lake 13 (Lake Jackson, 51ST10)(Figure 32). However, the change did not significantly affect the DO concentration of a downstream lake, lake 15 (Occoquan Reservoir, 51RE01)(Figure 33).

Discussion

The results of the sensitivity analysis and application seem to show that the parameters exert the correct effects on pollutant concentrations, that the modeling procedure works. However, adjustments are still needed before the model can truly simulate future basin development and policy changes. Such adjustments would be part of a verification process, in which the predictive capacity of the model would be shown. One of the recommendations of this thesis is that a verification be performed.

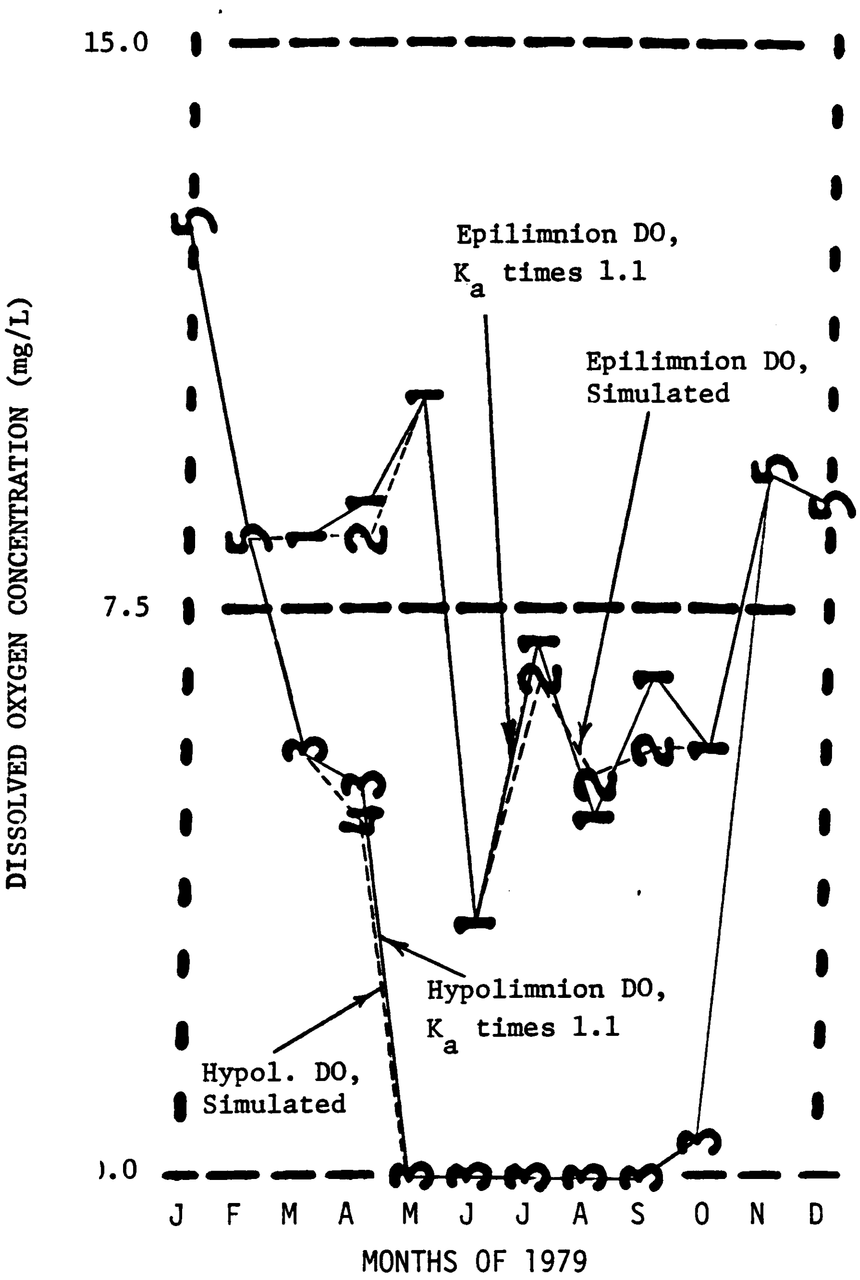

Figure 24. Sensitivity Analysis Number 1: DO Concentrations in Lake Jackson (lake 13) Resulting from Multiplying Reaeration Coefficients by 1.1

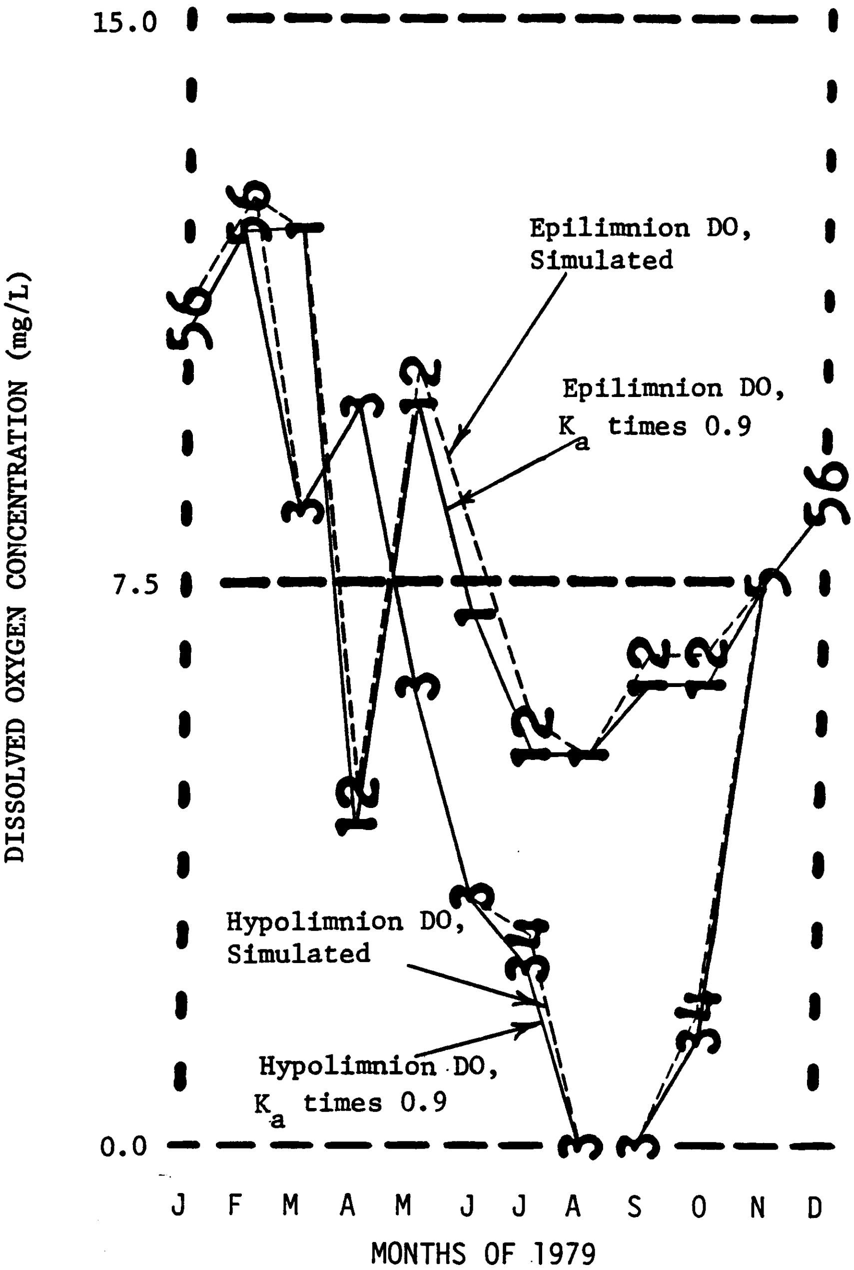

Figure 25. Sensitivity Analysis Number 2: DO Concentrations in Occoquan Reservoir (Lake 15) Resulting from Multiplying Reaeration Coefficients by 0.9

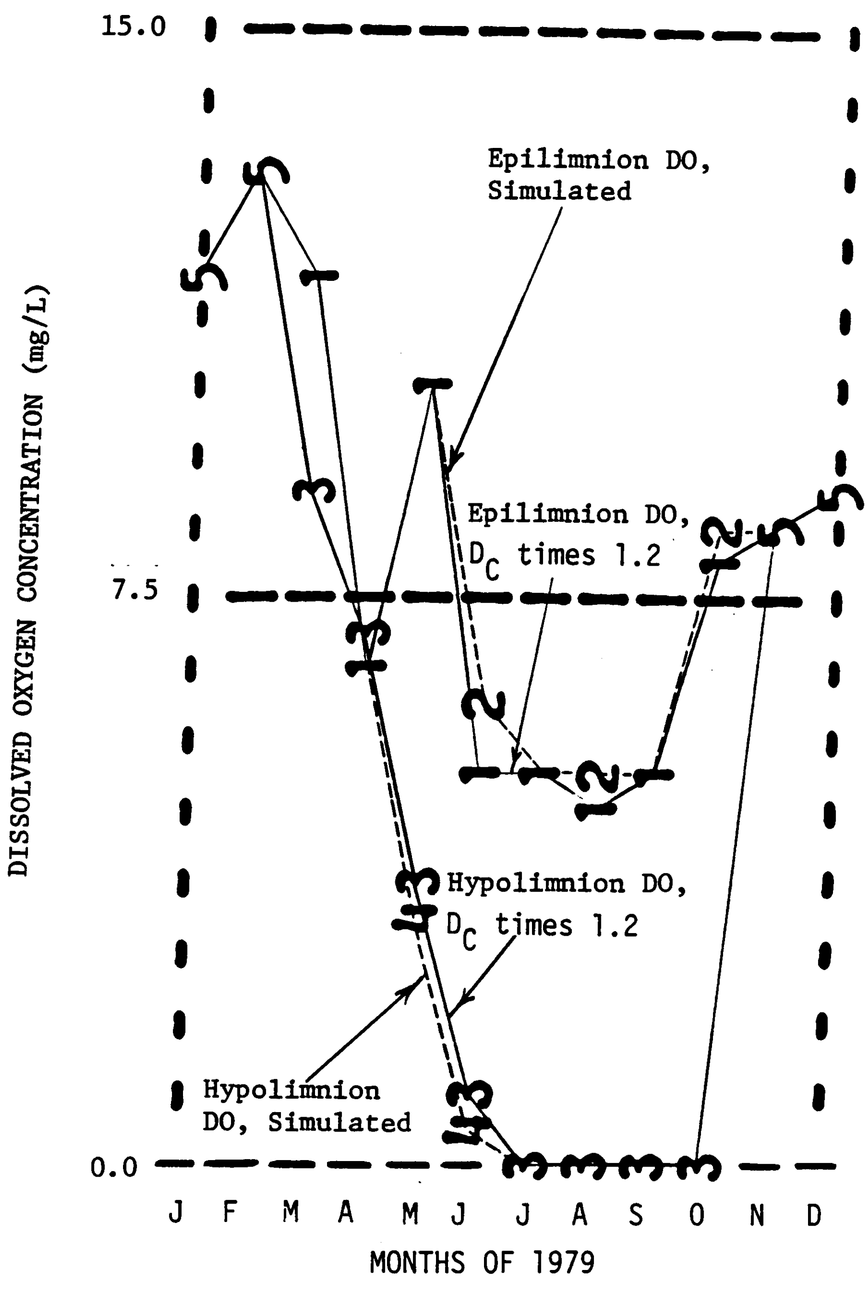

Figure 26. Sensitivity Analysis Number 3: DO Concentrations in the Occoquan River Arm of Occoquan Reservoir (Lake 14) Resulting from Multiplying Dispersion Coefficients by 1.2

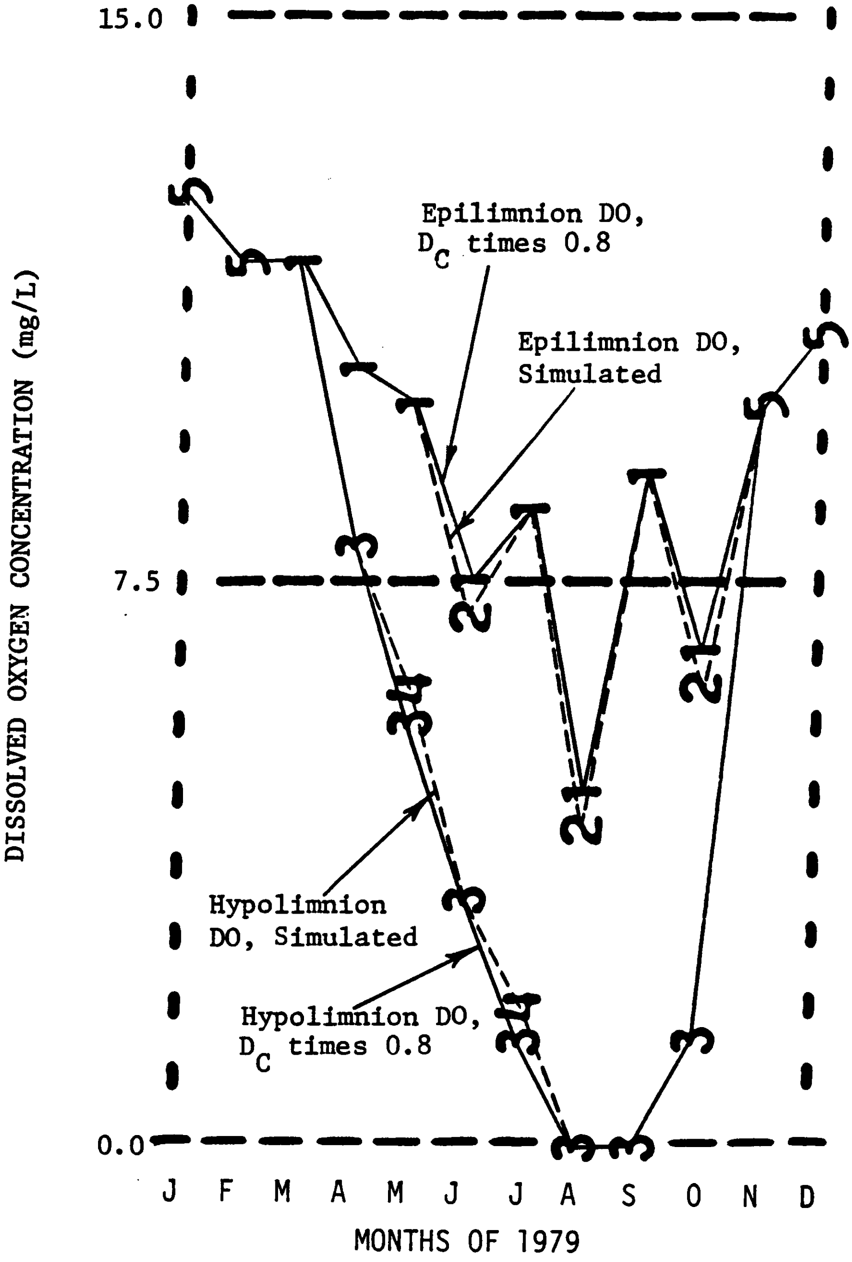

Figure 27. Sensitivity Analysis Number 4: DO Concentrations in Lake Manassas (Lake 5) Resulting from Multiplying Dispersion Coefficients by 0.8

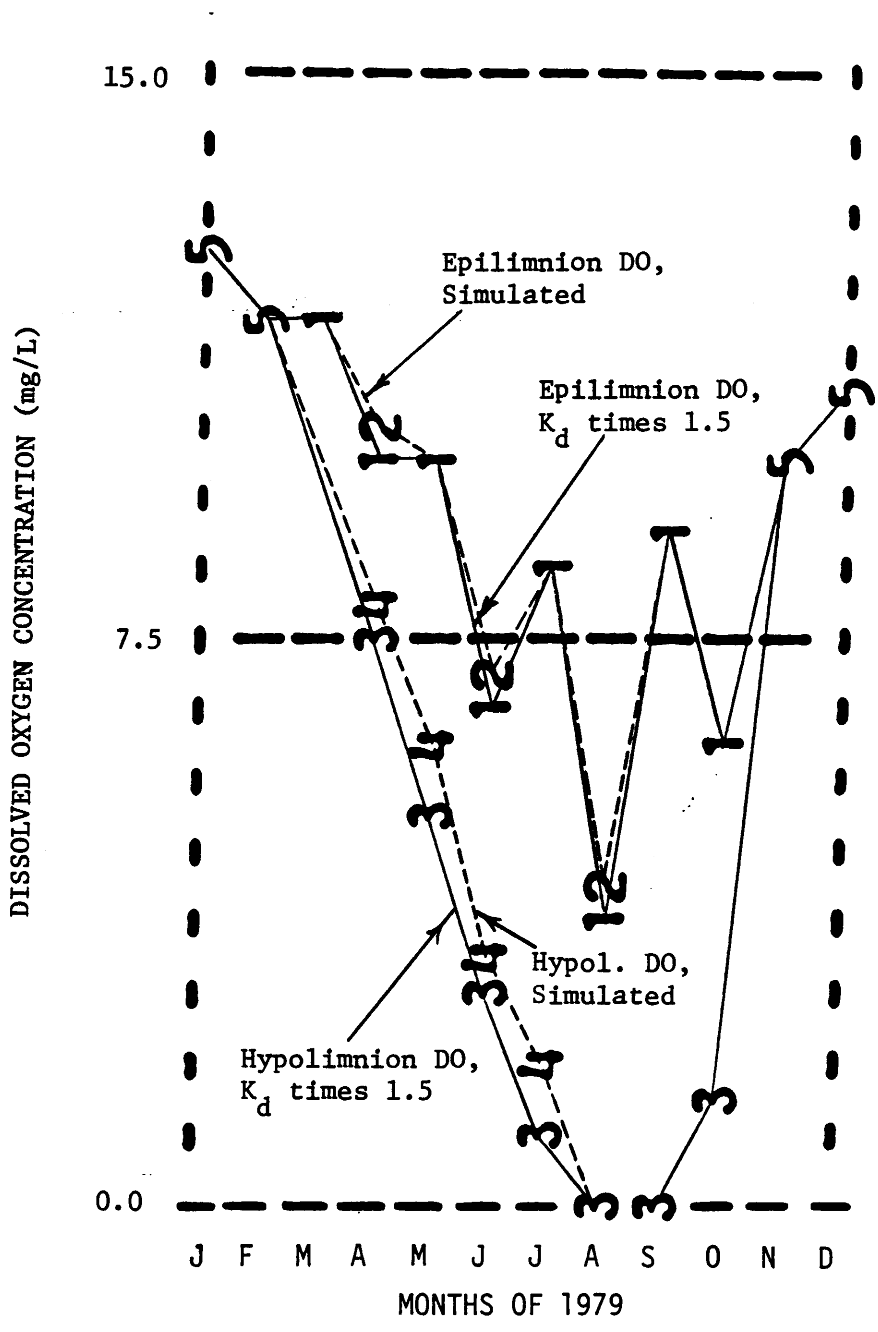

Figure 28. Sensitivity Analysis Number 5: DO Concentrations in Lake Manassas (Lake 5) Resulting from Multiplying Deoxygenation Coefficients by 1.5

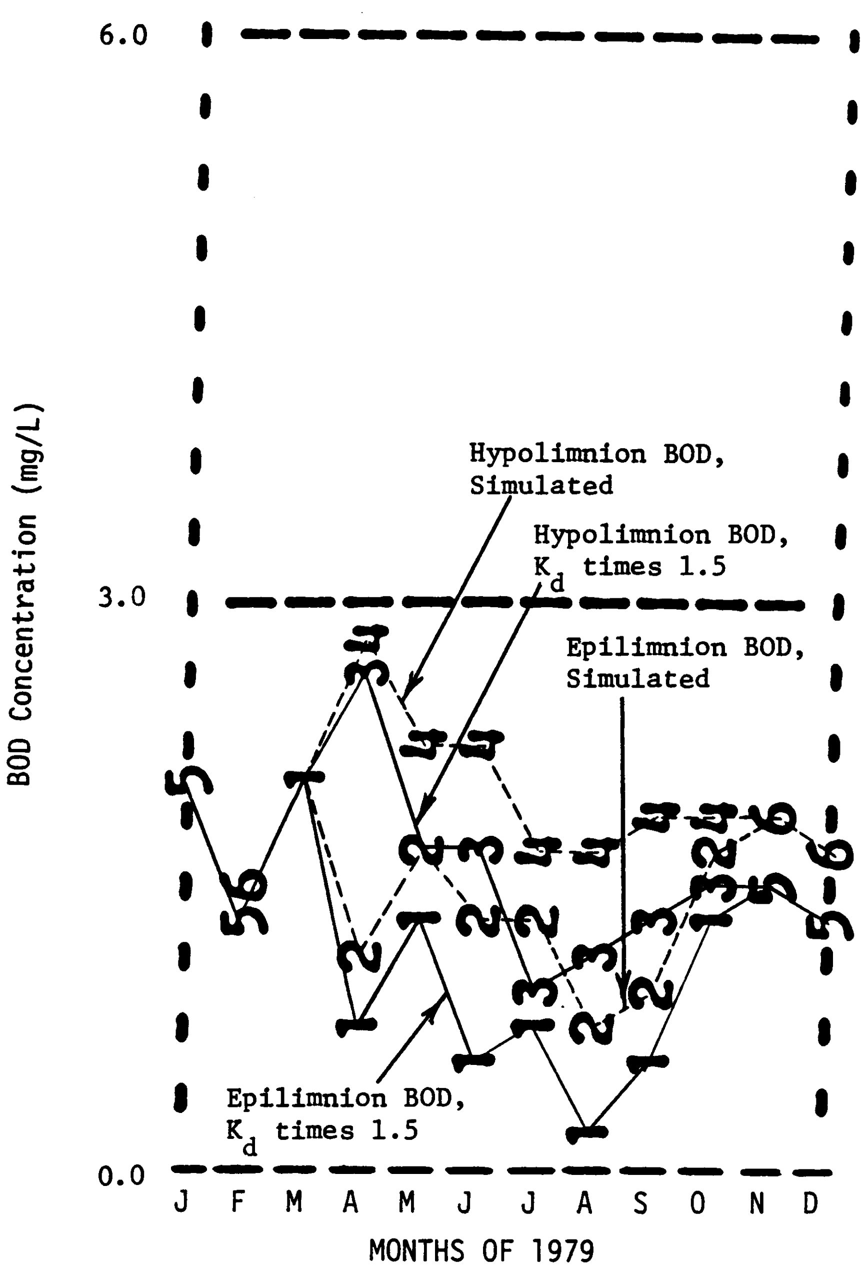

Figure 29. Sensitivity Analysis Number 5: BOD Concentrations in Lake Manassas (Lake 5) Resulting from Multiplying Deoxygenation Coefficients by 1.5

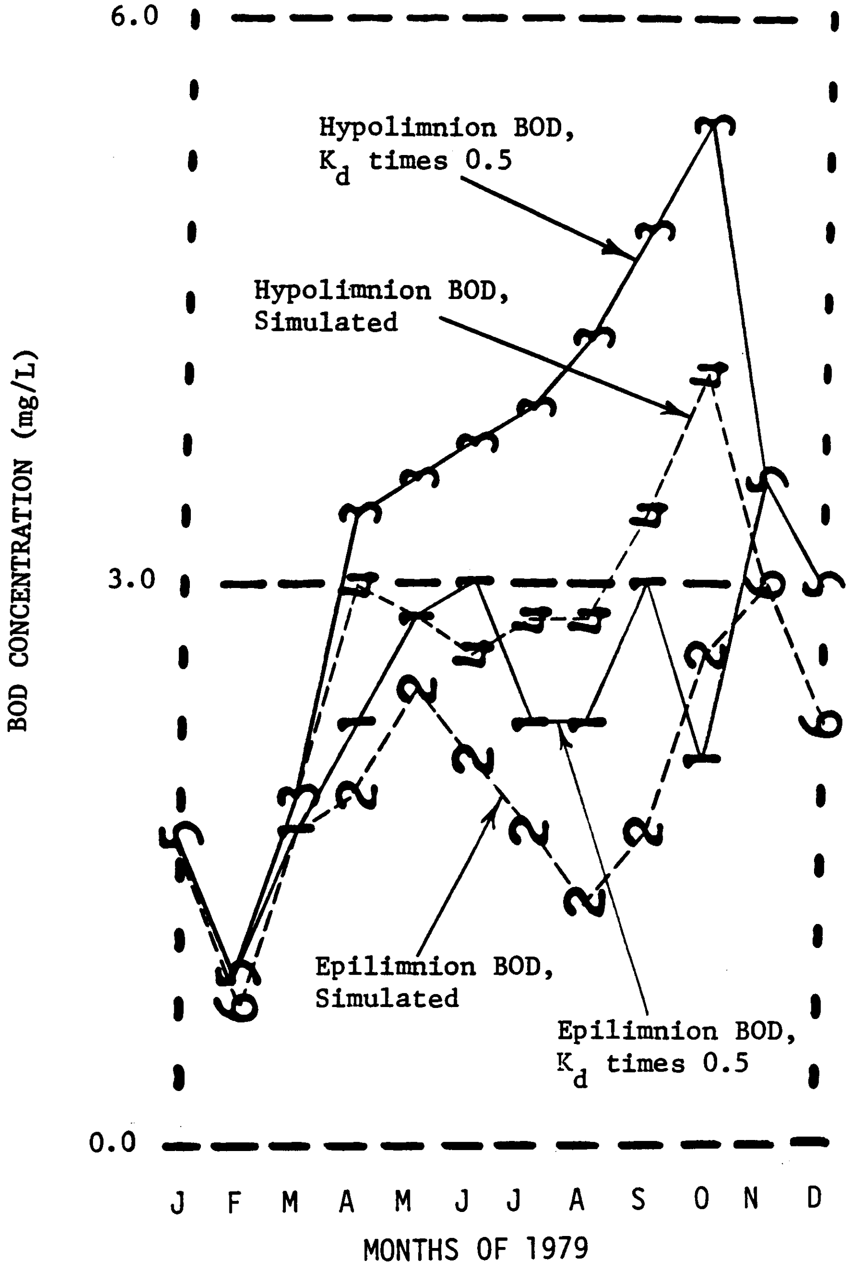

Figure 30. Sensitivity Analysis Number 6: BOD Concentrations in the Bull Run Arm of Occoquan Reservoir (Lake 12) Resulting from Multiplying Deoxygenation Coefficients by 0.5

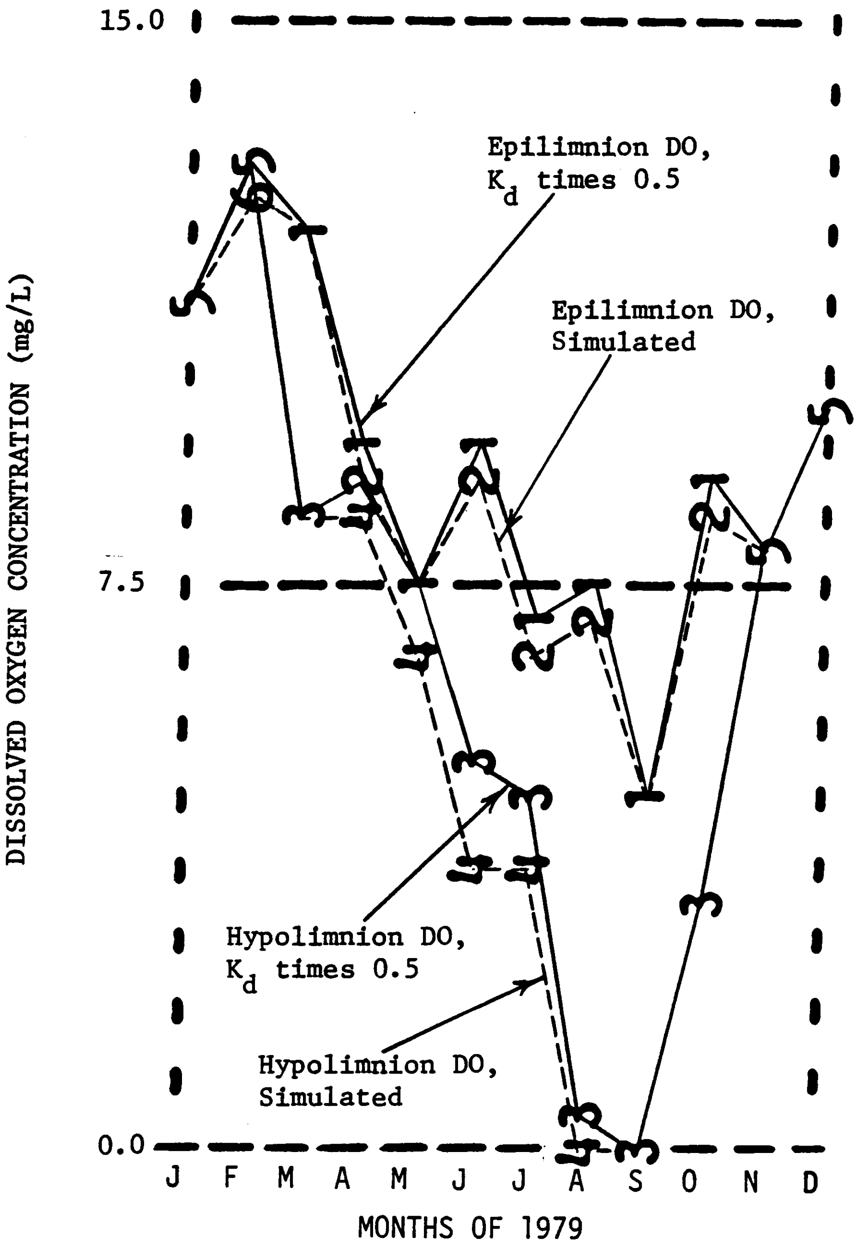

Figure 31. Sensitivity Analysis Number 6: DO Concentrations in the Bull Run Arm of Occoquan Reservoir (Lake 12) Resulting from Multiplying Deoxygenation Coefficients by 0.5

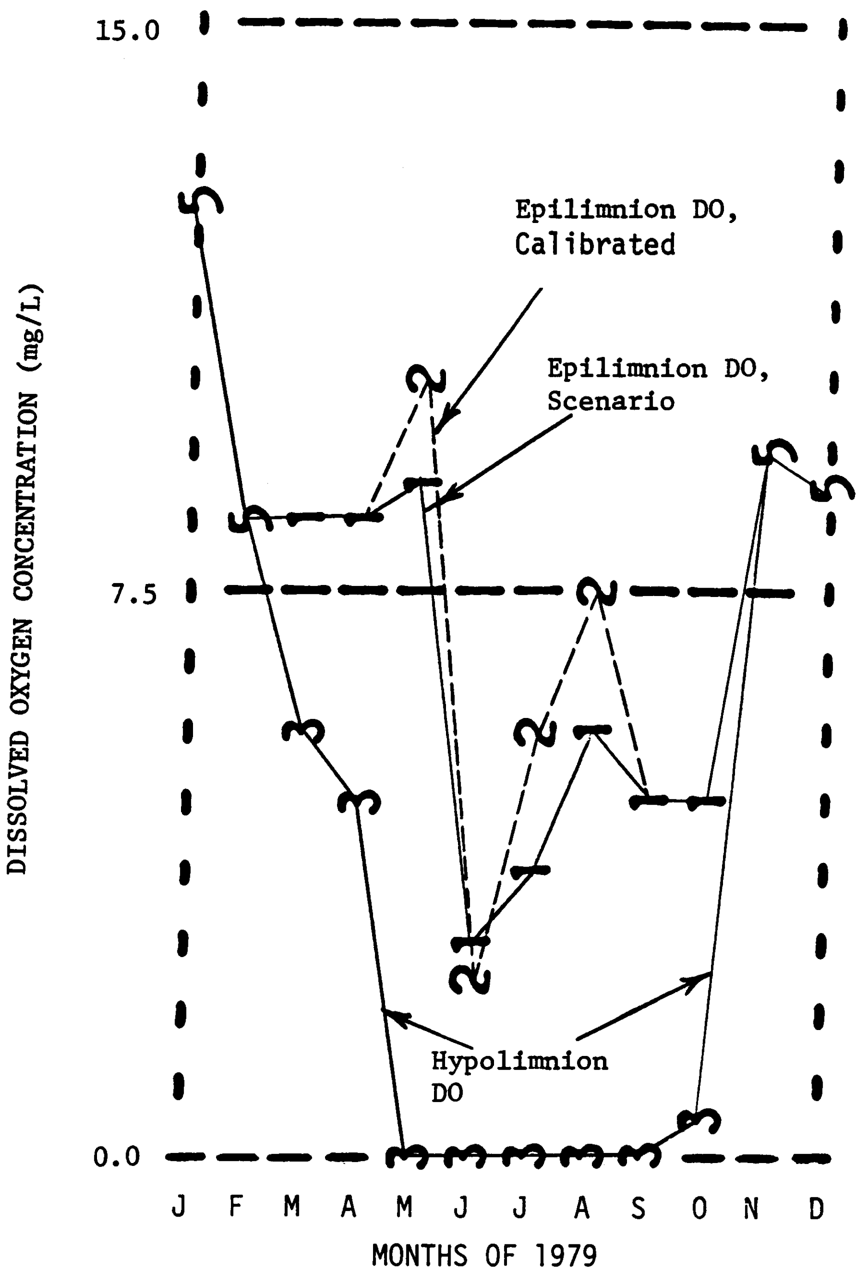

Figure 32. Scenario Test: DO Concentrations in Lake Jackson (Lake 13) Resulting from Increasing Commercial Land in Subbasin 13 from 0.0 Percent to 50.0 percent for the Entire Year.

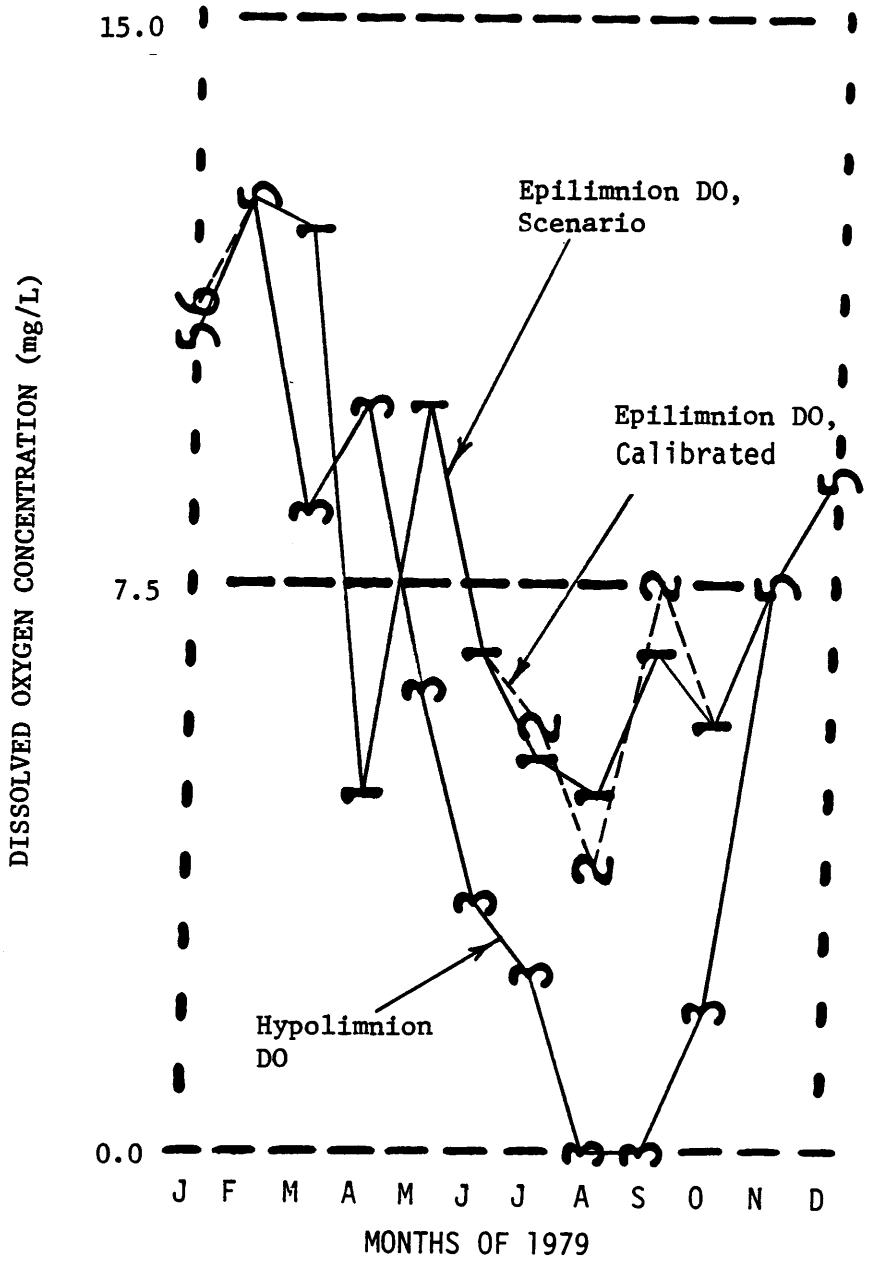

Figure 33. Scenario Test: DO Concentrations in Occoquan Reservoir (Lake 15) Resulting from Increasing Commercial Land in Subbasin 13 0.0 Percent to 50.0 Percent for the Entire Year.

CHAPTER VI

SUMMARY AND CONCLUSIONS

The original objective of this study, to develop a comprehensive water quality model capable of simulating the effects of population growth, development, and land use change, has only been partially completed. For one person, such an objective is an ambitious one indeed; even calibrating and verifying the model as it is presently developed would be a momentous task. On the other hand, with a group of workers it could obviously be done in a much shorter time.

This study has shown that the proposed method works and that there is a large data base available for expanding the model. The available data base includes masses of stream bottom material, periphyton biomasses, channel and floodplain dimensions, particle-size distributions in upland soil, heavy metals contents in stream sediments, phosphorus contents in upland soils, and phosphorus contents in stream sediments.

A model as descriptive as the proposed model offers much in the way of making management decisions and performing sensitivity analysis. How should land be zoned? Where and how should abatement facilities be constructed? What best-management practices should be promoted and where will they have the most effect? In what areas is research needed? A model such as proposed, in working form, would be better able to answer these questions than present basin-wide planning models.

In visualizing how the model could be used for management decisions, the idea of using the proposed model in conjunction with a linear cost optimization model, such as given by Jeng et al. (70), appears promising. The possibilities are many: zoning policies, abatement policies, and best management policies could be optimized together for any planning horizon. Another possibility follows the original idea: combining the proposed model with a more conventional DYNAMO model simulating social, technological, economic, and political interactions.

Using the proposed model in conjunction with dynamic runoff models such as SWMM and STORM is envisioned. In such a procedure, the proposed model would be used to help formulate overall basin-wide policy, while the dynamic models would be used for designing abatement facilities and for defining best operating policies. Thus the proposed model would be "strategic", the dynamic runoff models "tactical."

Conclusions

1. The objective of this study, to develop a long-term, basin-wide, water-quality-planning model for the Occoquan Basin in Northern Virgina, was not realized. At present, the model is coded for lake DO, sediment, phosphorus, eutrophication, and stream dynamics, and input data have been found for all of these, but the model is calibrated only for lake DO.

2. The method proposed in this thesis for modeling transport and transformation of pollutants works. System dynamics may be used to develop highly-descriptive, water-quality-planning models.

3. A large data base exists for expanding the model, a data base that includes masses of stream-bottom material, periphyton biomasses, particle-size distributions in upland soil, channel and floodplain dimensions, heavy metals contents in stream sediments, phosphorus contents in upland soils, and phosphorus contents in stream sediments. Such data have never before been used in a water-quality-planning model.

Recommendations

1. Before the Lake DO Submodel may be applied to making management decisions, the model needs to be verified. Verification will involve adjusting parameters so that the predictive capacity of the model is shown.

2. Levels and rates for the eleven stream channels need to be duplicated and modified to simulate both base-flow and runoff conditions. The simulation time interval, DT, would remain 1.0 month, and each level and rate applying to a stream channel would be multiplied by a factor indicating the fraction of the month in which base flow and runoff conditions occur.

3. The other parameters included in the model -- phosphorus compounds, sediment, stream dynamics, and eutrophication -- need to be calibrated, tested with sensitivity analyses, and verified.

4. The important pollutants not simulated -- stream dissolved oxygen, coliforms, nitrogen compounds, heavy metals, and pesticides -- need to be coded, calibrated, tested with sensitivity analyses, and verified.

CHAPTER VII

REFERENCES CITED

1. Metcalf and Eddy, Inc. (1970). 1969 Occoquan Reservoir study. Report prepared for the State Water Control Board, Commonwealth of Virginia, Richmond, Virginia.

2. To, Yan Pui Samuel (1974). Effects of sediment on water quality in the Occoquan Reservoir. PhD Thesis, Virginia Polytechnic Institute and State University.

3. Chaney, Gael Marshall (1975). The availability of sediment phosphate for algal growth. M.S. Thesis, Virginia Polytechnic Institute and State University.

4. Shugart, Stephen Lee (1976). Phosphorus readsorption on Occoquan sediments. M.S. Thesis, Virginia Polytechnic Institute and State University.

5. Markley, William E., III (1976). The occurence of select heavy metals, phosphorus, and nitrogen in the Occoquan Reservoir, Virginia. M.S. Thesis, Virginia Polytechnic Institute and State University.

6. McLaughlin, Stephen Gannon (1981). Reservoir sediment exchange of phosphate, ammonia, and metals under anaerobic and aerobic conditions. M.S. Thesis, Virginia Polytechnic Institute and State University.

7. Grizzard, Thomas G. (1985). Director, Occoquan Monitoring Laboratory, Manassas, Virginia. In a personal interview.

8. Sherman, Theresa Ellen (1983). The effect of nitrate on oxidation-reduction potentials and the adsorption and release of phosphate by reservoir sediment. M.S. Thesis, Virginia Polytechnic Institute and State University.

9. Streeter, H.W. and Phelps, E. B. (1925). A study of the pollution and natural purification of the Ohio River. Public Health Bulletin 146, U.S. Public Health Service, Washington, D.C.

10. Thomann, Robert V. (1984). Physiochemical and ecological modeling the fate of toxic substances in natural water systems. Ecol. Modell. 22, 145-170.

11. Texas Water Development Board (1970). DOSAG I, simulation of water quality in streams and canals. Report RA-202-974. Austin, Texas.

12. Systems Control, Inc. and Snohomish County Planning Department (1974). Water quality management plan for the Snohomish River Basin and the Stillaguamish River Basin, Volume IV -- computer program documentation, Part A: steady state stream model (SNOSCI), Snohomish County Planning Department, Everett, Washington.

13. Masch, Frank D. and Associates, and the Texas Water Development Board (1971). Simulation of water quality in streams and canals, theory and description of the QUAL-I mathematical modeling system. Report 128, the Texas Water Development Board, May 1971.

14. Roesner, Larry A., Monser, John R. and Evenson, Donald E. (1977). Computer program documentation for the stream quality model QUAL-II. EPA Cont. No. 68-01-0742, Water Res. Eng., Walnut Creek, California.

15. Grimsrud, G. Paul, Finnemore, E. John and Owen, H. James (1976). Evaluation of water quality models: A management guide for planners. Office of Research and Development USEPA-6000/5-76-004, Washington, D. C.

16. White, Jay D. and Dracup, John A. (1977). Water quality modeling of a high mountain stream. J. Wat. Pollut. Control Fed. 49, 2179-2189.

17. Bingham, David R., Lin, Chu-Hsien and Hoag, Robert S. (1984). Nitrogen cycle and algal growth modeling. J. Wat. Pollut. Control Fed. 56, 1118-1122.

18. Beck, M. B. (1983). A procedure for modeling. In Mathematical Modeling of Water Quality (Gerald T. Orlob, ed.), p. 19. Chichester, U.K.: John Wiley & Sons.

19. Loucks, D. P., and Lynn, W. R. (1966). Probabilistic models for predicting stream quality. Wat. Resour. Research 2, 593-605.

20. Thayer, R. P. and Krutchkoff, R. G. (1967). Stochastic model for BOD and DO in streams. Proc. Am. Soc. civ. Engrs, J. sanit. Engng Div. 9359-72.

21. Padgett, W. J., Schultz, G. and Tsokos, C. P. (1977). A stochastic model for BOD and DO in streams when pollutants are discharged over a continuous stretch. Int. J. Environ. Stud. 11, 45-55.

22. Tiwari, J. L., Hobbie, J. E., Reed, J. P. and Miller, M. C. (1978). Some stochastic differential equation models of an aquatic ecosystem. Ecol. Modell. 4, 3-27.

23. Finney, B. A., Bowles, D. S. and Windham, M. P. (1982). Random differential equations in water quality modeling. Wat. Resour. Research 18, 122-134.

24. Somlyody, L. (1982). Water-quality modeling: a comparison of transport-oriented and ecologly-oriented approaches. Ecol. Modell. 17, 183-207.

25. Fontaine, Thomas D., III (1983). A nonequilibrium approach to modeling toxic metal speciation in acid, aquatic ecosystems. Ecol. Modell. 22,85-100.

26. Kuwabara, James S., Leland, Harry V., and Bencala, Kenneth E. (1984). Copper transport along a Sierra Nevada stream. J. environ. Engng Div. Am. Soc. civ. Engrs 110, 646-655.

27. Gundelach, Jose M. and Castillo, Jorge E. (1976). Natural stream purification under anaerobic conditions. J. Wat. Pollut. Control Fed. 48, 1753-1758.

28. Bartell, S. M., Gardner, R. H. and O'Neill, R. V. (1984). The fates of aromatics model (FOAM): description, application, and analysis. Ecol. Modell. 22, 109-121.

29. Chen, Carl W. and Wells, John T., Jr. (1976). Boise River ecological modeling. In Modeling Biochemical Processes in Aquatic Ecosystems (Raymond P. Canale, ed.) pp. 171-203. Ann Arbor, Michigan: Ann Arbor Science Publishers, Inc.

30. Randall, Clifford W., Grizzard, Thomas J. and Hoehn, Robert C. (1978). Impact of urban runoff on water quality in the Occoquan watershed. Virginia Water Resources Research Center Bulletin 80, Virginia Polytechnic Institute and State University, Blacksburg, Virginia.

31. Krenkel, Peter A. and Novotny, Vladimir (1980). Water Quality Management,p. 220. New York: Academic Press.

32. Sliter, G. T. (1976). Focusing on nonpoint sources. J. Wat. Pollut. Control Fed. 48, 3-6.

33. Metcalf & Eddy, Inc., University of Florida and Water Resources Engineers, Inc. (1971). Stormwater management model, volume 1 -- final report. Water Pollution Control Research Series, U.S. Environmental Protection Agency Report No. 11024DOC07/71, July, 1971.

34. Medina, Miguel A., Jr., Huber, Wayne C., Heaney, James P. and Field, Richard. (1981). River quality model for urban stormwater impacts. J. Wat. Resour. Manage. Plann. Div. Am. Soc. civ. Engrs. 107, 263-280.

35. Litwin, Yoram J. and Donigian, Anthony S., Jr. (1978). Continuous simulation of nonpoint pollution. J. Wat. Pollut. Control Fed. 50, 2348-2361.

36. Colston, N. V. (1974). Characterization and treatment of urban land runmoff. EPA 670/2 74 096, Environmental Protection Agency, Washington, D. C.

37. AVCO Economic Systems Corporation (1970). Stormwater pollution from urban land activity. Federal Water Quality Administration, Washington, D. C.

38. Radzini, J. V. (1975). Effects of nonpoint discharge on urban stream quality. Proc. of the Amer. Water Res. Assn., Annual Symposium.

39. Hydrologic Engineering Center (1976). Storage, treatment, overflow, runoff model STORM users manual. U.S. Army Corps of Engineers, Davis, California.

40. Crawford, N. H. and Donigian, A. S., Jr. (1973). Pesticide transport and runoff model for agricultural lands. USEPA 660/2-74-013, U.S. Environmental Protection Agency, Washington, D.C.

41. Donigian, Anthony S., Jr. and Crawford, Norman H. (1976). Modeling pesticides and nutrients on agricultural lands. USEPA 600/2-76-043, Athens, Georgia.

42. Tubbs, Lawrence J. and Haith, Douglas A. (1981). Simulation Model for Agricultural Non-Point-Souce Pollution. J. Wat. Pollut. Control Fed. 53, 1425-1433.

43. Novotny, Vladimir, Tran, Hue, Simsiman, Geronimo V. and Chesters, Gordon (1978). Mathematical modeling of land runoff contaminated by phosphorus. J. Wat. Pollut. Control Fed. 150, 101-112.

44. Hydrocomp, Inc. (1978). The Occoquan Basin computer model: calibration, verification, and users manual. Prepared for the Northern Virginia Planning District Commission, 7309 Arlington Boulevard, Falls Church, Virginia.

45. Jewell, Thomas K., and Adrian, Donald Dean (1981). Development of improved stormwater quality models. J. environ. Engng Div. Am. Soc. civ. Engrs 107, 957-974.

46. Bedient, Philip B., Lambert, Jeff L. and Springer, Nina K. (1980). Stormwater pollutant load-runoff relationships. J. Wat. Pollut. Control Fed. 52, 2396-2404.

47. Dillon, P. J. and Liggett, J. A. (1983). An ephemeral stream-aquifer interaction model. Water Resour. Research 19, 621-626.

48. Christopherson, Nils, Seip, Hans M. and Wright, Richard F. (1982). A model for streamwater chemistry at Birkenes, Norway. Wat. Resour. Research 18, 977-996.

49. Chapra, S. C. and Gordimer, S. (1973). A steady-state, one-dimensional, estuarine water quality model. Data Systems Branch, EPA Region II, New York.

50. Hydroscience, Inc. (1972). Simplified mathematical modeling of water quality. Water Programs, USEPA-1971-444-367/392, Environmental Protection Agency, Washington, D. C.

51. Feigner, K. D. and Harris, H. S. (1970). Documentation report, FWQA dynamic estuary model. Federal Water Quality Administration, U.S. Department of the Interior.

52. Pritchard, D. W. (1969). Dispersion and flushing of pollutants in estuaries. J. Hydraul. Div., Am. Soc. civ. Engrs. 95, 115-124.

53. Vollenweider, R. A. (1975). Input-output models (with special reference to the phosphorus loading concept in limnology). Schweiz. Z. Hydrol. 37, 53-84.

54. Bella, David A. (1970). Dissolved oxygen variations in stratified lakes. J. sanit. Engng Div. Am. Soc. civ Engrs 96, 1129-1146.

55. Snodgrass, William J. and O'Melia, Charles R. (1975). Predictive model for phosphorus in lakes. Environ. Sci. + Technol. 9, 937-944.

56. Snodgrass, W. J. and Dillon, P. J. (1983). A test of two models of different levels of complexity for predicting changes of phosphorus concentration in a lake's outflow. Ecol. Modell. 19, 163-187.

57. Bierman, Victor J., Jr. and Swain, Wayland R. (1982). Mass balance modeling of DDT dynamics in Lakes Michigan and Superior. Environ. Sci. + Technol. 16, 572-579.

58. Schwarzenbach, R. P. and Imboden, D. M. (1984). Modelling concepts for hydrophobic organic pollutants in lakes. Ecol. Modell. 22, 171-212.

59. Gordon, John A. (19181). LARM two-dimensional model: an evaluation. J. environ. Engng Div. Am. Soc. civ. Engrs 107, 877-886.

60. Halfon, E. (1984). Error analysis and simulation of Mirex behaviour in Lake Ontario. Ecol. Modell. 22, 213-252.

61. Revelle, C. S., Loucks D. P., and Lynn, W. R. (1967). A management model for water quality control. J. Wat. Pollut. Control Fed. 39, 1164-1183.

62. Loucks, D. P., Revelle, C. S. and Lynn, W. R. (1967). Linear programming models for water pollution control. Management Science 14, A-166 to A-181.

63. Marsden, J. R., Pingrey, D. E. and Whinston, A. (1973). Application of nonlinear programming to water quality control. Water Air & Soil Pollut. 2, 155-169.

64. Bayer, M. B. (1977). A modelling method for evaluating water quality policies in nonserial river systems. Wat. Resour. Bull. 13, 1141-1151.

65. Young, Peter and Beck, Bruce (1974). The modeling and control of water quality in a river system. Automatica. 10, 455-468.

66. Biswas, Asit K. (1981). Model of the Saint John River, Canada. In Models for Water Quality Management (Asit K. Biswas, ed.), pp. 68-90. New York: McGraw Hill, Inc.

67. Hahn, Hermann H. and Cembrowicz, Ralf G. (1981). Model of the Neckar River, Federal Republic of Germany. In Models for Water Quality Management (Asit K. Biswas, ed.), pp. 158-221.

68. Emsellem, Yves and Bordet, Jean-Pierre (1981). Model for the Seine-Normandy Basin, France. In Models for Water Quality Management (Asit K. Biswas, ed.), pp. 222-272.

69. Newsome, David H. (1981). Model of the Trent River System, England. In Models for Water Quality Management (Asit K. Biswas, ed.), pp. 34-67. New York: McGraw Hill, Inc.

70. Jeng, Tzay-Rong, Uchrin, Christopher G., Granstrom, Marvin L. and Hsueh, Shing-Fu (1983). A linear program model for point-nonpoint source control decisions: theoretical development. Ecol. Modell. 19, 249-262.

71. Krenkel, Peter A. and Novotny, Vladimir (1980). Water Quality Management, p 382. New York: Academic Press.

72. Tuffey, T. J., Hunter, J. V. and Matulewich, V. A. (1974). Zones of nitrification. Wat. Resour. Bull. 10, 555-564.

73. Krenkel, Peter A. and Novotny, Vladimir (1980). Water Quality Management, pp. 638-639. New York: Academic Press.

74. Forrester, Jay W. (1971). World Dynamics. pp. 0-142. Cambridge, Massachusetts: Wright-Allen Press, Inc.

75. Grizzard, Thomas J. (1985). Director, Occoquan Monitoring Laboratory, Manassas, Virginia. In a personal interview.

76. West, Elizabeth A. (1978). The Equilibrium of Natural Streams, pp. 0-205. Norwich, U. K.: Geo Abstracts, Ltd.

77. Schumm, S. A. (1968). Speculations concerning paleohydrologic controls of terrestrial sedimentation. Bull. geol. Soc. Am. 79, 1573-1578.

78. Lyons, Joseph K. and Beschta, Robert L. (1983). Land use, floods, and changes: Upper Middle Fork Willamette River, Oregon (1936-1980). Water Resour. Research 19, 463-471.

79. Ryden, J. C., Syers, J. K. and Harris, R. F. (1972). Potential of an eroding urban soil for the phosphorus enrichment of streams: II. application of adopted method. J. Environ. Qual. 1, 435-438.

80. Baker, James (1985). Associate Professor of Agronomy, Virginia Polytechnic Institute and State University, Blacksburg, Virginia. In a personal interview.

81. Loucks, D. P., Stedinger, J. R. and Haith, D. A. (1981). Water Resource Systems Planning and Analysis, pp. 458-461. Englewood Cliffs, New Jersey: Prentice-Hall, Inc.

82. Porter, H. C., Derting,J. F., Elder, J. H., Henry, E. F. and Pendleton, R. F. (1963). Soil survey of Fairfax County, Virginia. Prepared by the U.S. Department of Agriculture in cooperation with the Virginia Agricultural Experiment Station and Fairfax County, Virginia. Published by the U.S. Government Printing Office, Washington, D.C.

83. Donohue, S. J. (1983). Virginia soil test summary -- FY1981. Extension Division, Virginia Polytechnic Institute and State University, Blacksburg, Virginia.

84. Bass, Michael L. (1980). Assessment of the damage to Bull Run Creek resulting from the Colonial Pipeline kerosene spill in Prince William County, Virginia, March 6, 1980 -- phase 1 -- water chemistry, sediment analysis and periphyton community analysis. Report submitted to the Department of Biological Sciences, Mary Washington College, Fredericksburg, Virginia, 22301.

85. Dawson, Brenda Louise (1980). The effects of urban runoff on the heavy metal concentrations, productivity, and autotrophic index of the periphyton from the Occoquan watershed. M.S. Thesis, Virginia Polytechnic Institute and State University.

86. Lorenz, William D., Jr. (1978). Heavy metals partitioning in a stream receiving urban runoff. M.S. Thesis, Virginia Polytechnic Institute and State University.

87. Chen, Chang-Ning (1974). Evaluation and control of soil erosion in urbanizing watersheds. Proceedings of the National Symposium of Urban Rainfall and Runoff and Sediment Control, University of Kentucky Bulletin BU106, Lexington, Kentucky.

88. Meyer, L. D. and Ports, M. A. (1976). Prediction and control of urban erosion and sedimentation, Mini-Course 1. Paper presented at the National Symposium on Urban Hydrology, Hydraulics, and Sediment Control, Univer-

sity of Kentucky, Lexington, Kentucky, 26-29. July 1976.

89. Haan, C. T. and Barfield, B. J. (1978). Hydrology and Sedimentology on Surface-Mined Lands. Lexington, Kentucky: Office of Continuing Education and Extension, College of Engineering, University of Kentucky.

90. Krenkel, Peter A. and Novotny, Vladimir (1980). Water Quality Management, p.382. New York: Academic Press.

91. Voshell, J. Reese (1981). Final report -- assessment of damage to the Rapidan River and Bull Run Creek resulting from two Colonial Pipeline oil spills -- phase II -- benthic macroinvertebrates. Report prepared for the Rockwell International Corporation Environmental Monitoring and Services Center, 2421 West Hillcrest Drive, Newbury Park, California.

92. McHugh, James J. (1980). Colonial Pipeline oil and kerosene spill fishery damage assessment. Report prepared by the Virginia Commission of Game and Inland Fisheries, Fredericksburg, Virginia.

93. Buikema, Arthur L. (1985). Professor of Biology, Virginia Polytechnic Institute and State University, Blacksburg, Virginia. In a personal interview.

94. Chen, Carl W. and Smith, Donald J. (1979). Preliminary insights into a three-dimensional ecological-hydrodynamic model. In Perspectives on Lake Ecosystem Modeling (Donald Scavia and Andrew Robertson, eds), pp. 249-279. Ann Arbor, Michigan: Ann Arbor Science Publishers, Inc.

95. Randall, C. W. and Grizzard, T. J. (1983). Runoff Pollution. In Stormwater Management in Urbanizing Areas (William Whipple, ed.), pp. 85-86. Englewood Cliffs, New Jersey: Prentice-Hall, Inc.

96. Brady, N. C. (1974). The Nature and Properties of Soil, p. 48. New York: MacMillan Publishing Co., Inc.

APPENDIX A

TABLES

Table A-1. Phosphorus contents in bottom sediments, for for calibration for 1979. Estimations based on data from To (2), Chaney (3), Shugart (4), McLaughlin (6), and Sherman (8).

Stream Channel	Phosphorus Content in Bottom Sediment (Kg/Kg)
1	0.0005
2	0.0005
3	0.0005
4	0.0006
5	0.0007
6	0.0005
7	0.0007
8	0.0006
9	0.00085
10	0.00085
11	0.00085
12	0.00085
13	0.0007
14	0.00068
15	0.00085

Table A-2. Rates of adsorption and desorption of orthophosphate to/from stream sediments, as estimated from To (2), McLaughlin (6), and Sherman (8).

Type of Adsorption	Zero-order Rate Constant (Kg/Kg-day)	First-order Rate Constant (Kg/Kg-day)
Anaerobic release	0.000012	
Aerobic uptake		0.13
Aerobic release		0.0

Table A-3. Descriptions of Stream Stations and Stream Channels.

STREAM STATION	DESCRIPTION	OWMP DESIGNATION	STREAM NUMBER	DESCRIPTION
1	Cedar Run near Catlett		1	Cedar Run
2	Cedar Run near Aden	51ST20	2	Cedar Run
3	Mouth Cedar Run		3	Cedar Run
4	Broad Run at Buckland	51ST70	4	Broad Run
5	Broad Run below Lake Manassas		5	Lake Manassas
6	Mouth Kettle Run		6	Kettle Run
7	Mouth Broad Run		7	Broad Run
8	Bull Run below Confl. Little Bull Run		8	Bull Run
9	Cub Run near Bull Run	51ST50	9	Cub Run
10	Bull Run at Manassas		10	Bull Run
11	Bull Run near Manassas		11	Bull Run
12	Bull Run at Confl. Occoquan River	51RE30	12	Bull Run Arm
13	Occoquan River near Manassas	51ST10	13	Lake Jackson
14	Occoquan River at Confl. Bull Run	51RE25	14	Occoq. Riv. Arm
15	Occoquan R. below Occoquan Reservoir	51RE01	15	Occoquan Reservoir

Table A-4. Particle-size distributions in A horizons of upland soil, for calibration for 1979. Estimations based on County Soil Surveys for the Commonwealth of Virginia (82).

subbasin	percent clay	percent silt	percent sand	percent gravel	percent boulders
1	12.	62.	16.	5.0	5.0
2	15.	65.	20.	0.0	0.0
3	15.	65.	20.	0.0	0.0
4	12.	62.	16.	5.0	5.0
5	19.	62.	16.	2.0	0.0
6	18.	57.	20.	2.0	0.05
7	18.	57.	20.	1.0	0.05
8	19.	58.	19.	1.0	0.0
9	20.	58.	22.	0.1	0.06
10	18.	46.	20.	2.0	1.0
11	16.	61.	20.	0.5	0.4
12	15.	61.	20.	0.0	0.0
13	15.	65.	20.	0.0	0.0
14	14.	44.	32.	0.0	0.0
15	14.	44.	32.	0.0	0.0

Table A-5. Particle-size distributions in B horizons of upland soil, for calibration for 1979. Estimations based on County Soil Surveys for the Commonwealth of Virginia (82).

subbasin	percent clay	percent silt	percent sand	percent gravel	percent boulders
1	18.	49.	22.	6.0	5.0
2	20.	50.	25.	4.0	1.0
3	20.	50.	25.	4.0	1.0
4	18.	49.	22.	6.0	5.0
5	22.	49.	22.	6.0	0.5
6	37.	41.	14.	4.0	0.5
7	37.	41.	14.	4.0	0.5
8	37.	41.	15.	4.0	0.0
9	40.	41.	13.	0.2	0.06
10	38.	37.	14.	4.0	1.0
11	30.	46.	17.	2.0	1.0
12	31.	46.	19.	0.0	0.0
13	31.	48.	19.	0.0	0.5
14	28.	37.	32.	2.0	0.5
15	28.	37.	32.	2.0	1.0

Table A-6. Particle-size distributions in C horizons of upland soil, for calibration for 1979. Estimations based on County Soil Surveys for the Commonwealth of Virginia (82).

subbasin	percent clay	percent silt	percent sand	percent gravel	percent boulders
1	18.	49.	22.	6.0	5.0
2	20.	50.	25.	4.0	1.0
3	20.	50.	25.	4.0	1.0
4	18.	49.	22.	6.0	5.0
5	22.	49.	22.	6.0	0.5
6	19.	40.	25.	6.0	0.5
7	19.	40.	25.	6.0	0.5
8	22.	38.	25.	1.0	0.0
9	18.	40.	25.	0.4	0.3
10	19.	40.	25.	6.0	5.0
11	18.	43.	25.	7.0	3.0
12	13.	43.	24.	9.0	1.0
13	13.	51.	24.	9.0	1.0
14	23.	35.	34.	6.0	1.0
15	23.	35.	34.	6.0	1.0

Table A-7. Extractable phosphorus contents in upland soils of A Horizons, by subbasin, for calibration for 1979. Estimated from the Virginia Soil Test Summaries (83).

SUBBASIN	"A" HORIZON EXTRACTIBLE PHOSPHORUS CONTENT (PPM)					
	LAWNS	FOREST	PASTURE	INSTITU-TIONA	VEGETABLE GARDENS	COMMERCIAL FARMLAND
1	20.	2.0	19.	35.	33.	17.
2	20.	2.0	19.	35.	33.	17.
3	30.	2.0	14.	35.	39.	18.
4	22.	2.0	18.	35.	34.	17.
5	28.	2.0	15.	35.	38.	18.
6	30.	2.0	14.	35.	39.	18.
7	30.	2.0	14.	35.	39.	18.
8	31.	2.0	16.	35.	39.	19.
9	19.	2.0	19.	36.	40.	33.
10	29.	2.0	17.	36.	40.	26.
11	28.	2.0	19.	36.	40.	35.
12	29.	2.0	17.	36.	40.	28.
13	30.	2.0	14.	35.	39.	18.
14	30.	2.0	14.	35.	39.	18.
15	29.	2.0	17.	36.	40.	28.

Table A-8. Stream survey performed by the author on 21 March, 1985.

SAMPLING STATION	CHANNEL WIDTH (FT)	CHANNEL DEPTH (FT)	BANK DEPTH (FT)	BOTTOM EXCHANGE MATERIAL RIFFLES	EDDYS	PERCENT RIFFLES
SS-1	25.	3.0	2.5	10% fines 50% boulders 40% gravel	10% fines 50% boulders 40% gravel	20.
SS-2	30.	2.5	2.0	98% boulders 2% gravel	98% boulders 2% gravel	50.
SS-3	70.	3.0	2.0	60% gravel 40% boulders	70% boulders 30% gravel	25.
SS-4	60.	8.0	4.0	95% gravel 3% sand 2% boulders	60% gravel 20% detritus 9% sand 9% fines 2% boulders	15.
SS-5	80.	8.0	2.0		99% detritus	0.0
SS-6	75.	4.0	2.5		40% sand 40% fines 9% sand 15% gravel 5% boulders	5.0
SS-7	80.	11.	6.0		65% gravel 25% boulders 10% fines	0.0
SS-8	30.	4.0	2.5		85% fines 10% boulders 5% detritus	0.0
SS-9	35.	3.5	2.5	90% gravel 9% sand 1% boulders	90% fines 10% detritus	10.
SS-10	70.	9.0	3.0		70% boulders 29% fines 1% sand	0.0
SS-11	40.	6.0	5.0	60% gravel 30% boulders 10% sand	60% gravel 30% boulders 10% sand	20.
SS-12	30.	3.5	3.0		90% boulders 9% gravel 1% sand 1% fines	1.0
SS-13	70.	8.0	3.0	95% gravel 5% boulders	45% sand 25% fines 10% boulders 2% gravel	65.
SS-14	200.	8.0		70% gravel 20% sand 10% boulders	70% gravel 20% sand 10% boulders	20.

Table A-9. Masses of sediment material in the bed exchange layer of stream channels, for calibration for 1979. Estimated from a stream survey preformed on 21 March 1985 and from data presented by Bass (84), Dawson (85), To (2), Shugart (4), and Lorenz (86).

STREAM CHANNEL	MASSES OF SEDIMENT IN BED EXCHANGE LAYER* (TON)				
	CLAY	SILT	SAND	GRAVEL	BOULDERS
1	1.9	3.9	0.0	43.	80.
2	3.2	5.4	8.4	43.	1.4
3	4.0	7.9	8.6	13.	13.
4	13.	40.	47.	13.	4.4
5	70.	206.	90.	0.0	0.0
6	12.	32.	0.4	1.7	0.3
7	28.	61.	2.7	0.0	140.
8	1.3	5.1	8.3	21.	10.
9	0.2	0.2	0.3	1.7	19.
10	7.6	15.	24.	43.	23.
11	2.2	4.4	12.	43.	14.
12	35.	99.	23.	0.0	0.0
13	26.	76.	33.	0.0	0.0
14	36.	105.	46.	0.0	0.0
15	105.	300.	69.	0.0	0.0

* Assuming a bed exchange layer depth of 2.0 mm for streams, 0.5 mm for lakes. Also assuming a specific gravity of 2.65 for all sediments.

Table A-10. Seasonal variation in the Rainfall Factor, R, as used in the Universal Soil Loss Equation, for Fairfax County, Virginia. From Chen (87).

Month	Monthly Distribution of R	Rainfall Factor, R
JAN	0.03	6
FEB	0.03	4
MAR	0.04	8
APR	0.04	8
MAY	0.09	18
JUN	0.12	24
JUL	0.20	40
AUG	0.22	44
SEP	0.10	20
OCT	0.06	12
NOV	0.05	10
DEC	0.03	6

Table A-11. Soil erodibility factors for use the Universal Soil Loss Equation. Estimated from values for Fairfax County, Virginia, given by Chen (87), and from a nomograph given by Chen (87).

Subbasin	Soil Erodibility Factor, K
1	0.28
2	0.30
3	0.35
4	0.30
5	0.36
6	0.42
7	0.34
8	0.28
9	0.29
10	0.28
11	0.34
12	0.33
13	0.28
14	0.24
15	0.34

Table A-12. Length-slope factors, LS, for use the Universal Soil Loss Equation. Estimated from a nomograph given by Chen (87).

SUBBASIN	AVG. LAND SLOPE*	TYPICAL LENGTH OF SLOPE** (FT)	LENGTH-SLOPE FACTOR, LS
1	3.51	370.	0.6
2	3.50	425.	0.7
3	6.56	377.	1.6
4	7.77	366.	1.8
5	4.80	355.	0.6
6	3.44	32.	0.6
7	4.51	375.	1.0
8	6.81	344.	1.5
9	3.98	387.	1.8
10	5.28	430.	1.2
11	10.3	304.	2.6
12	14.1	309.	4.3
13	12.8	273.	3.4
14	13.3	282.	3.6
15	12.4	255.	3.3

* Average values given by Hydrocomp (44).

** From divide to first-order channel, as given by Hydrocomp (44).

Table A-13. Vegetal cover factors, C, applicable to the Occoquan Basin, for use in the Universal Soil Loss Equation. Based on values given by Haan and Barfield (89).

Land Use	Vegetal Cover Factor (C)
commercial	0.5
estate	0.01
forest	0.001
large lot residential	0.05
medium density residential	0.1
town house	0.1
industrial	0.2
institutional	0.01
conventional tillage	1.0
minimum tillage	0.9
pasture	0.4

Table A-14. Sediment delivery ratio's for the fifteen subbasins.

SUBBASIN	TYPICAL DRAINAGE AREA OF FIRST ORDER TRIBUTARIES TO THE CHANNEL* (SQ. MI.)	DELIVERY RATIO**
1	10.	0.32
2	8.	0.35
3	3.	0.40
4	7.	0.37
5	3.	0.40
6	3.	0.40
7	2.	0.42
8	4.	0.39
9	6.	0.38
10	3.	0.40
11	12.	0.30
12	1.	0.45
13	1.	0.45
14	2.	0.42
15	3.	0.40

* Estimated from 1:250000 scale USGS mapping.

** Based on Figure 2 of Chen (85).

Table A-15. Lengths and slopes of channels and valleys, by subbasin. Estimated from USGS mapping.

Subbasin	Channel Length (mi.)	Channel Slope	Valley Length (mi.)	Valley Slope
1	10.6	0.00229	9.7	0.00250
2	6.8	0.000863	5.9	0.000995
3	9.4	0.000443	8.3	0.000502
4	6.8	0.00448	6.8	0.00406
5	3.0	0.0	3.0	0.00360
6	6.1	0.00202	5.5	0.00224
7	15.6	0.000971	13.7	0.00111
8	6.1	0.00211	5.3	0.00243
9	4.1	0.00249	3.7	0.00276
10	8.3	0.000685	7.1	0.000800
11	5.2	0.000474	4.9	0.000502
12	5.3	0.0	5.3	--
13	4.6	0.0	4.4	--
14	8.0	0.0	7.5	--
15	8.9	0.0	8.9	--

Table A-16. Medians of monthly average flows, by stream station. Based on ten years of USGS Water Resource data and, where no data exist, drainage area ratios.

STR.	DRAINAGE	MEDIANS OF MONTHLY AVERAGE FLOWS (CFS)											
STA.	AREA (AC)	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	61600.	135.	106.	121.	78.	51.	25.	19.	24.	8.	20.	30.	95.
2	102300.	182.	205.	255.	120.	83.	31.	27.	66.	16.	27.	68.	153.
3	132000.	240.	260.	330.	160.	110.	40.	40.	80.	20.	40.	90.	200.
4	33300.	73.	67.	73.	56.	38.	23.	12.	24.	14.	16.	27.	57.
5	49300.	110.	100.	110.	80.	60.	34.	18.	36.	21.	24.	40.	84.
6	17000.	37.	34.	37.	28.	19.	12.	6.	12.	7.	8.	14.	29.
7	73300.	160.	149.	160.	123.	84.	51.	26.	53.	31.	35.	59.	125.
8	55000.	150.	97.	101.	75.	51.	24.	16.	17.	15.	12.	33.	171.
9	32900.	82.	59.	71.	61.	41.	19.	12.	12.	8.	16.	22.	42.
10	97700.	267.	172.	180.	133.	90.	42.	29.	30.	26.	21.	59.	303.
11	122100.	335.	289.	303.	366.	177.	117.	56.	56.	186	108.	133.	346.
12	126500.	347.	300.	310.	380.	180.	120.	58.	58.	190	110.	140.	360.
13	226400.	529.	420.	459.	445.	199.	70.	62.	47.	28.	65.	169.	405.
14	237000.	550.	440.	480.	465.	210.	73.	65.	49.	29.	68.	177.	420.
15	389000.	960.	790.	840.	900.	420.	210.	132.	115.	230	190.	340.	834.

Table A-17. Seven-day, ten-year low flows, by stream station. Based on USGS Water Resource data and, where no data exist, drainage area ratios.

Stream Station	Drainage Area (acre)	Seven-Day, Ten-Year Low Flow (cfs)
1	61600.	0.2
2	102300.	0.6
3	132000.	0.7
4	33300.	0.6
5	49300.	0.8
6	17000.	0.1
7	73300.	1.3
8	55000.	0.4
9	32900.	0.2
10	97700.	0.9
11	122100.	6.9*
12	126500.	7.0*
13	226400.	1.0
14	237000.	1.2
15	389000.	7.3*

* Affected by sewage flow.

Table A-18. Land use fractions for 1979, by subbasin. Estimated from a map prepared by the Northern Virginia District Planning Commission in 1977 and revised in 1979. See Table A-19 for a continuation.

SUBBASIN	LAND USE FRACTIONS FOR 1979.						
	LAKE	ESTATE	LARGE LOT RESIDENTIAL	MEDIUM DENSITY RESIDENTIAL	TOWN HOUSE	COMMERCIAL	INDUSTRIAL
1	0.000	0.044	0.019	0.000	0.000	0.005	0.002
2	0.000	0.016	0.002	0.000	0.000	0.000	0.000
3	0.000	0.000	0.010	0.000	0.000	0.001	0.000
4	0.000	0.013	0.002	0.000	0.000	0.000	0.000
5	0.032	0.029	0.092	0.000	0.000	0.005	0.009
6	0.000	0.013	0.042	0.000	0.000	0.000	0.000
7	0.000	0.000	0.027	0.006	0.000	0.006	0.039
8	0.000	0.000	0.049	0.000	0.000	0.001	0.001
9	0.005	0.033	0.034	0.007	0.002	0.078	0.006
10	0.000	0.000	0.015	0.101	0.025	0.015	0.024
11	0.000	0.019	0.082	0.038	0.004	0.012	0.002
12	0.104	0.000	0.061	0.000	0.000	0.000	0.000
13	0.030	0.000	0.147	0.000	0.000	0.000	0.000
14	0.013	0.000	0.083	0.002	0.000	0.002	0.000
15	0.045	0.037	0.049	0.051	0.000	0.001	0.000

Table A-19. Land use fractions for 1979, continued from Table A-18.

SUBBASIN	LAND USE FRACTIONS FOR 1979.				
	INSTITUTIONAL	PASTURE	CONVENTIONAL TILLAGE	MINIMUM TILLAGE	FOREST
1	0.004	0.373	0.148	0.034	0.354
2	0.001	0.180	0.284	0.022	0.497
3	0.002	0.299	0.000	0.071	0.617
4	0.000	0.288	0.397	0.213	0.364
5	0.024	0.215	0.019	0.042	0.532
6	0.016	0.265	0.021	0.098	0.545
7	0.003	0.218	0.000	0.081	0.641
8	0.001	0.208	0.085	0.118	0.536
9	0.006	0.104	0.054	0.140	0.583
10	0.024	0.088	0.011	0.026	0.671
11	0.005	0.084	0.000	0.019	0.734
12	0.000	0.061	0.000	0.026	0.748
13	0.000	0.334	0.000	0.000	0.789
14	0.000	0.037	0.000	0.029	0.834
15	0.004	0.022	0.000	0.000	0.791

Table A-20. Dissolved oxygen rate constants, by month. Estimated from values given by Chen and Wells (29) and Krenkel and Novotny (90).

MONTH	DEOXYGENATION COEFFICIENT FOR DISSOLVED BOD, K1 (1/MONTH)	DEOXYGENATION COEFFICIENT FOR SUSPENDED BOD, KS1 (1/MONTH)	NITRIFICATION COEFFICIENT, KN (1/MONTH)
JAN	0.01	0.01	0.1
FEB	0.05	0.01	0.1
MAR	0.2	0.05	0.4
APR	1.0	0.15	1.0
MAY	2.0	0.25	1.3
JUN	3.5	0.40	1.6
JUL	5.0	0.50	2.0
AUG	6.0	0.45	1.9
SEP	5.0	0.40	1.7
OCT	3.0	0.25	1.0
NOV	0.8	0.10	0.5
DEC	0.05	0.03	0.2

Table A-21. Periphyton biomasses in stream channels, for calibration for 1979. Based on data given by Bass (84).

CHANNEL	AREA OF THE CHANNEL BOTTOM (SQ. FT.)	PERCENT BOULDERS AND GRAVEL IN THE BOTTOM EXCHANGE LAYER	DRY, ASH-FREE BIOMASSES OF ALGAL PERIPHYTEN (LB)
1	1680000.	97.	180.
2	2510000.	63.	140.
3	3970000.	20.	220.
4	2690000.	30.	90.
6	966000.	6.0	7.0
7	5770000.	70.	320.
8	1290000.	75.	110.
9	648000.	98.	70.
10	3070000.	66.	160.
11	1920000.	81.	120.

Table A-22. Periphyton productivity rates for the summer of 1979. From Dawson (85).

Month	Subbasin	Mean Periphyton Productivity Rates (mg/sq m-day)
JUL	10 11 12 15	50.3 91.2 41.7 53.5
AUG	10 11 12 15	48.8 123. 212. 53.0
SEP	12 15	95.0 184.
OCT	12 15	48.3 232.

Table A-23. Benthic macroinvertebrate biomasses to be used for calibration for 1979. Estimations based on the data of Voshell (91).

CHANNEL	DRY, ASH-FREE BENTHIC BIOMASSES (LB/SQ FT) TIMES 10^5											
	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC
1	6.3	6.4	6.5	6.6	6.8	6.8	7.0	6.8	6.8	6.6	6.5	6.4
2	10.2	10.2	12.3	14.3	14.3	15.3	15.8	15.8	14.7	13.8	12.3	11.4
3	14.3	15.9	17.8	19.4	21.3	23.1	24.5	24.5	22.7	20.8	18.8	16.6
4	6.3	6.4	6.5	6.6	6.8	6.8	7.0	6.8	6.8	6.6	6.5	6.4
6	6.3	6.4	6.5	6.6	6.8	6.8	7.0	6.8	6.8	6.6	6.5	6.4
7	14.3	15.9	17.8	19.4	21.3	23.1	24.5	24.5	22.7	20.8	18.8	16.6
7	14.3	15.9	17.8	19.4	21.3	23.1	24.5	24.5	22.7	20.8	18.8	16.6
8	1.5	1.6	1.7	1.8	1.9	2.0	2.0	4.1	3.7	2.4	1.8	1.6
9	1.5	1.6	1.7	1.8	1.9	2.0	2.0	4.1	3.7	2.4	1.8	1.6
10	7.0	6.4	5.9	5.4	4.9	4.4	5.1	2.7	4.6	5.3	6.0	6.5
11	12.5	13.0	13.5	14.0	14.5	15.0	15.5	14.6	14.2	13.8	13.4	13.0
14	12.5	13.0	13.5	14.0	14.5	15.0	15.5	14.6	14.2	13.8	13.4	13.0

Table A-24. Benthos emergence rates for the Boise River, Idaho. From Chen and Wells (29).

Month	Emergence Rate (mg/m^2-month)
JAN	0.4
FEB	0.0
MAR	0.4
APR	0.0
MAY	0.1
JUN	0.1
JUL	0.1
AUG	0.15
SEP	0.1
OCT	0.07
NOV	0.0
DEC	0.0

Table A-25. Fish biomass estimations, for calibration for 1979. Based on McHugh (92).

Channel	Dry Weight of Fish per Mile (lb)	Channel Length (mi)	Dry Fish Biomass (lb)
1	29.	10.6	310.
2	70.	6.8	480.
3	170.	9.4	1600.
4	29.	6.8	200.
5	2700.	3.0	8100.
6	29.	6.1	180.
7	170.	15.6	2650.
8	29.	6.1	180.
9	29.	4.1	120.
10.	170.	8.3	1410.
11	170.	5.2	880.
12	990.	5.3	5250.
13.	900.	4.6	4140.
14	900.	8.0	7200.
15	780.	8.9	6940.

Table A-26. Zooplankton concentrations for calibration for 1979. Taken from values presented for Lake Ontario by Chen and Smith (94).

Season	Herbivorous Zooplankton Concentration (mg/l)	Carnivorous Zooplankton Concentration (mg/l)
Winter	0.01	0.14
Summer	0.005	0.07

Table A-27. Lake Volumes. From values given by McLaughlin (6), Markley (5), Dawson (85) and from a topographic map prepared by the Northern Virginia District Planning Commission.

Lake	Winter Pool Volume (ac-ft)	Epilimnion Volume (ac-ft)	Hypolimnion Volume (ac-ft)
5	17680.	5360.	12990.
12	4790.	1220.	2760.
13	2760.	570.	2190.
14	6410.	1870.	4140.
15	21110.	6250.	12990.

Table A-28. Pollutant export rates in runoff. Estimated from a tabulation of values from previous stormwater monitoring programs compiled by Randall and Grizzard (95).

LAND USE	EXPORT OF DISSOLVED BOD IN RUNOFF (LB/ACRE-YR)	EXPORT OF DISSOLVED ORTHOPHOSPHATES IN RUNOFF (LB/ACRE-YR)
estate	45.	0.6
large lot residential	30.	0.15
medium density residential	65.	0.5
town house	80.	0.8
commercial	80.	1.0
industrial	80.	0.3
institutional	45.	0.04
forest	10.	0.04
pasture	45.	0.09
conventional tillage	45.	0.1
minimum tillage	30.	0.1

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