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INTRODUCTION

Water problems are centuries old, and problems of industrial pollution date back to the beginning of the industrial revolution. Expanding population and industry, together with increasing abuse of water resources, only accentuated the seriousness of the problems.

The sixth volume of the Proceedings is concerned about the impact of the water quality on the environment and the availability of water resources to the increasing needs. The "Annual December Meeting in Washington, D.C." with the World Bank as host became a traditional review of the world situation in water resources distribution in the past three academic years.

On December 4-8, 1972 in Mexico City the International Symposium on Water Resources Planning was held and four papers were delivered by our Seminar members.

In June 1973 in Madrid the Symposium on the Design of Water Resources Projects with Inadequate Data was organized by UNESCO, WMO and IAHS. The Seminar participated with two papers. Similarly, on March 4-8, 1974 one paper represented the Seminar in the UNESCO sponsored International Symposium on Hydrology of Volcanic Rocks, Canary Islands.

On July 30-August 2, 1974 IFIP Conference on Modeling and Simulation of Water Resources at Ghent University, Belgium, a report on the water resources data bank (LORDS) of New Jersey was presented by the Seminar.

The editors of the Proceedings wish to express their gratitude to all members contributing articles and lectures to foster the Seminar. The publication was made possible only by the generous help and cooperation of the U.S. Department of the Interior, Geological Survey and the State of New Jersey, Department of Environmental Protection in the series of U.S. Geological Survey--Water Resources Investigation.

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HYDROLOGICAL INVESTIGATION

OF THE UNSATURATED ZONE

by

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According to the terms and definitions generally accepted throughout the world, the water stored below the surface of the Earth is divided into two basicly different parts. Ground water is the larger part and completely fills all pores, hollows, fissures and fractures of the crust below a continuous water surface called water table. Above this level only a part of pores is occupied by water and the other part is filled with air. The relatively very thin layer between the surface and the water table is called, therefore, unsaturated zone or the zone of aeration. The second type of subsurface water is soil moisture stored in this zone.

Although the thickness of the unsaturated zone (a few meters, sometimes several decimeters) is negligible compared to the thousands of meters of thickness of the crust, its importance is not proportional to this ratio. This zone forms the surface of the Earth and includes the arable topsoil. Thus the result of any agricultural activity is not only closely connected to but basically determined by the behavior of the unsaturated zone. In this role of the unsaturated zone the importance of water is predominant, because it is well known that a sufficient ratio of water to air in the pores is a precondition of agricultural production. For this reason the investigation of water movement in the pores of soil has great practical importance.

From a purely hydrological standpoint as well, the processes occurring in the unsaturated zone have important roles. This is the zone of contact between the two terrestrial branches of the hydrological cycle (i.e., between surface and ground water), and together with vegetation governs evaporation and transpiration from the continents, and influences interchange between terrestrial and the atmospheric sections of the cycle as well. Surface runoff depends on infiltration, local storage, and evaporation, and these parameters are basically affected by the condition and behavior of the unsaturated zone. Ground water is recharged mostly through overlying layers and a considerable proportion of drainage interchanged between saturated and unsaturated zones. Evaporation and transpiration are always functions of actual moisture content of the soil and the latter depends on the storage capacity of the layers above the water table. Thus the effect of the unsaturated zone on some hydrological and hydrometeorological processes is also evident.

The central role of the unsaturated zone in the hydrological cycle proves the importance of investigations of processes occurring in the layers near the surface. The high number of the influencing factors inherent in this role causes, however, difficulties at the same time. Although any type of hydrological study has to be carried out considering the largest possible field of the hydrological cycle as a unit, in this case the investigation has to be limited to a relatively small prism of the unsaturated zone and the external effects have to be substituted as inputs and outputs of the system. Even after this restriction of the analysis there are problems remaining which hinder the correct study of the unsaturated zone. When applying water balance equations, a basic requirement is to measure all components separately and to use the equations in a form reduced to zero. In this case the measuring errors are combined as the closing errors of the equations. If one of the components is not measurable and is eliminated from the water balance equation, all measuring errors are included with this amount and its reliability is questionable. In the case of the present investigation, because of the high number of phenomena occurring in the unsaturated zone and also because of their interwoven character, water balance equations can only be applied in the incorrect form mentioned. It is necessary, therefore, to raise the accuracy of the observations and to develop special measuring equipment (lysimeters combined with soil moisture measurements). Theoretical investigations concerning storage capacity of and water movement through the unsaturated zone can also decrease the uncertainties in the hydrological description of layers above the water table.

According to aspects explained in the previous paragraph, the summarization of hydrological investigations concerning the unsaturated zone can be divided into three parts. The first chapter includes the detailed description of hydrological phenomena and their interactions together with the evaluation of data collected with lysimeters. The second part deals with the theoretical analysis of the pF curve, which is an important aid for the characterization of storage capacity in the unsaturated zone. Finally, the investigations of hydraulic resistivity of porous media can be extended to cases in which pores are only partly filled with water, containing also air. The physical relationships used in description of vertical water movement in the unsaturated layer can give important information for the analysis of the process of infiltration as it is summarized in Chapter 3.

1. HYDROLOGICAL PROCESSES OCCURRING IN THE UNSATURATED ZONE

The investigation of these processes is a boundary field of surface water hydrology, ground water hydrology (hydrogeology), and pedology (soil science and agronomy). Because of this interdisciplinary character and partly because of the very many influencing phenomena and factors, the collected data and the results of basic research concerning the unsaturated zone are not yet sufficient to describe correctly and completely these processes, although the solution of many practical problems requires the synthesis of a well founded mathematical model.

For clarification of hydrological phenomena occurring in the unsaturated zone and their interaction, a physical model of this zone was established to indicate all acting effects. As shown schematically in fig. 1, the physical model does not include only the unsaturated zone but also the zone of plants covering it, as well as a part of the gravitational ground water space, which is the lower boundary of the zone of aeration. The path of water within or through the unsaturated zone can be easily followed in this model.

The physical model can be regarded also as the vertical section of a lysimeter. It can be used, therefore, for detailed analysis of the reliability of this very important measuring instrument and for evaluation of data collected by lysimeters (Kovács and Péczely, 1973).

1. Analysis of relevant hydrological processes

Regarding the model as a closed system, the water amounts moving through the boundaries of the selected column are the inputs and the outputs of the system, and are indicated by arrows in fig. 1. The investigated prism is divided into three subsystems: zone of plants, zone of aeration, and zone of saturation. The water exchange between the subsystems can also be represented by arrows. The surface has a special role in the system, being the border between the zone of plants and the unsaturated zone, although the roots are crossing it. At the same time, a part of precipitation reaching the surface is turned back into the zone of plants by evaporation. The sur- face could be regarded, therefore, as a fourth subsystem, the special effect of which is indicated by dotted arrows.

Apart from inputs and outputs a system is characterized by the operations within the system itself. Storage within the zone of plants and aeration as well as the fluctuation of the water table (which represents the storage in the zone of saturation) is indicated in the figure as such internal operations. Some characteristic values governing the operation of the system are also mentioned (such as: pF curve, moisture distribution).

For better understanding of the hydrological phenomena and their interactions, it is useful to group and classify the various processes influencing water movement through and within the unsaturated zone. For this grouping the physical model sketched in fig. 1. can be used.

The investigated column is in connection at its upper boundary with the atmosphere. The input through this surface is precipitation, either liquid or solid, while the outputs are combined under the term of actual evapotranspiration.

Along the vertical faces the model is bordered by the same zones as are in the prism, i.e., zone of plants above the surface, unsaturated zone between the surface and the water table, and finally gravitational ground water space below the water table. The lower horizontal boundary of the column is similar to the lower part of the vertical face; it is in contact with the saturated zone. By separating the model from its surroundings, a discontinuity is caused along the listed boundaries, which has to be replaced by inputs and outputs acting on and originating from the system respectively. Such replacing factors are:

- Horizontal vapor movement in the zone of plants;
- Horizontal moisture movement in the unsaturated zone;
- Surface runoff into and out of the prism; and ground water flow.

The listed types of water movement may be either inputs or outputs of the system depending on the direction of the flow (whether it is directed into or out of the investigated prism).

Further groupings of acting processes can be distinguished according to the subsystems mentioned previously. Storage in the zone of plants and the evaporation of the water stored here may be combined into the investigation of interception. Storage on the surface and the direct evaporation from here are closely related to the former group, although these processes already belong to the next subsystem (i.e., the surface itself), which is characterized by surface runoff as one of its inputs (inflow on the surface to the investigated space), and also as the output of this subsystem (outflow on the surface). The water exchange between the zones of plants and aeration is the resultant of infiltration through the surface as well as the evaporation and transpiration from soil moisture. The two draining processes mentioned (evaporation and transpiration) are only a part of the actual evapotranspiration, because the latter includes the direct evaporation from the surface of both plants and earth. The next subsystem is the unsaturated zone, where the storage process is governed by infiltration, direct evaporation from soil moisture, transpiration of plants from the root zone, and water holding capacity of the unsaturated soil, which can be characterized by the pF curve or by the gravitational pore space compared to the actual moisture content of the layer. The final group of phenomena is water exchange between the saturated and unsaturated zone, composed of the vertical recharge and drainage of ground water and influenced by the change of the stored amount of the latter indicated by the fluctuation of the water table. Surveying the processes listed, those can be selected which are most closely related to the hydrological investigations of the unsaturated zone.

The distribution of precipitation in time and space is investigated appropriately by hydrometeorologists. Equipment and methods are mostly standardized or standardization is in progress. The same is true for meteorological measurements which may be used for establishing relationships suitable for calculation of some unmeasurable processes (e.g., temperature, radiation, potential evaporation, wind velocity, sunshine hours, etc).

There are factors which affect the water balance of the investigated prism only very slightly. These are horizontal vapor and moisture movements. It is assumed, therefore, that the further investigation of these phenomena can be neglected.

The measurement of surface runoff and ground water fluctuation is a common practice in operational hydrology. The determination of ground water flow belongs to operational hydrology as well, although this measuring problem is not yet completely solved.

Actual evapotranspiration, interception, and evaporation from the surface of both plants and soil are phenomena closely related to the hydrology of the zone of aeration, but occurring outside the unsaturated layer (only a part of actual evapotranspiration originates from there). The measuring techniques (i.e., the use of lysimeters for the quantitative characterization of the processes listed) create, however, very close links between the investigation of both the zone of plants and the unsaturated layer.

The processes not yet listed are those which are most closely related to the unsaturated zone:

- Infiltration through the surface;
- Evapotranspiration from soil moisture;
- Storage in the unsaturated layer; and
- Water exchange between soil moisture and ground water.

Among problems influenced by the four topics mentioned, there are some which can be investigated separately, using special measurements and observation (e.g., infiltration through the surface, relationship between storage capacity and the physical characteristics of the soil layer, etc.). The complete understanding and the comprehensive description of hydrological phenomena occurring in the zone of aeration, however, can only be given by evaluation of lysimeter data combined with observation of changes of soil moisture. This type of data can assist also with the better explanation of the special problems mentioned previously.

This is the reason why the remaining objective of the first chapter of the paper is to classify the types of lysimeters and methods of measurements. This is to make the collected data comparable and has the long range aim of standardization of equipment.

1.2 Classification of lysimeters

According to the most simple and very general definition, lysimeters are soil columns separated from their surroundings in which some of the components of water balance in the unsaturated layer are measurable. There are many possible solutions for construction of such a closed space in the soil. Lysimeters may differ not only in their size (depth, surface area) but also in their construction and operation. Variable aspects include: type of surface (bare or covered with vegetation); type of soil (homogeneous or layered, cohesive or cohesionless material), position of the water table; recharge of water (natural, or artificial, in the second case recharged through the surface, or by ensuring water supply in the gravitational ground water space); measuring techniques of various components of the water balance; etc.

The constructional and operational aspects influence not only the reliability and correctness of measurements but they determine at the same time what combination of the phenomena or which group of components are included in the data measured by the lysimeter. This is the reason data obtained using different equipment are not comparable.

It is not possible, however, to give preference to one type of construction or operation over the others because there is no way to measure all components separately. Only a combined or summarized effect of a group of phenomena can be observed. The purposes served by the lysimeter determine, therefore, which group should be measured and thus which type of construction should be chosen. In other cases the comparison of data of two different lysimeters allows characterization of a special component, which is included in one group only while other components measured with the two lysimeters are identical. Thus the difference of the observed data describes the phenomenon in question.

Considering the facts explained previously, there is no possibility for complete standardization of lysimeters. Nevertheless the data can be made comparable by classification of the equipment used and by determination of which components are measured with a given type of lysimeter. The proposed steps of this indirect standardization are as follows:

- To classify the types of lysimeters;

- To determine the components measured either separately or in groups by the various types (qualification);

- To investigate which type of lysimeter can measure a given component or group of components (evaluation);

- To propose standardization of a set of equipment suitable to provide research-workers with reliable information on all acting phenomena;

- To collect standard sets of compared data measured with the various types of lysimeter proposed to be included into the unified system of equipment.

The proposed classification is based on 21 members divided among 7 groups each composed of 3 members. Each group describes a special character of the lysimeter using three figures which can be any integer between 1 and 9. Thus the character in question is given by three data each classified at most into nine categories. Indicating the members of the basic figure of classification by letters it has the following form:

abc def ghi klm nop rst uvz.

The meaning of the groups and the special characteristics indicated by each of the letters are listed below, while the categories belonging to the various letters are given in Table 1.

A(abc) description of the container
- a - surface area
- b - depth
- c - material of the container

B(def) composition of the soil column investigated
- d - soil layers
- e - effective diameter of the basic layer
- f - porosity of the basic layer

C(ghi) location of the lysimeter
- g - related to the surface of the surroundings
- h - related to the vegetation of the surroundings
- i - related to the surrounding layers

D(klm) composition (formation) of the lysimeter surface
- k - slope of surface
- l - type of vegetation
- m - depth of the root-zone

E(nop) water balance of the lysimeter
- n - surface runoff
- o - water table
- p - recharge of the soil column

F(rst) methods of basic measurements
- r - method of measuring the stored amount of water
- s - methods of soil moisture measurements
- t - period of basic measurements

G(uvz) supplementary measurements
- u - meteorological measurements
- v - agronomical measurements
- z - other measurements

Some of the features listed do not influence the character of the measured data but others determine basically the type of data obtained by a given lysimeter. A detailed investigation can be carried out to select those parameters influencing the character of the measured data and the lysimeters can be classified into four main groups.

LA bare lysimeter without groundwater;
LB bare lysimeter with groundwater;
LC lysimeter covered by vegetation without groundwater;
LD lysimeter covered by vegetation with groundwater.

The various possible types within each main group can be evaluated considering the number and reliability of the data collected by different constructions (Table 2.).

1.3. Evaluation of the various types of lysimeters

On the basis of analysis of various types of lysimeters mentioned in the previous chapter it can be determined which constructions provide the most detailed information on the hydrological phenomena occurring in the unsaturated zone and which types of lysimeters are suitable, therefore, for general use and for standardization in the future within the different main groups. There are some statements which can be drawn up directly from the analysis. These are as follows:

- The two basic types (i.e. bare lysimeters and those covered by vegetation) investigate different phenomena. It is impossible to give preference to either of them. The type used should be chosen according to the purpose of the investigation.

- Lysimeter with watertable always gives more information than a dry lysimeter. The application of the latter may be justified only in the case of very deep watertable, when the construction of lysimeter including groundwater would be difficult and costly. (It has to be considered that dry lysimeters deform the natural conditions, because drying influences the soil column from both the upper and the lower end, and, therefore, the dynamic balance of moisture distribution in dry lysimeters differs from the pF curve.)

- The correct application of water balance equations requires the form reduced to zero (measuring all components separately). The separate observation of all parameters is not possible in lysimeters. Some components have to be calculated from water balance equations. It has to be taken into consideration, therefore, that these calculated components include all measuring errors.

- There are three methods of measuring the components of water balance: i.e. weighing; weighing together with the determination of the amount of recharged or drained water; and measuring only the recharged or drained water. The second solution (weighing and measuring outflow and inflow) gives the most complete information. The application of weighing without observing recharge and drainage is not justified, because the execution of these measurements does not solve any special technical problem. The reliability of weighing is expressed always in percentage of the total weight. There are cases, therefore, when the probable error in weighing is higher than the value to be observed. In these cases the construction of very expensive lysimeters capable of weighing is not reasonable, and preference should be given to the third solution (observation only of recharge and drainage);

- Soil moisture measurements always gives important supplementary information. In some cases it is the only way to separate components measured only as a group by lysimeters. It is always advisable to apply this observation in lysimeters.

- Hydrological phenomena in lysimeters covered by vegetation are always strongly influenced by the type and the grade of development of the plants used. Detailed agronomical observations are necessary, therefore, for the evaluation of data in this case. It is advisable to include the measurement of the total dry material of plants in this group of observations as well.

Considering the aspects listed previously some constructions can be selected from each main group which might be proposed for general use in the future and probably for standardization. (The symbols used there are identical with those in Table 2.)

LA bare lysimeter without groundwater

The most complete information can be collected by lysimeters which weigh as well as measure the drained water and soil moisture (LA_4). It is not reasonable to construct a lysimeter capable of weighing and neglect the measurement of drained water. LA_1 and LA_2 types should be excluded from the possible variations (this remark refers to all types with index 1. and 2. and, therefore, they will not be mentioned again). Data provided by LA_5 are insufficient. The components measured by LA_6 are the same as by LA_4. The advantage of LA_4 is the greater accuracy of data and the control of storage in the unsaturated zone. At the same time the construction of LA_6 is considerably cheaper than that of LA_4, especially in the case of a thick soil column. It has to be considered, however, that the application of lysimeters without groundwater is basically a rough approximation acceptable only when water table is very deep. In this case the depth of the lysimeter is not determined by any factor to be simulated in the lysimeter. The thickness of the layer investigated can be chosen, therefore, according to the requirements of weighing (the error of measurements should be smaller than the components observed). Thus the final recommendations is to accept type LA_4 as the generally used bare lysimeter without groundwater and to apply type LA_6 only as members of larger networks when cheaper construction allows a greater number of lysimeters.

LB bare lysimeter with groundwater

As before the lysimeter capable of weighing as well as measuring recharge, drainage and soil-moisture (LB_4) provides the largest amount of information. Equipment capable only of weighing (LB_1 and LB_2) or unable to measure soil moisture (LB_3, LB_4 and LB_5) may be excluded from the advisable constructions. A special problem is to determine how to control the water table. There are two possible ways:

- To drain and recharge the groundwater with a given amount of water (which can be constant or changing according to a seasonal program) and leave the water table to develop freely as a result of natural and artificial effects, or

- To keep the water table at a determined level (which can be constant or fluctuating according to seasons) and to ensure the recharge or drainage necessary for maintenance of this level.

The most perfect solution would be to keep the water table within the lysimeter at the same level as in the surroundings and to measure recharge or drainage necessary for this operation. The technical solution of this construction raises difficulties, and therefore, either the maintenance of constant waterlevel (LB_4 and LB_{62}) or the application of constant recharge or drainage (LB_{61}) are the generally accepted measuring methods. The latter type (constant drainage or recharge) can hardly be constructed with capability of weighing, because the fluctuation of the water table requires a deep lysimeter and in this case the accuracy of weighing is generally lower than the amounts to be measured. This is also the reason why weighing cannot be used for investigation of a thick unsaturated zone. It is necessary to note, that the maintenance of a constant water table or recharging (draining) a constant amount of water creates unnatural conditions (conditions different from the ground water regime in the surrounding areas) and, therefore, a group of such lysimeters has to be constructed. In this way a suitable model of the surroundings can be selected from the group in all periods of the year. As a final summary of the evaluation of this group it can be stated, that the construction of LB_4 type is advisable only in the case of a shallow water table. In other cases type LB_6 is the suitable construction. This gives almost the same amount of information (except interception). Within the latter type LB_{61} operates with a fluctuating water table and constant recharge or drainage, while in LB_{62} the level of ground water is constant. The complete investigation of the unsaturated zone requires the construction of a group of such lysimeters in the same area (in the case of LB_{61} with different constant discharges and LB_{62} with different constant levels).

LC lysimeter covered by vegetation without groundwater

Following the same reasoning as in the case of type LA, the lysimeter capable of weighing and measuring discharge as well as soil moisture can be brought into the limelight as the best construction. It can be stated, therefore, that type LB_4 should be the generally used lysimeter and type LB_6 can be applied only as a member of large networks.

LD lysimeter covered by vegetation, with groundwater

As in the case of LC lysimeters, it is not necessary to repeat the reasoning given in connection with the bare lysimeters. The final conclusions can be applied for lysimeters covered by vegetation as well. Thus the construction of LD_4 type is advisable only in the case of shallow water table. If the unsaturated zone is thick or the purpose is the modeling of groundwater fluctuation, type LD_6 is the proposed construction either with constant recharge-drainage (LD_{61}), or with constant level (LD_{62}).

2. THEORETICAL ANALYSIS OF THE pF CURVE

It was already mentioned in Chapter 1, that some theoretical investigations could help the evaluation of the measured data and the clarification of the influence of some hydrological processes on the water balance in the unsaturated zone. Storage in this layer was mentioned as an example.

It is well known that there are physical parameters used in soil science and soil mechanics for describing both the actual water content and the storage capacity of a sample. In the present investigation, however, the characterization of the whole system is the problem to be solved. It is necessary, therefore, to enlarge the methods established for point measurements and to construct a combination of these parameters suitable for description of the balanced condition along a vertical profile of the soil between the surface and the watertable.

As will be proven in this chapter, theoretical analysis gives the solution of the problem. Before discussing the application of the pF curve for the investigation of storage in the unsaturated zone, it is necessary to summarize some elementary knowledge concerning the measurement of water content.

2.1 Determination of water content of soil samples

Water content of a sample is either the weight or the volume of water in the pores related to the total dry weight of the sample and its volume respectively. The water is bound to the grains with adhesion increasing with the decrease of distance between the investigated water molecule and the grain surface. It is necessary, therefore, to have some standard method to determine the extent to which water should be drained from the sample. Drying the sample at 105°C until its weight became constant was chosen as reference level. This definition summarizes the classical way of measuring soil moisture: weighing moist sample (G) and its weight after drying (G_o) at 105°C. The difference between the wet and oven dry weight related to the latter gives the water content expressed as ratio of weights:

$$w = \frac{G - G_o}{G_o}; \qquad 1.$$

The same parameter related to volumes can be calculated knowing the specific weight of the dry sample (γ_o) and of water (unity) using the dimension of P/cm^3 or mp/m^3 (γ_v=1):

$$W = \frac{G - G_o}{\gamma_v} : \frac{G_o}{\gamma_o} = \frac{G - G_o}{G_o} \gamma_o = w\,\gamma_o. \qquad 2.$$

This way of measuring requires removal of a sample and excludes both repetition of the investigation at the same point and continuous observation of the change of soil moisture. There is equipment for non-disruptive measurement of soil moisture based on electric resistivity or capacity (e.g. gypsum block); on absorbtion of radioactive rays by hydrogen atoms (neutron probe) and on infrared photography. None of these can be regarded as a final solution. Electric measurements are disturbed by the change of temperature and chemical composition of water. Neutron probe measures hydrogen ions and thus the results are influenced by the organic content of soil especially in the root-zone. Quantitative evaluation of infrared air photography is not yet perfected. It can be stated, however, that these methods indicate very important developments in continuous observation of soil moisture and in general characterization of large areas.

Discussion of methods for measuring soil moisture would lead, however, far from the original topic, which is the hydrological investigation of the unsaturated zone. It is necessary, therefore, to turn back and continue the physical interpretation of water content. The water content determined in the way explained is an instantaneous value describing the momentary state of the investigated sample, point or section (vertical line) without giving any information on the behaviour of the soil containing the measured amount of water.

It is obvious that the same water content can saturate one sample, but leave considerable open pore space in another sample of greater porosity. The coefficient of saturation, (the quotient of the volumetric water content and porosity) gives, therefore, very important supplementary information

$$s = \frac{W}{n} ; \qquad 3.$$

showing the saturated ratio of the pores. (s=1 if the sample is saturated; s=0 in the case of completely dry sample. It may have any value between the two limits given).

One can easily argue that the knowledge of the ratio of saturation is still insufficient information to judge the expected behaviour of the soil because a change of saturation in sand does not involve considerable modification as may be caused in a clay soil. Measuring water content at a given state of the sample gives guidance for complete understanding the effects of the actual or instantaneous soil moisture on the investigated soil. Knowing these specific values of water content of the soil in question and comparing the actual soil moisture to them the behaviour of the soil can be estimated.

When selecting the specific parameters, the most important requirement is that the state described by them should be characteristic and easily repeatable. From this aspect the parameters of plasticity used in soil physics are well determined values, although they belong to arbitrarily chosen states of the sample (W_L liquid limit is a water content described by Casagrande and W_P limit of plasticity is moisture content, when a string of 3 mm can be rolled from the sample). The index of consistency, which is the ratio of two differences (that between liquid limit and instantaneous water content related to the difference of W_L and W_P)

$$K_i = \frac{W_L - W}{W_L - W_P}, \qquad 4.$$

is a good example of how actual water content is compared to selected limit values.

Although the specific soil moisture values used generally in soil science as parameters belong to more natural conditions than the physical parameters of soils, their reproduction causes, however, some difficulties, because the conditions described are not determined precisely enough. E.g. field capacity (W_{FC}) indicates the water amount retained in the sample against gravity. This is a very important parameter, but it is influenced by numerous undetermined factors (e.g. temperature, relative humidity of air, etc. Among these the position of the investigated point related to the actual water table is perhaps the most important as will be demonstrated later). Therefore, field capacity can hardly be reproduced or physically interpreted. The same statement can be made of wilting point (W_{WP}) as well, because the suction of the roots differs from plant to plant.

The most stable and repeatable parameters describing specific moisture contents used in soil science are various measures of hygroscopic moisture content (or hygroscopicity) which measure the water content retained by the sample in closed space in the presence of sulfuric acid. Thus Mitscherlich's hygroscopicity (W_{HY}) is determined with 10% concentration of the acid while Kuron's hygroscopicity (W_{hy}) is measured with sulphuric acid of 50% concentration (Mitscherlich, 1932; Kuron, 1932). Because of the high stability of these parameters it is reasonable to accept their general use in the future and to regard the others only as rough approximations which can be estimated as functions of hygroscopicity using linear relationships. There are many of such equations proposed in the literature (Mádos 1939; 1941; Juhász 1967). A few of these are listed here:

$$\begin{aligned} w_{FC} &= 4\, w_{hy} + 12; \\ w_{WP} &= 4\, w_{hy} + 2; \\ w_{L} &= 2{,}0\, w_{HY} + 12; \\ w_{P} &= 1{,}7\, w_{HY} + 6{,}5; \\ w_{hy} &= 0{,}45\, w_{HY}. \end{aligned} \qquad 5.$$

2.2 Interpretation of field capacity and gravitational porosity

As was already mentioned, the water holding capacity of a soil cube depends on the position of the investigated sample (whether it is a sample separated from its surroundings or is in a soil profile and in the latter case what is its elevation above the water table). The reliability of this statement can be easily understood. In the case of an isolated sample the effect of gravity is expressed by the weight of the water contained in the pores. If the soil cube (the water holding capacity of which is investigated) is part of a continuous soil profile, the sample is fitted into a space of gravitational potential, the datum (reference level) of which is the water table where the surplus pressure is zero (the gravitational potential is zero at this level). Everywhere in this space the effect of gravity should be expressed with respect to this datum. Thus above the reference level gravity causes a suction proportional to the height of the investigated point above the water table. Physically this process can be explained by imagining that the continuous chain of water films composes a closed system in which the pressure on a water particle (in this case negative pressure i.e. suction because the particle is above the water table with zero pressure) is proportional to the weight of a straight water column between the particle and the reference level, independent of the form of the container (the form of the chain composed of the water films). This is the reason field capacity will be larger near the water table, where the suction caused by gravity is smaller, than at a higher point of the profile, and why water holding capacity measured in a separated sample can be regarded as a meaningless parameter.

There is another parameter used generally in the investigation of the unsaturated zone which becomes questionable if one accepts the interpretation of field capacity given previously and determines the field capacity as a function of the elevation above the water table. This parameter is the free or gravitational porosity (generally indicated with the symbol of $\underline{n_o}$), the classical definition of which tells that this is a part of total porosity, in which the water is not bound to grains by adhesion and moves, therefore, freely affected by gravity. It is proposed consequently, that gravitational porosity should be calculated as the difference between total porosity and water holding capacity. Accepting the concept of field capacity as a function of the position of the investigated point, it must be stated that the gravitational porosity can be expressed only as the function of elevation above the watertable.

In all types of soil profile a line could be determined which divides the total porosity into two parts one is field capacity and the other one is gravitational porosity. It is evident, that field capacity is relatively larger near the water table and its value decreases going upwards in the profile, while gravitational porosity changes inversely. It is also obvious that the sum of the two parameters at a given elevation is equal to the total porosity, and the sum is constant if porosity does not change in the profile (Fig. 2.).

There is a further condition which can be considered as well when determining the position of this dividing line in the soil profile. If that part of porosity covered by field capacity is filled with water and the remaining part is occupied by air, soil moisture is in a dynamic equilibrium in the profile. There is water movement only if an external force (e.g. evaporation from or infiltration to the top soil: raising of watertable; etc.) induces it. The dynamic equilibrium can develop only when the acting internal forces balance each other. In an unsaturated soil profile the internal forces are the tension on the surface of water films and gravity. Their balanced state can be expressed by equaling the total hydraulic gradient to zero both in horizontal and vertical direction. Investigating the process in a horizontal plane, this condition requires that the vertical moisture distribution should be identical at each profile in a homogeneous medium while in vertical direction the condition gives relationship between tension and gravity

$$I = \frac{d(h + \frac{1}{\gamma}\Psi)}{dx} = \frac{1}{\gamma}\frac{d\Psi}{dx} - 1 = \frac{1}{\gamma}\frac{d\Psi}{dW}\frac{dW}{dx} - 1 = 0. \qquad 6.$$

From this equation field capacity (water content belonging to the state of dynamic equilibrium at different elevations in the profile) can be calculated as a function of the height of the investigated point above watertable ($\underline{h}$) if the relationship between tension and moisture content is known. The equation of

$$W_{fc} = f(h), \qquad 7.$$

achieved as final result describes the position of the dividing line of Fig. 2.

A further consequence must be deduced from the conditions explained. It was already mentioned that the water content does not give sufficient information on the behaviour of the soil. It is necessary to compare these data to parameters belonging to special conditions of the sample. This restriction should be enlarged. Point measurements, even compared to such specific characteristics as hygroscopic moisture content, liquid limit or limit of plasticity are insufficient to describe field conditions. The complete vertical distribution of moisture content must always be determined in a profile and the result must be compared to soil moisture distribution belonging to the dynamic equilibrium. Only the differences between the actual distribution and the matching curve shows where water deficit or surplus exists in the profile. This indicates also the possible vertical water movement either upwards or downwards. The total hydraulic gradient can be calculated from the curves and the existence of a gradient not equal to zero is the precondition of movement.

The only remaining problem is the determination of the equation of the line dividing field capacity and gravitational porosity, which describes the state of equilibrium of soil moisture in a profile, as was proved earlier. It was also shown that in homogeneous media this problem can be reduced to the investigation of the relationship between tension and watercontent. This condition immediately suggests that the pF curve could be used for determination of or can be identical with the desired matching curve, since, according to its definition, the pF curve represents the relationship mentioned, being the tension in the height of the water column plotting on a logarithmic scale. This is the reason the physical interpretation of the pF curve is dealt with in detail in the next section.

2.3 Construction and calculation of pF curves

The usually accepted way for the determination of a pF curve is to apply various suctions on the investigated sample and to measure retained soil moisture. After plotting the points with suction - which is supposed to be equal with the tension on the surface of water films - as the logarithm of the height of the equivalent water column and water content as an arithmetic value, the pF curve can be easily constructed (Fig. 3.). Various methods are used to create suction on the sample. The choice of method depends mostly on the range of suctions to be applied.

Most commonly pF curves are composed of three clearly recognizable sections (Fig. 4-a) (Kovács, 1968). The upper part of the curve is almost vertical and is followed by a nearly horizontal section. The curves are completed by a vertical line at a moisture content equal to the porosity (W n; .s = 1). There are only a few exceptions, always in the case of very fine materials, when the first two stretches are replaced by a curved line of motonically decreasing slope as water-content increases (Fig. 4-b).

This character of the pF curve can be easily explained considering that in the unsaturated zone gravity is balanced by two different intermolecular forces, i.e.: adhesion and capillarity.

At the upper part of the pF curve, far from the water table, the water covers grains in the form of a thin film. The force keeping the water here against gravity is adhesion. Without investigating the character of this force in detail, its existence can be explained as the attraction between solids and water molecules created by the electrostatic charges of grains and the orientation of dipolar water molecules (Van der Waals force). This type of force is generally approximated in theoretical physics by relating the tension at the surface of the water film (ψ) to the thickness of the film (δ) in the form of a hyperbola of sixth order

$$\psi = \left(\frac{A}{\delta}\right)^6 \qquad 8.$$

It is quite evident, that the thickness of the water film is closely correlated with the water content of the sample. Using some approximations this relationship can be determined:

$$W = 4n \frac{\delta}{d_o} \left(1 - \frac{\delta}{d_o}\right); \quad s = 4\frac{\delta}{d_o} \left(1 - \frac{\delta}{d_o}\right) ; \qquad 9.$$

where d_o is the average diameter of the pores, or that of a model pipe hydraulically equivalent to the network of channels composed of the pores. The correctness of Eqs. 8 and 9 was proved by comparing calculated and measured parameters of numerous samples (Kovács, 1972. Fig. 5.).

As was already mentioned, in the state of dynamic equilibrium the tension on the surface of the water film balances the effect of gravity which is proportional to the elevation of the point investigated above water table:

$$\psi = h \gamma . \qquad 10.$$

Substituting this value together with Eq.9 into Eq.8 the vertical distribution of soil moisture at equilibrium (W_B or s_B) can be determined

$$W_B = \frac{A}{(h\gamma)^{1/6}} \frac{4n}{d_o} \left[1 - \frac{1}{d_o} \frac{A}{(h\gamma)^{1/6}}\right];$$

$$s_B = \frac{A}{(h\gamma)^{1/6}} \frac{4}{d_o} \left[1 - \frac{1}{d_o} \frac{A}{(h\gamma)^{1/6}}\right] . \qquad 11.$$

(It is necessary to note, that accepting Eq. 10. as a basic principle, any kind of $\psi = f$ (W) function will obviously satisfy the condition given in Eq. 6. This equation cannot serve, therefore, as a control, and the reliability of the proposed relationship between tension and water content must be checked by measurements as was already referred in connection with Eq.9).

Continuing the theoretical analysis, the constant of Eq.8 can be expressed as the function of the soil physical parameters D_h (effective diameter), α (shape coefficient of grains) and n (porosity). This theoretical relationship is in a good accordance with the empirical result gained from measurements (Fig. 5) except the power of D_h/α , which is 1 in theory.

Experiments give a value of 0.8. The theoretical and empirical formulae to be compared are as follows:

theoretical: $$\frac{W\,\Psi^{1/6}}{1-n} = C_1 \frac{\alpha}{D_h} \left(1 - \frac{C_2}{\psi^{1/6}} \frac{\alpha}{D_h}\right);$$

validity zone $$\frac{C_2}{\psi^{1/6}} \frac{\alpha}{D_h} < 0.5;$$ 12a.

empirical $$\frac{W\,\Psi^{1/6}}{1-n} = 0.75.10^{-3} \left(\frac{\alpha}{D_h}\right)^{0.8};$$

validity zone $$\frac{\alpha}{D_h} > 10^4;$$

empirical $$\frac{W\,\Psi^{1/6}}{1-n} = 1,5.10^{-3} \left(\frac{\alpha}{D_h}\right)^{0.8} \left(1 - 5.10^{-5} \frac{\alpha}{D_h}\right);$$

validity zone $$10^4 > \frac{\alpha}{D_h} > 10^2;$$ 12b.

empirical $$\frac{W\,\Psi^{1/6}}{1-n} = 1,5.10^{-3} \left(\frac{\alpha}{D_h}\right)^{0.8};$$

validity zone $$10^2 > \frac{\alpha}{D_h};$$

or using a unified formulae in the whole zone important from practical point of view.

empirical approximation $$\frac{W\,\Psi^{1/6}}{1-n} = 2.5.10^{-3} \left(\frac{\alpha}{D_h}\right)^{2/3};$$ 12c.

validity zone $$2.10^4 > \frac{\alpha}{D_h} > 5.10^1.$$

(In the empirical formulae the factors and the limits of the validity zone have dimensions. The effective diameter has to be substituted, therefore, in Cm-s).

On the basis of the equations given the position of the upper part of the pF curve can be determined from the physical parameters of the soil sample or these parameters can be calculated from the measured upper section of the curve. As two unknown parameters (n and D_h/α) have to be determined, it is sufficient to have two measured points. Having three, there is a possibility of control as well. The number of necessary measurements raises possibility of using Kuron's and Mitscherlich's hygroscopic moisture contents for characterization of the upper part of pF curves. Knowing that the suctions created by sulphuric acid in a concentration of 10 and 50 percents are pF=4.62 and pF=6.16 respectively, and the measurement of water content associated with these values accurate and well repeatable, the curve and the characteristic soil-physical parameters can be measured with simple instruments. For control the use of concentration of 20 or 30 percent can also be used which give points at pF=5.28 or 5.62 values (Péczely, and Zotter 1973).

There are some few cases, when the curve described by the equations listed previously remains valid in the whole zone of $0 < W < n$. These are very fine grained soils having a pF curve without break (see Fig. 4-b). The intersection of $\Psi = f(W)$ curve with the vertical $W=n$ indicates the limit value of tension (ψ_n) and if the suction caused by gravity ($h\gamma$) is smaller than ψ_n the sample remains saturated, because the tension, even in the centre of the pores, greater than the suction:

$$\psi_n = \left[4 \frac{A}{d_o} \left(1 - \frac{A}{d_o} \frac{1}{\psi_n^{1/6}} \right) \right]^6 ; \qquad 13.$$

or considering that this case is characteristic in the zone of very fine grains, and using the empirical relationships mentioned

$$\psi_n = \left[\left(\frac{1}{n} - 1\right) 0.75.10^{-3} \left(\frac{\alpha}{D}\right)^{0.8} \right]^6 ;$$

or

$$\psi_n = \left[\left(\frac{1}{n} - 1\right) 2.5.10^{-3} \left(\frac{\alpha}{D}\right)^{2/3} \right]^6 . \qquad 14.$$

In a layer composed of coarser grains (generally the characteristic condition) complete saturation can occur in the presence of suction greater than the limit mentioned in the previous paragraph because there is another molecular force acting against gravity, i.e. capillarity. The character of this force is well known. There is attraction between water molecules, which in the interior of the medium is balanced, because the same forces act on a molecule from each direction. At the surface of water, however, the assymetrical and thus unbalanced condition creates stress, which becomes observable in the form of curved surface, where the water surface contacts the solid wall. Generally speaking the same phenomenon occurs at the boundary of two different fluids or that of a liquid and a gaseous medium. If the container of the water is small enough, it can be observed that the total stresses around the wall can act against gravity raising the water above the water table of zero pressure.

For numerical characterization of capillary force this capillary height is generally used. It is proportional to the linear capillary tension (ω) and inversely proportional to the horizontal area of the capillary pore (in the case of a circular cross-section of its diameter). Both capillary tension and the coefficient of proportionality depend on the contacting materials. Thus in the case of the contact of quartz, water and air as solid, liquid and gaseous media respectively (and this is the general case of soils), the capillary height in a tube of d diameter can be calculated from the following simple equation:

$$h_k\,[\mathrm{cm}] = \frac{4\omega}{\gamma d} = \frac{0.30}{d\,[\mathrm{cm}]} \qquad 15.$$

On the basis of former investigations a method can be proposed for the calculation of the probable average (d_o), minimum (d_1) add maximum (d_2) diameter of the pores using the physical parameters of soils as independent variables (Kovács, 1972):

$$d_o = 4\,\frac{n}{1-n}\,\frac{D_h}{\alpha};\; d_1 = \frac{d_o}{1.5};\; d_2 = 1.25\, d_o;\; d_2 = 1.86\, d_1. \qquad 16.$$

The formulae were derived by determining a model pipe, the hydraulic resistivity of which was equal to that of the channels composed of the pores. It was, however, proved by comparing the results to Stakman's (1966) air-bubbling measurements, that the two extreme diameters can be regarded as the probable maximum and minimum pore sizes.

Substituting d_1 and d_2 into Eq.15. the minimum and maximum of the expected capillary height can be calculated

height of the closed capillary zone:

$$h_{k\,min} = \frac{0.30}{d_2};$$

height of the open capillary zone:

$$h_{k\,min} = \frac{0.30}{d_1}; \qquad 17.$$

which determines the two ends of the nearly vertical section of the pF curves.

The size of the pores can be considered as a random value, a given probability can be attached, therefore, to both d_1 and d_2, while the ratio of the various pore sizes can be characterized by a probability distribution curve. The pF curve describes the relationship between suction and water content, thus in the open capillary zone (between $h_{k\,min}$ and $h_{k\,max}$) it shows which part of the pores can be saturated at an elevation of h in question (when $h_{k\,max} > h > h_{k\,min}$) by capillarity. viz. which is the ratio of pores having a capillary height equal to or greater than h. Considering Eq.15. this ratio depends only on pore diameter, and therefore, this section of pF curve can also be approximated by a probability distribution function (Réthází, 1960).

The network of pores is, however, a system of channels with changing cross-section and not straight pipes with constant diameters. The capillary height is influenced, therefore, not only by the distribution of the pore sizes in a horizontal section but by the vertical change of the diameters as well. This is the reason, why some pores are not saturated when the dry sample is wetted from the direction of the water table, while the same pores can keep capillary water when the process starts with the complete saturation of the sample and the dynamic equilibrium is achieved by drainage. This phenomenon accounts for the hysteresis of the pF curve (the nearly horizontal section of the curve has a lower position if it is determined by wetting and a higher in the case of drainage) which has to be considered in the development of a method suitable for characterization of the pF curve in the open capillary zone by a well fitting probability distribution function.

The random character of pore diameters explains the form of the closing section of the pF curve as well. Theoretically all pores are completely saturated in the close capillary zone (below $h_{k\ min}$) thus the second section runs to the point $\Psi = \gamma h_{k\ min}$; W=n, and the curve is closed here by a vertical line. It was, however, proved, that the pores could only be partly saturated below this level. Réthâti (1960) found, that the degree of saturation (which is s=0.85-1.0) depends on the uniformity of grain size distribution and the initial water content of the sample, but it is independent of both grain diameter and porosity. The incomplete saturation can be caused partly by air bubbles closed in the pores and partly by large pores the occurrence of which has very low probability. If a given probability of d_2 diameter (and thus that of $h_{k\ min}$ value) is used for the calculation of the parameters of the probability distribution function describing the second section of the pF curve and it is determined by considering the expected rate of saturation, the actual form of the closing section of the pF curve can be well approximated at the same time. Thus finally the whole curve can be composed of two parts, viz. the hyperbole for the zone of adhesion and the probability distribution function in the open and closed capillary zones.

3. INFILTRATION THROUGH THE SURFACE INTO THE UNSATURATED ZONE

Similarly to the process of storage, infiltration from the surface into the unsaturated layer can be investigated theoretically. The better understanding of this phenomenon provides a check on the reliability of lysimeter measurements. A further purpose of this type of investigation is to determine a method for numerical characterization of infiltration, the result of which could help the generalization of lysimeter measurements for large catchments.

The first attempt, and the most practical one, for determination of infiltration as a function of time was the construction of various infiltrometers which made actual infiltration measurable in the field. From the measurements different approximate functions were derived, the constants of which could be determined in each case at the spot at which infiltration had to be calculated. An obvious advantage of these methods is that the parameters express the actual local conditions. At the same time the inhomogenity of soils, the relatively limited size of the equipment and hydraulic uncertainties of the measurements can cause considerable errors.

Infiltration through the surface is only a boundary condition of a more complex process, the change of moisture content of the unsaturated zone in time and space. Theoretically the solution of a system of two differential equations (i.e. continuity and equation of movement) gives the control of any kind of infiltration function. This solution, however, requires the application of some simplifying hypothesis, which may make the results sometimes questionable.

There are quite recent investigations concerning the hydraulic conductivity of fine materials, in which movement is influenced by adhesion between grains and water as well. This study was extended to include the investigation of unsaturated media. Using the results of this analysis a further step can be made toward the theoretical explanation of the infiltration process.

3.1. Short summary of classical investigation of infiltration

Two different ways of investigations were mentioned in the introduction for the characterization of infiltration, the practical and the theoretical.

Measuring actual infiltration on the investigated area is an essential part of the practical methods. For this purpose various equipment (so called infiltrometers) were constructed. The common basis of their operation is the attempt to create vertical (or nearly vertical) water movement in the unsaturated zone and measure the discharge of this flow. The surface of the soil is covered with water having a relatively shallow depth (h_o) and a constant level maintained by adding measured amounts of water. It is supposed that this amount is moving downwards with a constant horizontal cross-section similar to movement in a vertical tube. A further hypothesis is that above the water front moving downwards the soil is completely saturated and hydraulic conductivity is constant while moisture content is not influenced below this level.

It is evident that according to the suppositions listed the discharge decreases gradually and tends to a constant value. The area (A) and hydraulic conductivity (k) are constant, the gradient calculated as the ratio of pressure head (h_o); depth of seepage (z); and capillary suction (h_k) to the depth of seepage becomes unity if h_o and h_k are negligible compared to z (Fig. 6.):

$$Q(t) = A\,k\,\frac{h_o + z + h_k}{z}; \quad I = \frac{h_o + z + h_k}{z};$$

$$\frac{dz}{dt} = v_{eff} = \frac{k}{n} I; \text{ and } I \rightarrow 1; \text{ if } z \rightarrow \infty; \qquad 18.$$

The Q(t) function can be determined from this relationship.

The supposed approximations can hardly be acceptable in the case of field measurements. The biggest problem is raised by the nonvertical character of the movement, viz. a part of the discharge is used for saturation of the layer around the theoretically supposed vertical tube. Most of the differences between the proposed equipment are caused by special solutions, the purpose of which is to decrease the effect of the lateral saturation on the measurements (application of double cylinders, measuring the discharge only in the internal one, while the water in the external cylinder supplies the horizontal flow; or the use of relatively large wetted surface to decrease the ratio of lateral flow compared to the vertical water movement; etc.).

The suction at the water front can only be roughly approximated with capillary height. It is obvious that the error decreases with increasing seepage depth, but it may be considerable at the beginning of the measurements. This error during the first phase of the movement can also be decreased by applying deeper water cover on the surface. The constant water cover, however, creates unnatural conditions and, therefore, the sprinkling type of water supply is proposed in some cases. This solution, however, causes further uncertainties, because this way of recharge does not saturate the layer and thus hydraulic conductivity remains a varying factor depending on the degree of saturation.

Eq.18. itself is very uncertain, because the seepage of water along certain channels of pores can be observed instead of the development of a wetted front. The correct measurement requires, therefore, the observation of moisture content along the entire profile during the recharge period. This is the reason why there are only very rare cases in which the complete investigation of the infiltration process (the determination of soil moisture in time and space between surface and water table) was the purpose of measurements. In many cases the determination of one boundary condition (recharge at the surface) was regarded as sufficient information. There are always many local factors (root zone, secondary porosity, layered unsaturated zone and other inhomogenities, etc.) influencing and disturbing the process of infiltration. This is the reason, why the most simple mathematical formulae are used in the practice instead of Eq.18. for describing infiltration as the function of time. The single requirement is that the curve representing the relationship should be monotonically decreasing and tends to a horizontal asymptote. The usually applied form is the exponential equation (Horton's formula):

$$q = (f_c - f_o) \exp(-at) + f_o; \qquad 19.$$

where q is the specific infiltration (recharge through a unit area);
f_c is the initial and f_o the final value of infiltration; and
a is a parameter of the relationship depending on the type and the actual condition of the soil.

There are further proposals as well, using hyperbole or other simple mathematical formulae satisfying the basic requirements mentioned previously, the parameters of which can be determined with local measurements in a similar manner as in Horton's equation.

In contrast to practical methods, which describe only infiltration through the surface, the purpose of the theoretical investigations is the determination of W(x,t) through the entire zone of aeration. The best known and usually accepted and applied solution is the Philip's equation (Philip 1957). The basis of this method is a generalized form of the Fokker-Planck equation. Its final form describes the vertical isothermal water transport through a homogeneous porous medium under the potential gradient arising from capillarity and gravity.

$$\frac{\partial W}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial W}{\partial x}\right) - \frac{\partial K}{\partial x}; \qquad 20.$$

subject to the conditions

$$W = W_1; \quad t = 0; \; x > 0;$$
$$W = W_0; \quad x = 0; \; t \geq 0; \qquad 21.$$

and where D and K are both single-valued functions of W. Using approximations this partial differential equation is reduced to the numerical solution of a set of ordinary differential equations.

Although the results of this method--as Philip has indicated--agree with experimental measurements and provide important improvements in the understanding of the phenomenon of infiltration, it is necessary to continue the theoretical investigations taking into consideration the known physical relationships between water content on the one hand and hydraulic conductivity and gradient of the total hydraulic potential respectively on the other. One of the starting points of the analysis is the equation describing the tension at the surface of water films as a function of water content (Eq.12). The other essential formula is provided by the hydraulic investigation of seepage through unsaturated porous media, the results of which are summarized in the following section.

3.2 Seepage through unsaturated layer

A series of papers was presented at the 13th Congress of IAHR in 1969. The first of these papers gives the general dynamic interpretation of the various types of seepage, and--on the basis of the classification--the zones of validity of the types discussed (Kovács, 1969 a). The classification includes only the investigation of seepage through saturated porous media. The second and third paper supplement the first one, giving detailed interpretation and proposing practical methods for describing seepage with lower velocity than that in the validity zone of Darcy's law (microseepage) (Kovács, 1969 b) and with high velocity (transition and turbulent zones) (Kovács, 1969 c).

Apart from dynamic interpretation, the use of a physical model constructed from straight pipes with varying diameter instead of the actual channels of pores in the porous medium was the common basis of the previously mentioned investigations. The pipe model is the same as was used for deriving the pF curve and of which the diameters are given in Eq.16. The correctness of Kozeny-Carman's equation for calculation of the coefficient of permeability in the Darcy-zone can be proved by this physical model and practical modification of this formula can be justified. Thus the use of the model created a common theoretical basis for the characterization of seepage within the entire range of flow in saturated porous media.

Summarizing the results of the investigation, the final formulae for calculation of hydraulic conductivity (k) in the linear relationship between seepage velocity (v) and hydraulic gradient (I)

$$v = kI \qquad 22.$$

can be listed. (It is necessary to note that Eq.22 remains linear only within the laminar--or Darcy--zone, where $k=k_D$ is constant. In other cases the coefficient of proportionality itself is the function of either velocity or gradient.) These formulae are:

Darcy's coefficient of permeability (K_D) which is equal to the hydraulic conductivity if $Re_p < 10$ and $I/I_o > 12$:

$$k_D \frac{1}{5} \frac{g}{\nu} \frac{n^3}{(1-n)^2} \left(\frac{D}{\alpha}\right)^2 ; \qquad 23.$$

(the symbols characterizing the physical parameters of soils were already explained; ν is the kinematic viscosity;

$$Re_p = \frac{vD_h}{\nu} \frac{4}{\alpha} \frac{1}{(1-n)}$$

is the Reynolds number calculated for the model pipe; and I_o is the threshold gradient indicating the gradient below which gravity is balanced completely by adhesion and, therefore, lower gradient do not induce flow through the porous medium).

When adhesion is negligible (in saturated media $I/I_o > 12$ is proposed as the lower limit of this zone) Eq.22 can be transformed to a general form which is independent of velocity and from which the reciprocal value of the hydraulic conductivity can be derived:

$$\frac{1}{k} = \left[\left(\frac{1}{k_D}\right)^{3/4} + \left(\frac{do}{nk_D} \frac{0{,}01}{\nu}\right)^{3/4} v^{3/4}\right]^{4/3} . \qquad 24.$$

This generally applicable form can be approximated with more simple formulae in the different validity zones of seepage, in the laminar zone with Eq.23, in the zones of higher velocity with the following equations:

in the first transition zone ($10 < Re_p < 100$)

$$k_{T1} = \frac{k_D}{0.8+0.02\ Re_p} ; \qquad 25.$$

in the second transition zone ($100 < Re_p < 1000$)

$$k_{T2} = \frac{k_D}{2.0 + 0.008\ Re_p} \qquad 26.$$

in the turbulent zone ($1000 < Re_p$)

$$k_F = k_D \frac{100}{Re_p} \; ; \qquad 27.$$

When adhesion is considerable ($I/I_o < 12$)

$$k_M = 0{,}714 \; k_D \frac{\left(I - I_o\right)}{I \cdot I_o \quad 0.1} \; ; \qquad 28.$$

and when adhesion has to be considered in the laminar zone as well

$$k_L = k_D \left(1 - 2 \frac{I_o}{I}\right) \qquad 29.$$

is the correct form of hydraulic conductivity, which has to be substituted in Eq.22.

This series of papers was supplemented later by another study applying the same physical model for investigation of the unsaturated seepage (Kovács, 1971). Dynamically this type of seepage can be characterized by the effects of gravity and molecular forces as main accelerating forces while the dominant resistive forces are friction and adhesion. The process is made more complicated by the fact that there is a possibility of water movement not only in liquid but also in vapour phase because on the surface of water films evaporation and condensation can occur. In hydrodynamical investigations this phenomenon has to be neglected for simplification, treating the water phase as a closed system without interaction with air.

The thickness of the water film and the tension on its surface vary continuously in response to water movement. It is very rare therefore, that steady movement can develop because the difference of tension between two points is one of the dominant accelerating forces. Thus the supposition of a steady state is also a simplifying approximation.

It was shown by previous investigations, that the resistance of an unsaturated layer is higher than that of a saturated medium. The hydraulic conductivity (k_H) is proportional to that in a saturated state. The coefficient of proportionality can be expressed as a function of water content (or degree of saturation) in the sample. The relationship between the two variables can be given in the form of graphs (Kézdi, 1962), measured points (Polubarinova Kotchina, 1962) or formulae (Averjanov, 1949 a; 1949 b; Irmay, 1945) as is shown in Fig. 7. The common form of Irmay's and Averjanov's formula is

$$k_H = k \left(\frac{s - s_o}{1 - s_o}\right)^{\beta} ; \qquad 30.$$

where s_o is the minimum degree of saturation. The power is given by Irmay as β=3.0 and by Averjanov as β=3.5.

The ratio of the hydraulic conductivities of a sample in unsaturated and saturated condition was theoretically determined as well, using the physical model of the channels composed of pores and considering the effect of adhesion on the seepage (Kovács, 1971). As is shown in Fig. 7, the approximations proposed by Irmay and Averjanov are in good accordance with both theoretical results and experimental measurement. It can even be stated that a value between 3 and 4 is acceptable as the power of Eq.30, and the effect of the minimum degree of saturation (which can hardly be higher than 0.1) is practically negligible in most cases.

It is evident that when calculating seepage velocity in an unsaturated layer a further difference should be considered apart from the modification of hydraulic conductivity, i.e. the total hydraulic gradient is composed of the variation of gravitational potential and tension along flow lines:

$$v = k_H \frac{d\,/h + \Psi(\tau)}{dx} \quad . \qquad 31.$$

Considering Eq.12, which gives the relationship between tension and saturation, it can be recognized, that the gradient is also a function of saturation and changes along flow lines. Its value cannot be taken into consideration, therefore, as a constant calculated from the known boundary conditions at the entry and exit faces of the layer even in the case of constant cross-section of the seepage field when the constancy of the gradient is a correct supposition in saturated media.

Taking into account the approximations mentioned previously (the use of Eq.30 and the negligible effect of minimum saturation) the final form of seepage velocity downwards through the unsaturated zone can be given as follows:

$$-v = k_D \; s^{\beta} \left[\frac{6A}{\tau s^7} \frac{\partial s}{\partial x} + 1 \right] \text{; because} \qquad 32.$$

$$\frac{\partial \Psi}{\partial x} = \frac{d\Psi}{ds}\frac{\partial s}{\partial x} \; ; \; \frac{d\Psi}{ds} = -\frac{6A}{s^7} ; \; h = H - x ; \; \frac{dh}{dx} = -1 ;$$

where $s = s(x,t)$ and the partial differential has to be used when differentiating saturation or tension according to the depth. (More precisely Eq.32 can be used only if the pF curve is described by Eq.12 in the whole zone of saturation. It must be supplemented with the consideration of capillary effects in other cases.)

3.3 Theoretical investigation of infiltration

It was already mentioned that the theoretical investigation of infiltration should be based on hydrodynamical derivations and their approximations related to seepage through unsaturated porous media because in this way all known and experimentally proved physical relationships can be considered for the description of this process. The main aspects which have to be taken into account are as follows:

- The hydraulic conductivity of an unsaturated medium is proportional to Darcy's coefficient and to the third or fourth power of saturation (Eq.30).

- In the unsaturated zone the hydraulic gradient is composed of two members. The effect of gravity is expressed with negative units in the case of a vertical flow directed downwards. The effect of tension differences along the unit length of a flow line must be added to the former (Eq.32 or its supplemented version).

- The relationship between the thickness of the water film and the tension on its surface can be approximated with a hyperbole of the sixth power. The same formula--after transformation of the constants--can be related to the dependence of tension on water content or saturation (Eq.12). This relationship is valid only if the capillary effect is negligible. In other cases this influence has to be considered as well.

- Considering the previous two points the gradient inducing infiltration can be expressed as a function of the vertical distribution of saturation (Eq.32).

- The relationship between water content and tension also determines the upper section of the pF curve above the open capillary zone, where water content is not influenced by capillarity. This limit (maximum capillary height) can be calculated from Eq.17.

- When there is a dynamic equilibrium between the acting forces (gravity and tension differences) the vertical distribution of water content in a homogeneous soil profile is also in a balanced condition. This state can be described in the form of a function of water content depending on the elevation of the investigated point above groundwater table. The equation in question can be derived from the pF curve, and in the upper zone of the latter is also a hyperbole of sixth power (Eq.11).

- The pressure of water above the meniscus in a capillary tube is transferred directly by the water column to the lower end of the tube and, therefore, the outflow of the same amount of water (but not the same particles) starts immediately from the tube into the gravitational water space (Major, 1972).

- Because of the process mentioned in the previous point the investigation of infiltration has to be divided into three parts. In the zone of adhesion ($x < H-h_{kmax}$) the general description of water transport can be used, while in the closed capillary zone (where all capillary pores are completely saturated, $x < H-h_{kmin}$) the pressure transfer and not the water transport is characteristic. In the open capillary zone (between the two zones mentioned previously; $H-h_{kmax} < x < H-h_{kmin}$) both phenomena (i.e. water transport and pressure transfer) are significant. A combined method must be used for the investigation of mixed processes (Fig. 8).

For the description of water transport through the zone of adhesion two basic differential equations can be used. The equation of continuity describes the indestructibility of matter.

$$\frac{\partial W}{\partial t} = \frac{\partial q}{\partial x} \; ; \text{ or } \quad n\,\frac{\partial s}{\partial t} = \frac{\partial q}{\partial x} \; ; \qquad 33.$$

where q is the flux (the flow rate through a unit area perpendicular to the direction of flow). The other relationship is the equation of movement expressing the conservation of energy which (in the case of negligible capillarity) is equal to Eq.32. Because seepage velocity is equal to flux, the former being the ratio of flow rate to cross-sectional area, Eq.31 can be written in the following form:

$$-q = k_D s^{\beta}\left[\frac{6A}{s^7}\frac{\partial s}{\partial x} + 1\right] = k_D s^{\beta-7}\,\frac{6A}{\gamma}\,\frac{\partial s}{\partial x}\,k_D s^{\beta}. \qquad 34.$$

Combining Eqs. 33 and 34 the following partial differential equation can be achieved as the basis of further investigation:

$$-n\,\frac{\partial s}{\partial t} = \frac{k_D A}{\gamma}(6\beta-42)\,s^{\beta-8}\left(\frac{\partial s}{\partial x}\right)^2 + \frac{k_D A}{\gamma}\,6.s^{\beta-7}\frac{\partial^2 s}{\partial x^2} + k_D\,\beta s^{\beta-1}\frac{\partial s}{\partial x}\,. \qquad 35.$$

The initial condition is described by the pF curve

$$s(x,t) = s_B(x); \text{ if } \; t = 0 \; \text{ and } x \geqslant 0; \qquad 36.$$

and the boundary conditions can be determined at two sections, i.e. at the surface and at the depth were the total pore-space is under the influence of adhesion (see Eq. 13). (This second condition supposes once again that there is no capillary effect on the sample, or the section of the pF curve describing capillary suction is covered by the tension curve.) The boundary condition at the lower section can be easily determined

$$s(x,t) = 1 \; ; \quad \text{if } \; t \geqslant 0 \quad \text{and } x = x_n = H - \Psi_n/\gamma\,. \qquad 37.$$

At the same time the boundary condition is more complicated at the surface, where

$$\begin{aligned} &s(x,t) = s_B(0); \quad \text{if } \; t = 0 \; \text{ and } x = 0; \\ &s_B(0) < s(x,t) = \varphi(t) < 1 \quad \text{if } t_n > t > 0 \text{ and } x = 0; \\ &s(x,t) = 1 \qquad \text{if } \; t \geqslant t_n \; \text{ and } x = 0; \end{aligned} \qquad 38.$$

and t_n is known.

To avoid the difficulties caused by the very complex boundary conditions, it is advisable to choose a fictive starting level at an elevation of x_o above the surface, where a more simple boundary condition can be accepted

$$\begin{aligned} &s(x,t) = s_B(-x_o) \quad \text{if } t = 0 \; \text{ and } x = x_o. \\ &s(x,t) = 1\;; \qquad \text{if } t > 0 \; \text{ and } x = x_o. \end{aligned} \qquad 39.$$

This simplification requires the determination of x_o as a new parameter from the supposition that the function s(x,t)--which is the solution of the partial differential equation 35--satisfies the conditions summarized as Eq. 28 when substituting $x=x_o$.

The mathematical solution of the problem can be achieved by reducing the partial differential equation to an ordinary differential equation. This can be accomplished by substituting a new variable sufficiently combining the two original variables x and t [e.g. z = exp (ax-bt)]. The following steps can be made either numerically or in closed form in some special cases. The determination of the different variations and the selection of the most convenient function among the possible solutions by comparing them to observed data is under the way now. The result, which can be already drawn up from the present investigation, is that the process of infiltration is influenced by the depth of watertable as well, although this parameter was generally neglected in the past. This statement is quite evident when the thickness of the unsaturated zone is smaller than the capillary height (even than h_{kmax}), but it can be proved, also that infiltration is a function of the position of pF curve which depends on the depth of watertable.

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Table 1. Classification of various types of lysimeters.

Main group "A" Description of the soil container

subgroup "a" surface area of the container sq.m

category	Surface Area		
1	A		0,05
2	0,051	-	0,30
3	0,31	-	0,80
4	0,81	-	2,00
5	2,01	-	6,00
6	5,01	-	20,00
7	20,01		A.

subgroup "b" depth of the soil column in the container m

category	Depth		
1	d		0,50
2	0,51	-	0,80
3	0,81	-	1,00
4	1,01	-	1,50
5	1,51	-	2,00
6	2,01	-	2,50
7	2,51	-	3,00
8	3,01		d

Subgroup "c" material of the container

category	material
1	steel
2	concrete
3	artifical
4	combination of steel and concrete
5	combination of steel and artificial
6	other materials

Table 1--Continued.

Main group "B" Composition of the investigated soil column

subgroup "d" soil layers

category	type of soil
1	homogenous cohesive soil /$D_{effective} < 0,1$ mm/
2	cohesive basic layers with bottom filter /$D_{effective}$ varies from 0,4 to 20 mm/
3	cohesive basic layer with humus top soil
4	cohesive basic layer with humus and filter
5	homogenous and cohesionless layer /$D_{effective} > 0,1$ mm/
6	cohesionless basic layer with bottom filter
7	cohesionless basic layer with humus top soil
8	cohesionless basic layer with humus and filter
9	undisturbed soil sample

subgroup "e" the effective diameter of grains in the basic layer/of the soil column mm

category	effective diameter
1	$D_{eff} > 2,01$ /cohesionless/
2	2,00 - 0,41 /cohesionless/
3	0,40 - 0,11 /cohesionless/
4	0,10 - 0,021 /cohesive/
5	0,020-0,0021 /cohesive/
6	$0,002 > D_{eff}$ /cohesive/

subgroup "f" porosity /n/ of the basic layers of the soil column

category	porosity
1	n < 0,25
2	0,26 - 0,30
3	0,31 - 0,35
4	0,36 - 0,40
5	0,41 - 0,45
6	0,46 - 0,50
7	0,51 - 0,60
8	0,61 - 0,70
9	0,71 ≤ n

Main group "C" Location of the soil column /or lysimeter/

subgroup "g" location of the soil column related to the surface of the surroundings

category	vertical position
1	soil column installed at the surface /placed on the ground/
2	soil column is recessed into the soil but the elevation of its surface is higher than the average level of the ground surface
3	soil column is recessed into the ground having a surface elevation equal to the average level of the ground surface
4	soil column is recessed into the ground and the elevation of its surface is lower than the average level of the ground surface

subgroup "h" location of the lysimeter related to the vegetation of the surroundings

category	horizontal position
1	located in a closed space
2	located at an observation station /in garden for measuring instruments/ and separated from the environment
3	situated into natural environment with a surface cover equal to the surroundings
4	located into natural environment with a surface cover different from the surroundings
5	situated into natural environment and its surface is periodically or continuously covered with water

subgroup "i" location of the soil column related to the surrounding layers

category	contact with the soil space
1	soil column not completely separated from its environment
2	container of the soil column directly contacted with the surrounding soil space
3	container surrounded with air /in a shaft for the lysimeter/
4	vessel surrounded with water /if it is floating in the water/

Main group "D" Composition /formation/ of the surface of the lysimeter

subgroup "k" surface slope of the lysimeter

category	slopes
1	soil column has horizontal surface; slope = 0%
	surface slope:
2	between 1% and 5%
3	between 6% and 10%
4	between 11% and 15%
5	between 16% and 20%
6	between 21% and 30%
7	between 31% and 40%
8	between 41% and 50%
9	surface slope higher than 50%

subgroup "l" species or vegetation covering the surface of the lysimeter

category	
1	bare soil surface without any treatment
2	bare soil surface, the topsoil is kept in loose condition to a depth of 5 to 10 cm
3	surface covered with cereals in dormant season the surface is kept in a loose and bare condition
4	same treatment as in point 3 but the vegetation is root crop
5	same treatmen as in point 3 but the vegetation is vegetable
6	surface covered with leguminous plant
7	surface covered with sod
8	surface planted with orchard or vinegard
9	surface covered with other plants

subgroup "m" the effective depth of the active root zone

category	depth /cm/
1	d ≤ 30
2	31 - 50
3	51 - 80
4	81 - 100
5	101 - 150
6	151 - 200
7	201 - 250
8	251 - 300
9	300 < d

Table 1--Continued.

Main group "E" Water balance of the lysimeter

subgroup "n" surface runoff

category	
1	both incoming and outflowing runoff are excluded
2	incoming runoff is excluded but the outflowing runoff can occure and measured
3	both incoming and outflowing runoff are measured
4	both incoming and outflowing runoff can occure but not measured

subgroup "o" watertable

category	
1	drained soil column without permanent watertable
2	regulation of watertable according to a constant or a defined control program with a device being able either to draine or to recharge a changing amount of water. Modelling the horizontal groundwater flow in the device the depth of phreatic surface is measured
3	equipment which produces constant watertable with recharging and drainaging a changing amount of water
4	watertable regulation according to a defined program with an equipment recharging or drainaging changing amount of water
5	equipment for measuring the elevation of water table without influencing the development of it

subgroup "p" water recharge of the soil column

category	
1	only natural recharging from precipitation
2	artificial recharging through the surface with sprinkling irrigation
3	artificial recharge of the soil column with flooding
4	recharge of water artificially directly into the gravitational groundwater space

Main group "F" Methods of basic measurements of lysimeter

subgroup "r" method of measuring the stored amount of water

category	measuring method
1	weighing the soil column by lifting the cointainer/from its shaft/,which has no device for water table regulation
2	weighing with scales installed on the container which is not supplemented with a device for the regulation of watertable
3	measuring the /liquid/ pressure change of the hydraulic /jack/ system supporting the conrainer which is not supplemented with a device for the regulation of water table
4	weighing method according to point 1 but the cointainer is installed with water table regulating device
5	weighing method according to point 2 but the cointainer is installed with water table regulating device
6	weighing method according to point 3 but the cointainer is installed with water table regulating device
7	measuring the water volume recharging and drainaging the soil column by estimating the difference between natural recharge /precipitation/ and surface runoff

subgroup "s" Method of soil moisture measurements

category	measuring method
1	there is no soil moisture measurement at all
2	weighing /the determination of the difference in weight between an oven dry and wet soil sample/
3	measuring the moisture content with electric resistivity
4	measuring the moisture content with electric capacitor
5	measuring the moisture content with neutron probe
6	measuring the moisture content with the combination of electric resistivity and neutron probe
7	determination of soil moisture content with other suitable method

subgroup "t" period of basic measurements

category	period
1	continuous registration of data
2	periodical measurements several times within an hour
3	periodical measurement several times within a day but not more frequently than an hour
4	periodical measurement several times within one decade but not more frequently than one day
5	periodical measurement not more frequently than one decade.
6	irregular observations

Table 1--Continued.

Main group "G" Supplementary measurements

subgroup "u" meteorological measurements /continuity of observations and at least daily repetition of measurements is necessary/

category	
1	there is no meteorological observation at all
2	measurement of precipitation
3	measurement of air temperatura and precipitation
4	measurement of relative huminidity of air and precipitation
5	measurement of wind velocity and precipitation
6	measurement of temperatura and relative humidity of air as well as precipitation
7	measurement of wind velocity and relative humidity of air as well as precipitation
8	measurement according to point 6 completed with wind velocity
9	meteorological observations at a 1st order station /measurements listed in point 8 supplemented with water surface evaporation--using "A" and GGI 300 type pans-, sunshine duration, soil temperature of the upperlying layers, radiation e.c.t. observations/

subgroup "v" agronomicel measurement /density of stand crop which is equal to the number of plants within a unit area, supposed to be known/

category	
1	there is no agronomical measurement at all
2	weighing the crop only in the final phase of growth
3	weighing only in the final phase of growth the dry matter of plants emerging above the ground surface
4	weighing the total dry matter of plants only in the final phase of growth /comprising roots and the part of plants emerged above the surface/
5	continous weighing the dry matter of plants emerging above the ground surface
6	continous weighing the dry matter and the surface area of the leaves of plants emerging above ground surface
7	continous weighing of the total dry matter of plants
8	continous weighing of the total dry matter plants and the surface area of leaves

subgroup "z" other measurements

category	measurement
1	depth and surface area measurement of stagnant pools occuring on the surface of the investigated soil column after water recharging processes through the surface
2	soil temperature measurement in the lysimeter
3	air temperature measurement in the closed shaft where lysimeter is recessed in
4	measuring the change in porosity of the soil column in a profile
5	joint-measurement of factors listed in point 1 and 2
6	" " " " 1,2 and 3
7	" " " " 1 and 4
8	" " " " 2 and 3
9	" " " " 1,2,3 and 4

Table 2. Evaluation of lysimeters in the form of waterbalance-equations.

Type of lys. I.	Directly measured parameters II.	Parameters calculated from measured values III.	Remarks IV.
LA_1	$P_T = P_s$	$\Delta S_2 = \Delta G/\eta A$	
	$\Delta R = R_i - R_o$	$E + I_s = P_s - \Delta R$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$E_s = \Delta S_2$	2.
LA_2	$P_T = P_s$	$\Delta S_2 = \Delta G/\eta A$	
	$\Delta R = R_i - R_o$	$E + I_s = P_s - \Delta R$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$E_s = \Delta S_2$	2.
	$W/x,t/$	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	3.
LA_3	$P_T = P_s$	$\Delta S_2 = \Delta G/\eta A$	
	$\Delta R = R_i - R_o$	$E + I_s = P_s - \Delta R$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$I_s = \Delta S_2 - /-D/$	1.
	$/-D/$	$E = P_s - \Delta R - \Delta S_2 + /-D/$	1.
		$E_s = \Delta S_2$	2.
LA_4	$P_T = P_s$	$\Delta S_2 = \Delta G/\eta A$	
	$\Delta R = R_i - R_o$	$E + I_s = P_s - \Delta R$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$I_s = \Delta S_2 - /-D/$	1.
	$/-D/$	$E = P_s - \Delta R - \Delta S_2 + /-D/$	1.
	$W/x,t/$	$E_s = \Delta S_2$	2.
		$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	3.

Type of lys. I.	Directly measured parameters II.	Parameters calculated from measured values III.	Remarks IV.
LC_1	P_T	$\Delta S_1 + \Delta S_2 = \Delta G/\eta A - \Delta P1$	4.
	$\Delta R = R_i - R_o$	$E + \Delta S_1 + E_1 + I_s = P_T - \Delta R$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$ET_A = E + E_I + E_s + T_s = \Delta G/\eta A - \Delta P1$	2.
	$P1$		
LC_2	P_T		
	$\Delta R = R_i - R_o$	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_1 = \Delta G/\eta A - \Delta S_2 - \Delta P1$	4.
	$\Delta P1$	$P_s = P_T - \Delta S_1 - E_I$	1.
	$W/x,t/$	$E + E_I + I_s = P_T - \Delta R - \Delta S_1$	1.
		$E_s + T_s = \Delta S_2$	2.
		$ET_A = E + E_I + E_s + T_s = \Delta G/\eta A - \Delta P1$	2.
LC_3	P_T	$\Delta S_1 + \Delta S_2 = \Delta G/\eta A - \Delta P1$	4.
	$\Delta R = R_i - R_o$	$E + \Delta S_1 + E_1 + I_s = P_T - \Delta R$	1.
		$I_s = \Delta S_2 - /-D/$	1.
	$\Delta G = G/t_2/ - G/t_1/$	$ET_A = E + E_I + E_s + T_s = \Delta G/\eta A - \Delta P1$	2.
	$\Delta P1$		
	$/-D/$		
LC_4	P_T	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$\Delta R = R_i - R_o$		
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_1 = \Delta G/\eta A - \Delta S_2 - \Delta P1$	4.
	$\Delta P1$	$P_s = P_T - \Delta S_1 - E_I$	1.
	$/-D/$	$I_s = \Delta S_2 - /-D/$	1.
	$W/x,t/$	$E + E_I = P_T - \Delta R - \Delta S_1 - I_s$	1.
		$E_s + T_s = \Delta S_2$	2.
		$ET_A = E + E_I + E_s + T_s = \Delta G/\eta A - \Delta P1$	2.

Table 2--Continued.

I.	II.	III.	IV.
	$P_T = P_s$	$E+I_s = P_s - \Delta R$	1.
	$\Delta R = R_1 - R_o$	$\Delta S_2 = I_s + /-D/ = P_s - \Delta R - E + /-D/$	
	$/-D/$		
LA_5	$V/t/ = S_{2max} - S_2/t/$	$\Delta S_2 = S_2/t_2/ - S_2/t_1/ = V/t_1/ - V/t_2/$	
	periodically saturating the soil column until maximum water capacity	$E_s = \Delta S_2$ only approximation	2.
	$P_T = P_s$	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$R = R_1 - R_o$		
LA_6	$/-D/$	$E+I_s = P_s - \Delta R$	1.
	$W/x,t/$	$I_s = \Delta S_2 - /-D/$	1.
		$E = P_s - \Delta R - \Delta S_2 + /-D/$	1.
		$E_s = \Delta S_2$	2.
	$P_T = P_s$	$\Delta S_3 = n \cdot \Delta H = I_g - E_g$	
	$\Delta R = R_1 - R_o$	$\Delta S_2 = \Delta G/\eta A - \Delta S_3$	
LB_1	$\Delta G = G/t_2/ - G/t_1/$	$E+I_s = P_s - \Delta R$	1.
	$\Delta H = -[H/t_2/ - H/t_1/]$	$I_s = \Delta G/\eta A$	1.
		$E = P_s - \Delta R - \Delta G/\eta A$	1.
		$E_s = \Delta G/\eta A$	2.
	$P_T = P_s$	$\Delta S_3 = n \cdot \Delta H - I_g - E_g$	
	$\Delta R = R_1 - R_o$	$\Delta S_2 = \Delta G/\eta A - \Delta S_3$	
	$\Delta G = G/t_2/ - G/t_1/$	$E+I_s = P_s - \Delta R$	1.
LB_2	$\Delta H = -[H/t_2/ - H/t_1/]$	$I_s = \Delta G/\eta A$	1.
	$W/x,t/$	$E = P_s - \Delta R - \Delta G/\eta A$	1.
		$E_s = \Delta G/\eta A$	2.
		$\Delta S_2 = \int_0^M [/W/x,t_2/ - W/x,t_1/]\,dx$	3.

I.	II.	III.	IV.
	P_T	$E+\Delta S_1+E_1+I_s = P_T - \Delta R$	1.
	$\Delta R = R_1 - R_o$	$\Delta S_2 = I_s + /-D/ = P_T - \Delta R - E - \Delta S_1 - E_1$	
	$/-D/$		
LC_5	$V/t/ = S_{2max} - S_2/t/$	$\Delta S_2 = S_2/t_2/ - S_2/t_1/ = V/t_1/ - V/t_2/$	
	periodically saturating the soil column until maximum water capacity	$E_s+T_s = \Delta S_2$ only approximation	2.
	P_T	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$\Delta R = R_1 - R_o$		
LC_6	$/-D/$	$I_s = \Delta S_2 - /-D/$	1.
	$W/x,t/$	$E+E_I+\Delta S_1 = P_1 - \Delta R - I_s$	1.
		$E_s+T_s = \Delta S_2$	2.
	P_T	$\Delta S_3 = n \cdot \Delta H = I_g - E_g$	
	$\Delta R = R_1 - R_o$	$\Delta S_1 + \Delta S_2 = \Delta G/\eta A - \Delta S_3 - \Delta P1$	4.
LD_1	$\Delta G = G/t_2/ - G/t_1/$	$E+I_s+\Delta S_1 = P_T - \Delta R$	1.
	$\Delta H = -[H/t_2/ - H/t_1/]$	$I_s = \Delta G/\eta A$	1.
	$\Delta P1$	$\Delta S_1 + E = P_T - \Delta R - \Delta G/\eta A$	1.
		$ET_A = E_s + T_s + E + E_I = \Delta G/\eta A - \Delta P1$	2.
	P_T	$\Delta S_3 = n \cdot \Delta H = I_g - E_g$	
	$\Delta R = R_1 - R_o$	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$\Delta G = G/t_2/ - G/t_1/$		
LD_2	$\Delta H = -[H/t_2 - H/t_1/]$	$\Delta S_1 = \Delta G/\eta A - \Delta S_3 - \Delta S_2 - \Delta P1$	4.
	$W/x,t/$	$P_s = P_T - \Delta S_1 - E_I$	1.
	$\Delta P1$	$E+E_I+I_s+\Delta S_1 = P_T - \Delta R$	1.
		$I_g = \Delta G/\eta A - \Delta P1$	1.
		$E+E_I = P_T - \Delta R - \Delta S_1 - \Delta G/\eta A - \Delta P1$	1.
		$ET_A = E_s + T_s + E + E_I = \Delta G/\eta A - \Delta P1$	2.

Table 2--Continued.

I.	II.	III.	IV.
	$P_T = P_s$	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_1 - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_2 = \Delta G/\eta A - \Delta S_3$	
	$\Delta H = -[H/t_2/ - H/t_1/]$	$E + I_s = P_s - \Delta R$	1.
	D	$I_s = \Delta G/\eta A - D$	1.
LB_3		$E = P_s - \Delta R - \Delta G/\eta A + D$	1.
		$E_s = \Delta G/\eta A - D$	2.
	in special case of maintenance of a given watertable, groundwater drainage and recharge are measured separately	$I_g = /-D/$ $E_g = /+D/$	
	$P_T = P_s$	$\Delta S_3 = n.\Delta H.$	
	$\Delta R = R_1 - R_o$	$I_g - E_g = \Delta S_3 - D$	
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_2 = \Delta G/\eta A - \Delta S_3$	
LB_4		$E + I_s = P_s - \Delta R$	1.
	$\Delta H = -[H/t_2/ - H/t_1/]$	$I_s = \Delta G/\eta A - D$	1.
	D	$E = P_s - \Delta R - \Delta G/\eta A + D$	1.
	W/x,t/	$E_s = \Delta G/\eta A - D$	2.
		$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	3.
	in special case of maintenance of a given water-table, groundwater drainage and recharge is measured separately	$I_g = /-D/$ $E_g = /+D/$	
	$P_T = P_s$	$\Delta S_3 = n.\Delta H$	
LB_{51}	$\Delta R = R_1 - R_o$	$I_g - E_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/ - H/t_1/]$	$E + I_s = P_s - \Delta R$	1.
	D	$\Delta S_2 = I_s - \Delta S_3 + D - P_s - \Delta R - E - \Delta S_3 + D$	1.

I.	II.	III.	IV.
	P_T	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_1 - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_1 + \Delta S_2 = \Delta G/\eta A - \Delta S_3 - \Delta P1$	4.
	$\Delta H = -[H/t_2/ - H/t_1/]$	$E + E_I + E_s + \Delta S_1 = P_T - \Delta R$	1.
LD_3	$\Delta P1$	$\Delta S_1 + I_s = \Delta G/\eta A - D - \Delta P1$	1.
	D	$E + E_I = P_T - \Delta R - \Delta G/\eta A + D + \Delta P1$	1.
		$ET_A = E_s + T_s + E + E_I = \Delta G/\eta A - D - \Delta P1$	2.
	in special case of maintenance of a given watertable, groundwater drainage and recharge are measured separately	$I_g = /-D/$ $ET_g = /+D/$	
	P_T	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_1 - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta G = G/t_2/ - G/t_1/$	$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
	$\Delta H = -[H/t_2/ - H/t_1/]$		
	$\Delta P1$	$\Delta S_1 = \Delta G/\eta A - \Delta S_3 - \Delta S_2 - \Delta P1$	4.
LD_4	D	$P_s = P_T - \Delta S_1$	
	W/x,t/	$E + E_I + I_s + \Delta S_1 = P_T - \Delta R$	1.
		$\Delta S_1 + I_s = \Delta G/\eta A - D - \Delta P1$	1.
		$E + E_I = P_T - \Delta R - \Delta G/\eta A + D + \Delta P1$	1.
		$ET_A = E_s + T_s + E + E_I = \Delta G/\eta A - D - \Delta P1$	2.
	in special case of maintenance of a given watertable, groundwater drainage and recharge is measured separately	$I_g = /-D/$ $ET_g = /+D/$	
	P_T	$\Delta S_3 = n.\Delta H$	
LD_{51}	$\Delta R = R_1 - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/ - H/t_1/]$	$E + E_I + I_s + \Delta S_1 = P_T - R$	1.
	D	$\Delta S_2 = I_s - \Delta S_3 + D$	1.
		$\Delta S_1 + \Delta S_2 = P_T - \Delta R - E - E_I - \Delta S_3 + D$	1.

Table 2--Continued.

I.	II.	III.	IV.
LB_{52}	$P_T = P_s$	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_i - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$I_g = /-D/$	
	D	$ET_g = /+D/$	
		$E+I_s = P_s-\Delta R$	1.
		$\Delta S_2 = I_s-\Delta S_3+D = P_s-\Delta R-E-\Delta S_3+D$	1.
LB_{61}	$P_T = P_s$	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_i - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$\Delta S_2 = \int_0^M [W/x,t_2/-W/x,t_1/]\,dx$	
	D	$E+I_s = P_s-\Delta R$	1.
	W/x,t/	$I_s = \Delta S_2+\Delta S_3-D$	1.
		$E = P_s-\Delta R-\Delta S_2-\Delta S_3+D$	1.
		$E_s = \Delta S_2+\Delta S_3-D$	2.
LB_{62}	$P_T = P_s$	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_i - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$I_g = /-D/$	
	D	$ET_g = /+D/$	
	W/x,t/		
		$\Delta S_2 = \int_0^M [W/x,t_2/ - W/x,t_1/]\,dx$	
		$E+I_s = P_s-\Delta R$	1.
		$I_s = \Delta S_2+\Delta S_3-D$	1.
		$E = P_s-\Delta R-\Delta S_2-\Delta S_3+D$	1.
		$E_s = \Delta S_2+\Delta S_3-D$	2.

I.	II.	III.	IV.
LD_{52}	P_T	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_i - R_o$	$I_g - ET_g = \Delta S_3 . D$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$I_g = /-D/$	
	D	$ET_g = /+D/$	
		$E+E_I+I_s+\Delta S_1 = P_T-\Delta R$	1.
		$\Delta S_2 = I_s-\Delta S_3+D$	1.
		$\Delta S_1+\Delta S_2 = P_T-\Delta R-E-E_I-\Delta S_3+D$	1.
LD_{61}	P_T	$\Delta S_3 = n.\Delta H$	
	$\Delta R = R_i - R_o$	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$\Delta S_2 = \int_0^M [W/x,t_2/-W/x,t_1/]\,dx$	
	D	$E+E_I+I_s+\Delta S_1 = P_T-\Delta R$	1.
	W/x,t/	$I_s = \Delta S_2+\Delta S_3-D$	1.
		$E+E_I+\Delta S_1 = P_T-\Delta R-\Delta S_2-\Delta S_3+D$	1.
		$P_s = P_T-E-E_I-\Delta S_1$	1.
		$E_s+T_s = \Delta S_2+\Delta S_3-D$	2.
LD_{62}		$\Delta S_3 = n.\Delta H$	
	P_T	$I_g - ET_g = \Delta S_3 - D$	
	$\Delta R = R_i - R_o$	$I_g = /-D/$	
	$\Delta H = -[H/t_2/-H/t_1/]$	$ET_g = /+D/$	
	D		
	W/x,t/	$\Delta S_2 = \int_0^M [W/x,t_2/-W/x,t_1/]\,dx$	
		$E+E_I+I_s+\Delta S_1 = P_T-\Delta R$	1.
		$I_s = \Delta S_2+\Delta S_3-D$	1.
		$E+E_I+\Delta S_1 = P_T-\Delta R-\Delta S_2-\Delta S_3+D$	1.
		$P_s = P_T-E-E_I-\Delta S_1$	1.
		$E_s+T_s = \Delta S_2+\Delta S_3-D$	2.

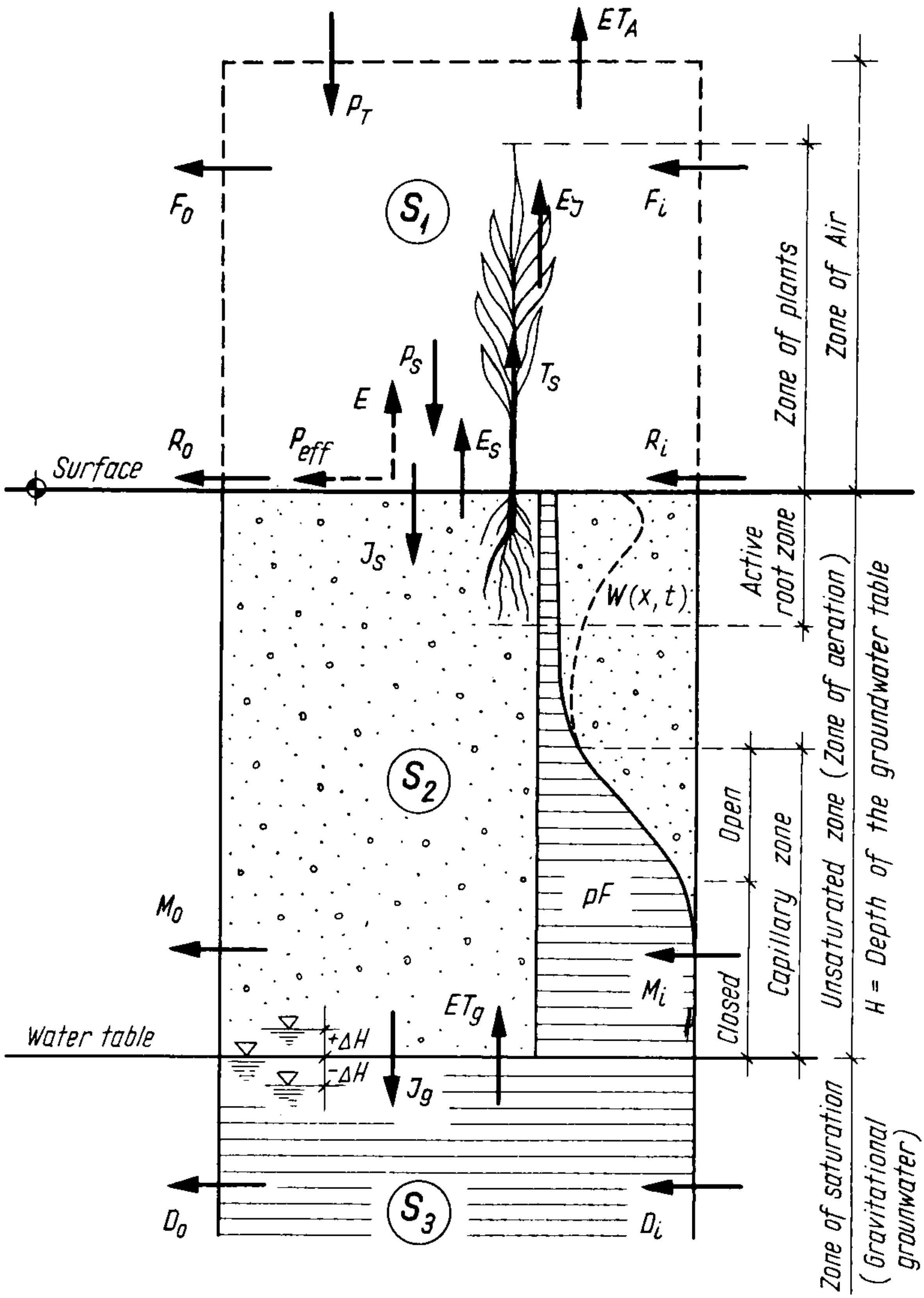

Figure 1. Physical model representing hydrological processes occurring in the unsaturated zone.

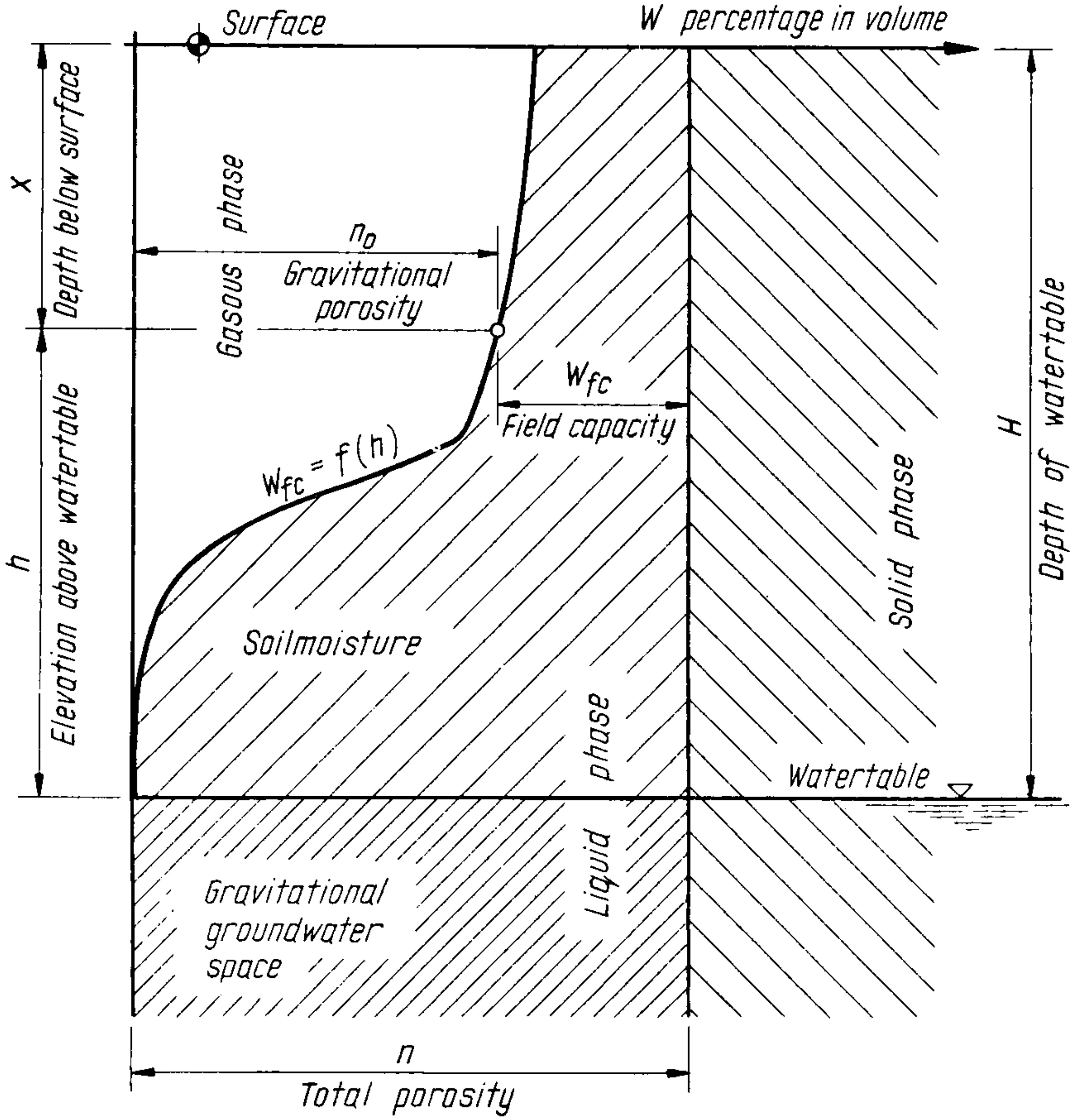

Figure 2. Interpretation of field capacity and gravitational porosity as functions of the elevation above the watertable.

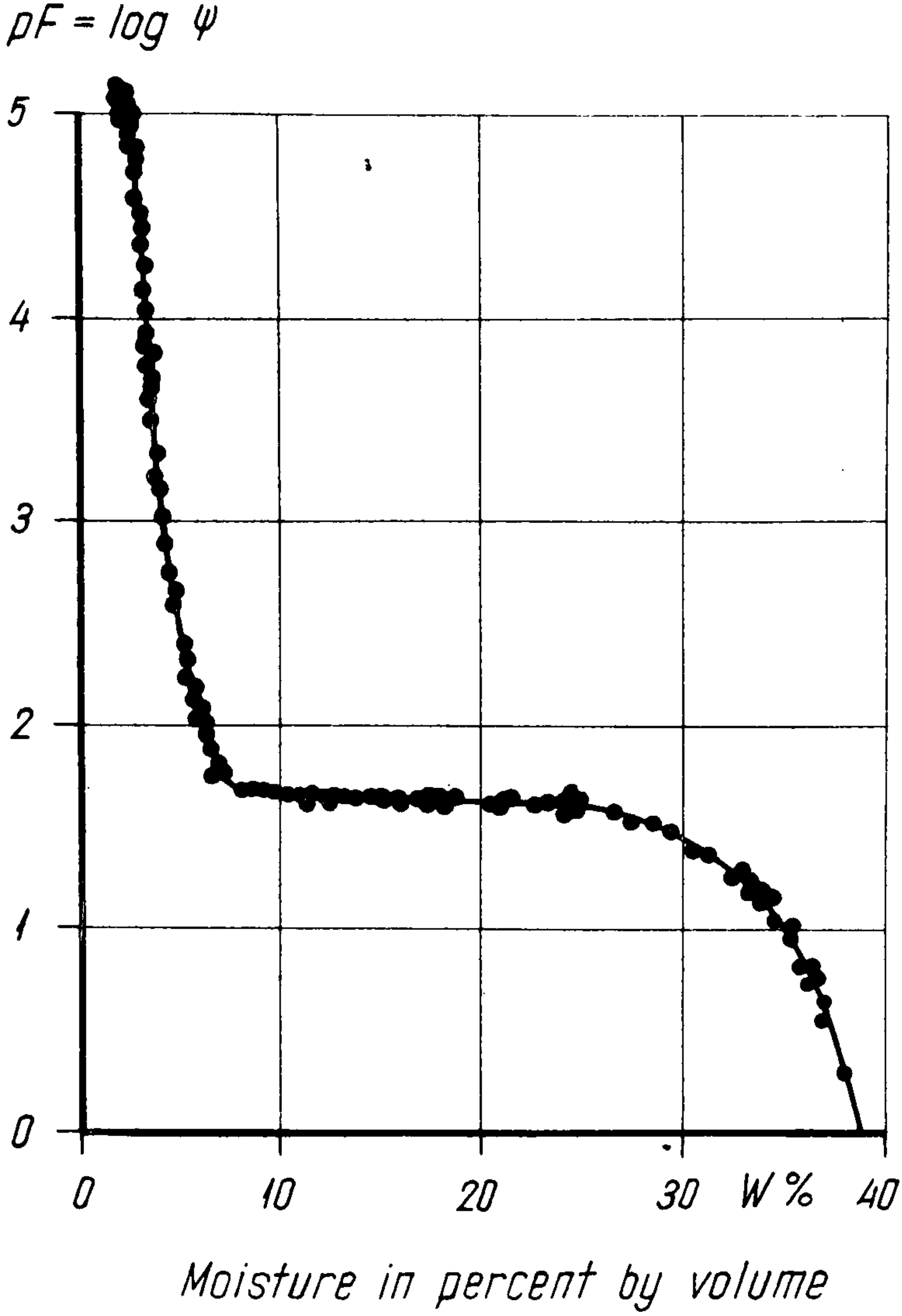

Figure 3. The general form of a pF curve determined with point measurements.

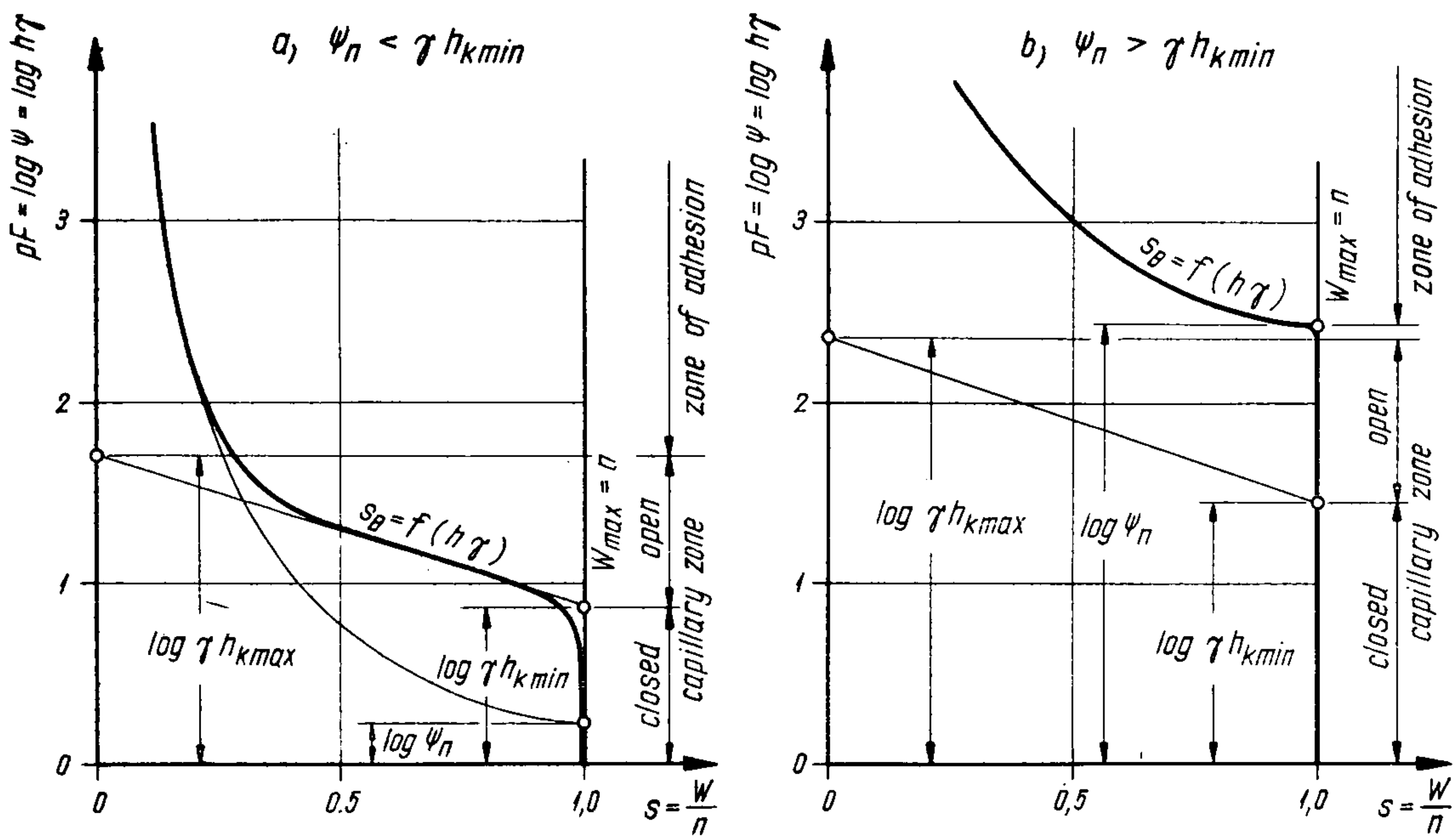

Figure 4. Two basic types of pF curves:
a/ composed of three stretches (general form);
b/ characterized by a monotonously decreasing curve (in the case of very fine material).

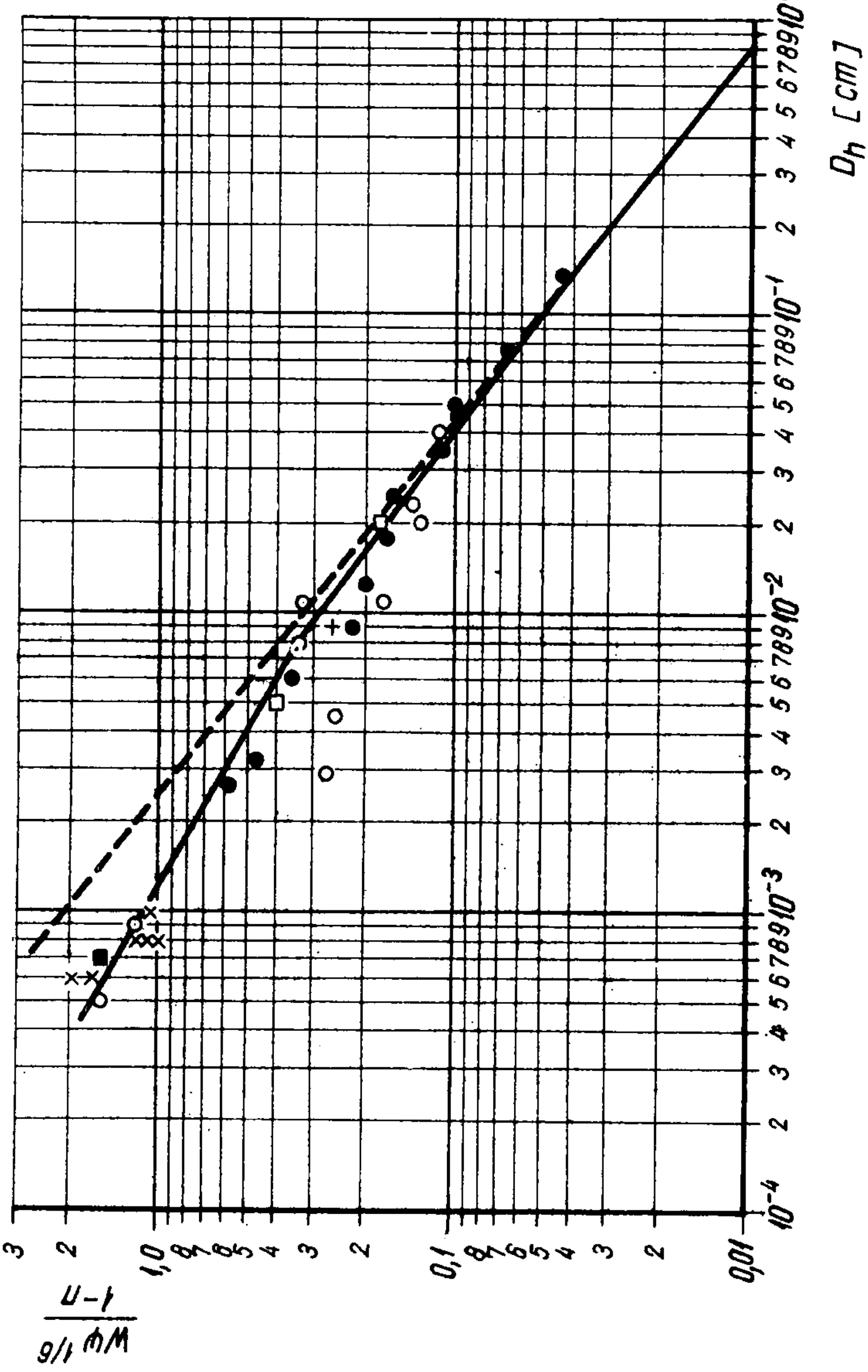

Figure 5. Evaluation of field measurements with infiltrometers.

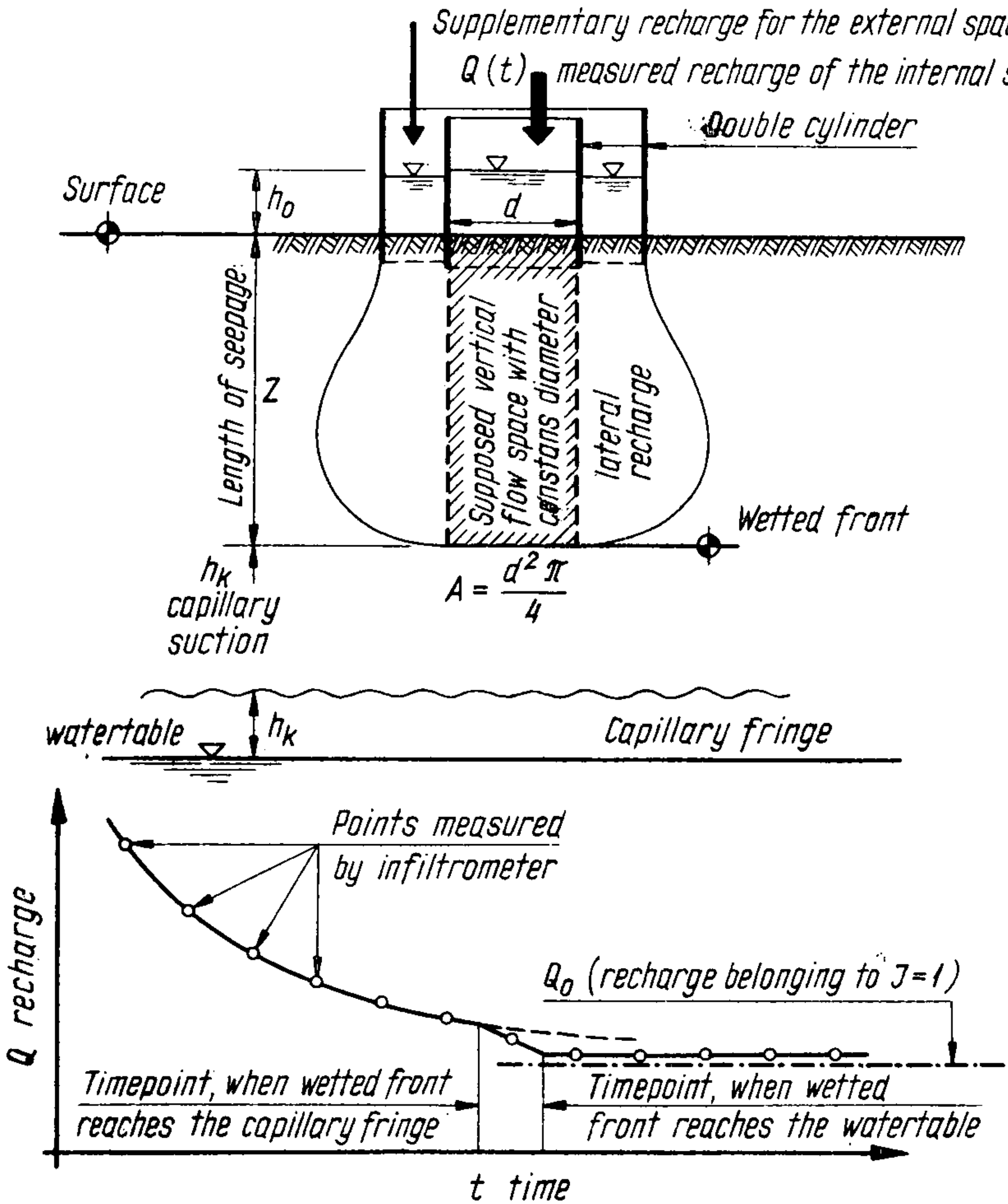

Figure 6. Hydraulic conductivity of the unsaturated zone, as the function of saturation.

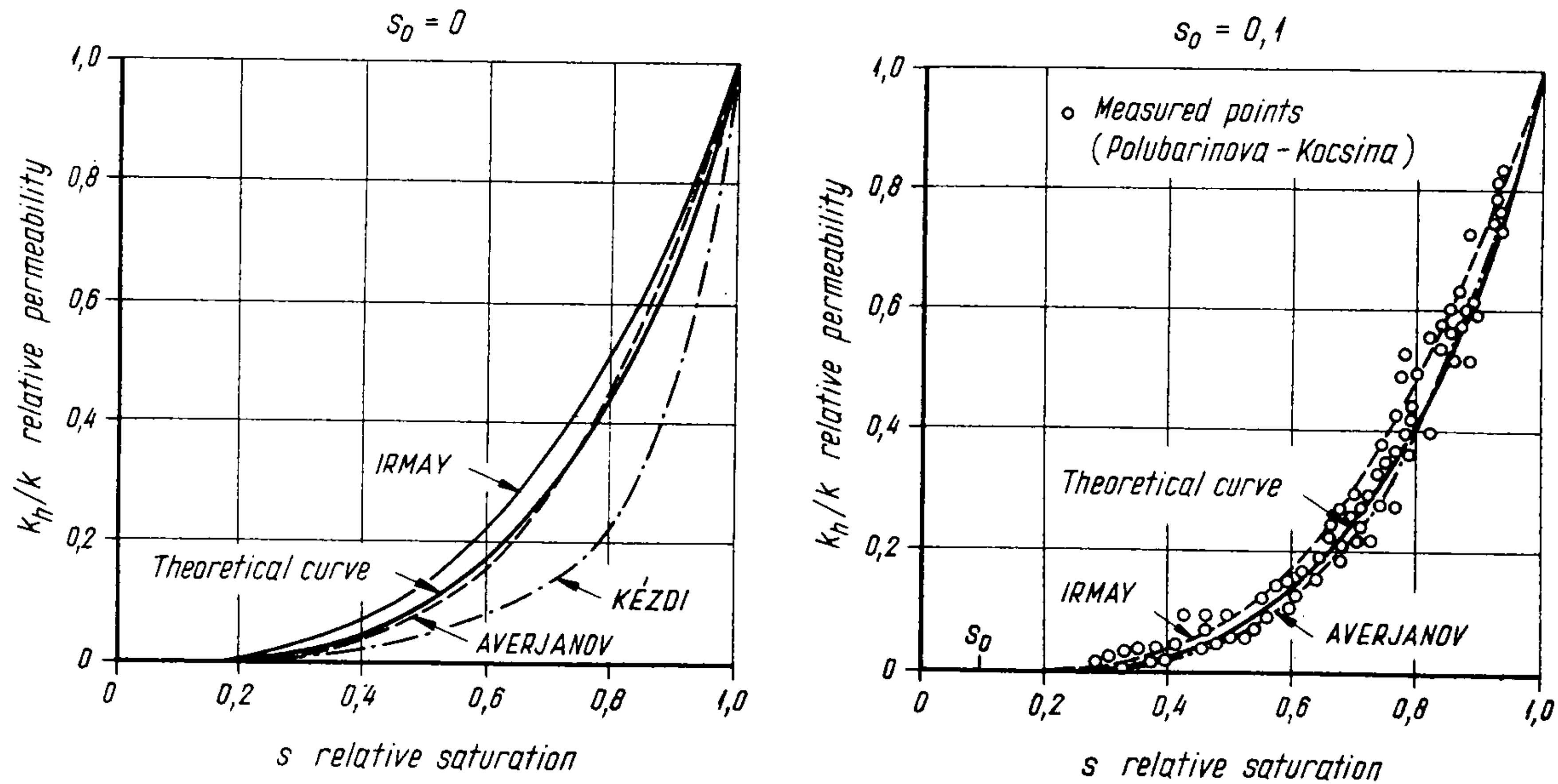

Figure 7. Representation of the process of infiltration in the form of saturation depending on time and depth.

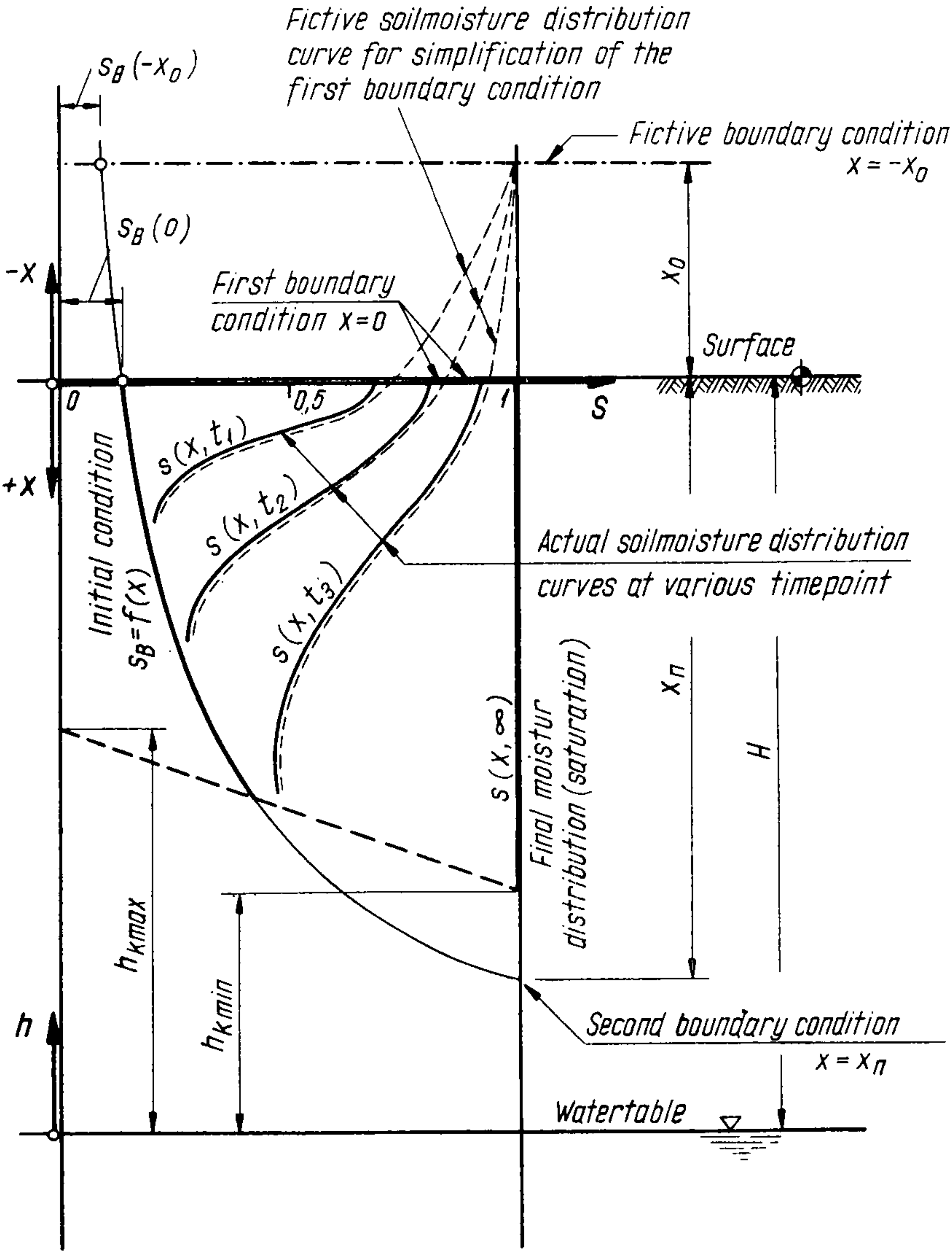
Fictive soilmoisture distribution curve for simplification of the first boundary condition
$s_B(-x_0)$
Fictive boundary condition $x = -x_0$
$s_B(0)$
x_0
-X
+X
First boundary condition x=0
Surface
0
0,5
1
S
$s(x,t_1)$
$s(x,t_2)$
$s(x,t_3)$
Initial condition $s_B = f(x)$
Actual soilmoisture distribution curves at various timepoint
$s(x,\infty)$
Final moistur distribution (saturation)
x_n
H
h_{Kmax}
h_{Kmin}
h
Second boundary condition $x = x_n$
Watertable

Figure 8

MODEL ECOSYSTEM STUDIES: MODELS OF WHAT?

by

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The concept that most of the chlorinated hydrocarbon insecticides are highly resistant to biodegradation and are retained in the environment for considerable time periods, whereupon they become sequestered in living organisms and subsequently magnified in both terrestrial and aquatic food chains, is one which has been so frequently repeated during the last decade that it appears to have become almost universally accepted. For the most part, this thesis rests on a large number of correlative field studies, the enumeration of which is beyond the scope of this paper. However, there have been attempts to duplicate this phenomenon under controlled laboratory conditions, mainly through the so-called "model ecosystem" approach. These studies have been carried out primarily at the University of Illinois by Metcalf and his coworkers, although some other works relevant to the topic are known (for instance, Reinert, 1972). In the present review we shall focus on the experiments of the Illinois investigators, reported in the following papers: Kapoor, Metcalf, Nystrom, and Sangha, 1970; Metcalf, Sangha, and Kapoor, 1971; Kapoor, Metcalf, Hirwe, Lu, Coats, and Nystrom, 1972; Metcalf and Kapoor, 1972; Kapoor, Metcalf, Hirwe, Coats, and Khalsa, 1973; and Metcalf, Kapoor, Lu, Schuth, and Sherman, 1973.

The original impetus for undertaking the the model ecosystem experiments seems to relate to the search for substitute chemicals which would retain the advantageous residual action against target insect species associated with DDT and other widely used pesticides of the organochlorine group, but which would be more "biodegradable"--especially by members of the vertebrate phylum. During the past few years Metcalf and his coworkers have synthesized a considerable number of "DDT analogs" and have tested these both for their insecticidal activity and their biodegradability (Metcalf, 1973). The behavior of these compounds in the model ecosystem has been compared with that of such insecticides as DDT, DDD, aldrin, dieldrin, endrin, lindane, hexochlorobenzene, etc., as well as with non-insecticidal but persistent metabolic products such as DDE.

The claims made regarding the efficacy of the model ecosystem as a screening technique for the evaluation of new pesticides and as a simple, practical, replicable methodology for determining the environmental effects of pesticides now registered for use are presented strongly in all of the publications emerging from the work of Metcalf and his coworkers. Since these claims appear to have been accepted without critical scrutiny by important decisionmaking bodies and even by scientists who defend the need for continued use of the well known chlorinated hydrocarbon insecticides for increases in food productivity or for disease vector control programs, it was felt that a critical evaluation of these publications and an attempt to partially replicate the findings of the Illinois group would be fruitful. The following, then, is a report of a review of the studies, and the results of our experiments bearing on confirmation. Our evaluation centers broadly on four topics: (1) the nature of the system, its components, and the techniques employed by Metcalf and his coworkers; (2) results of our algal growth studies; (3) the reported findings *per se* of the Metcalf group; and (4) the conclusions and claims put forth by the investigators.

The System

The model ecosystem as first described by Kapoor *et al.* (1970) consisted of a small glass aquarium 10 X 12 X 18 in., containing a shelf of 15 kg washed white quartz sand and 12 l "standard reference water." The sand is steeply sloped in such a way as to provide a small above-water portion where Sorghum halpense can be grown. The Sorghum seeds are planted on the first day of the experiment. The following members of the test ecosystem are introduced into the aquatic portion of the aquarium on the same day: phyto- and zooplankton from old aquarium water, the filamentous green alga Oedogonium cardiacum, Daphnia magna, and Physa sp. snails. The water is continuously aerated with a pump, and the system is kept at 26°C with 12 hour exposure to 5000 ft. candles in an environmental plant growth chamber. After 20 days, when the Sorghum reaches about 6 in. height, 5 mg of a radiolabeled insecticide is applied to the leaves of the plant. Ten larvae of the salt marsh caterpillar Estigmene acrea are placed in the aerial portion of the aquarium. The caterpillars completely devour the plants, and their feces--containing radiolabeled compounds--then contaminate the aquatic part of the system. After 26 days, 300 Culex quinquefasciatus mosquito larvae are added to the tank, and after 30 days, three Gambusia affinis fish are placed in the water. The experiment is terminated after 33 days, at which time weighed samples of fish, snails, mosquito larvae, algae, and water are removed, extracted, and assayed for radioactivity by a series of techniques (to be described later).

In the 1971 publication of Metcalf et al., some further details are given about the model ecosystem, with two specific changes (quantity of water and size of aquarium), and certain discrepancies in description. The size of the aquarium is there said to be 10 X 12 X 20 in. with 180 in.^{2} surface (sic), and only 7 liters of "standard reference water" are used. It is stated on p. 710 that a plexiglass cover 11 X 12 in. is placed over the aquatic portion of the chamber, and on the following page that ". . . the 4 in. open end of the aquarium covered (sic) with copper screen to confine the insects" (Metcalf et al., 1971, p. 711). No explanation is offered as to what might cover the missing 4 inches (12 + 4 = 16; the total length of the aquarium is stated to be 20 in.). The sand-water system is equilibrated for one day (day 0) before the introduction of any organisms. On day 1, 50 Sorghum seeds are planted in 5 rows, and several ml of old aquarium water, a "few" strands of Oedogonium cardiacum, 30 Daphnia magna, and 10 Physa snails are added to the water. The organismic composition of the old aquarium water is reported as follows: among the identified diatoms are Navicula, Coscinodiscus, Diploness (sic), and Diatomella. The zooplankton include the protozoa Nuclearia, Coleps, Vorticella and Paramecium, and the rotifera Asplanchnopus, Notomatta (sic), Euclaris, and Scaridium.

After 20 days, the Sorghum plants reach 4 in. height and are treated with 5 mg pesticide. The rate of application is said to correspond to about 1 lb./acre. On the same day, 10 5th instar larvae of the salt marsh caterpillar are placed onto the dry sand, with the expectation that they will consume nearly all of the treated leaves within 3 to 4 days.

After 26 days, when it is expected that the aqueous portion of the aquarium should be contaminated with the radiolabeled compound through the caterpillar feces, the leaf frass, and the caterpillar larvae themselves, 300 Culex pipiens quinquefasciatus larvae (here correctly named) are added to the water. Four days later, 50 of the mosquito larvae are removed from the system for analysis, at which time 3 Gambusia affinis mosquito fish are placed in the water. These are expected to eat the remaining 250 mosquito larvae and the 30 Daphnia. "The experiment is terminated after 33 days, when weighed samples of the organisms were (sic) examined for radioactivity. . . . Samples of sand are counted for radioactivity, together with duplicate 1-ml aliquots of water taken from the aquarium at 1, 3, 7, 14, and 28 days after treatment of the Sorghum" (Ibid., p. 711).

There are four problems with this description which are of more import than the confusing numbers referring to the surface dimensions of the aquarium or the misspellings of generic names and uncorrected grammar. First, of the four diatoms supposedly identified, two--Coscinodiscus and Diatomella--are not fresh water species. One would therefore hardly expect them to be present in old aquarium water. Secondly, while it is mentioned in all of the publications that samples of various organisms and other elements of the system were weighed, data regarding these weights are not presented. Calculated distributions of each radiolabeled compound under test, together with its breakdown products in certain of the organisms and in the water, are presented in the form of tables but are always expressed in terms of milligram per kilogram, and without information on the absolute quantities involved, any attempt to scrutinize the investigators' findings is rendered exceedingly difficult. Thirdly, even though residue values in the sand were said to have been determined, in none of the publications are those values reported. Lastly, since both publications describing the operation of the system state that the experiment is terminated "after 33 days," and since it is said that approximately 30 Daphnia magna are added to the model ecosystem at the beginning of the experiment (Metcalf et al., 1971), one is left with the clear impression that the duration of the entire experiment (from day 1) is 33 days. On the other hand, samples of sand and water are apparently still being extracted and assayed on days 34 and 48 (14 and 28 days after treatment of the Sorghum, which takes place on day 20). If the water was not extracted for chemical and radioactive assays on the same day as were the organisms, conclusions drawn from the experimental results (which are based on proportions of the investigated compound in water and in the organisms) would be completely invalid. This dilemma can only be resolved if one presumes that what the authors meant to say is that the experiments are terminated 33 days after treatment of the Sorghum leaves with an insecticide, or, in other terms, that the duration of the entire experiment is actually 53 rather than 33 days. Nowhere, however, do they so state.

Chemical and Radioassay Techniques

In addition to the model ecosystem studies reported in these publications, the investigators performed several other experiments in attempts to elucidate the metabolic pathways of different pesticides in the salt marsh caterpillar, in houseflies, and in mouse liver homogenates. They also studied the elimination of the compounds in urine and feces of mice following oral dosing of the animals. We do not intend to deal with these questions in the following discussions, except where comparison between the results reported in different publications are pertinent to evaluating the accuracy of radiotracer methods employed. Otherwise, we shall restrict our remarks to those topics which bear directly on the model ecosystem studies.

From the scanty descriptions in the several publications of the methodologies one arrives at the following rather imprecise understanding of the chemical and radiotracer analyses used by these investigators (given slight variations dependent upon whether the starting material was a ^{14}C or a ^{3}H labeled compound).

1. 1-ml aliquots of water were periodically assayed in "cocktail D" (100 g naphthalene and 5 g PPO in dioxane to make 1 liter) by scintillation counting.

2. Unspecified quantities of the organisms and water in the system were assayed at the termination of the experiments for quantitative and qualitative determinations of both parent compound and degradation products. All of the publications refer back to Kapoor et al. (1970) for basic information on the techniques employed; however, in two other papers there are summaries given which are at variance with that of Kapoor et al. (1970) and even the original description is far from being clear. For this reason we cite the appropriate passages from the three papers in question. After termination of the experiment ". . .weighed samples of fish, snails, mosquito larvae, algae, and water were removed and assayed to (sic) total radioactivity. These samples were homogenized and extracted with diethyl ether, and both water and ether layers examined by TLC to determine the qualitative and quantitative nature of the degradative (sic) products present, using radioautography and serial scintillation counting of the areas containing radioactivity" (Ibid., p. 1149). One page earlier the reader is informed that ". . .wherever animal extracts were investigated, . . . all such extracts were 'cleaned up' before chromatography by partitioning in acetonitrile petroleum ether 2:1. The acetonitrile fraction was evaporated and the radiolabeled metabolites taken up in acetone or ether for application to the TLC plates" (Ibid., p. 1148). In the publication of the year following, on the other hand, where the details of the model ecosystem are treated, the chemical methodology is as follows: ". . .weighed samples of the organisms were examined for radioactivity. (There is no mention of the water.) The samples are homogenized in water and extracted with equal volumes of diethyl ether. Both layers are examined by TLC to determine the qualitative and quantitative nature of the radiolabeled products with use of radioautography and scintillation counting of serial sections (sic)" (Metcalf et al., 1971, p. 711). At this time the acetonitrile petroleum ether "clean up" procedure is not mentioned, and the impression is that only aqueous extracts and those obtained with diethyl ether were assayed. By 1973, the procedure is outlined in an even less likely fashion: "After 33 days. . .the experiment was terminated, and the amount and nature of the ^{14}C determined by homogenization of the organisms, extraction with acetonitrile, TLC autoradiography, and liquid scintillation counting" (Metcalf et al., 1973, p. 36). From this one would deduce that the extraction was carried out with acetonitrile, although this is hardly probable since the chemical is water miscible.

3. The next step in the procedure seems to be the separation and identification of the parent compound and the different metabolites by applying unspecified quantities of the extracts to (apparently) three sets of silica gel TLC plates which contained fluorescein (Kapoor et al., 1970), specifically described in a later paper as fluorescent marker E. Merck GF-254 (Metcalf et al., 1973). Non-radioactive labeled parent compounds and model metabolites were cochromatographed with the "unknowns" in the extracts. The visualization of the spots after the development of the TLC plates in the appropriate solvents was achieved either through the quenching of fluorescence or by spraying with selected chromogenic agents. In order to localize

the unknowns, autoradiography was used by applying No-Screen(R) X-ray film (Eastman Kodak) to the plates for unspecified periods of time.

4. After identification of the compounds in the extracts through the development of the X-rays, the appropriate spots (1 cm^2 or more) from the plates were scraped into "cocktail D" for quantitation by liquid scintillation counting.

Although the determination of total radioactivity in animal tissues was carried out by Schöniger combustion technique for tritium labeled compounds, all other aspects of the separation and quantification of the metabolites were evidently the same as with ^{14}C labeled pesticides. From Kapoor et al. (1970) it would seem that the tritium labeled compounds were counted, after TLC separation, in "cocktail D," while "^{3}H cocktail" was used only for the oxygen combustion procedures. ("^{3}H cocktail" consists of 200 g naphthalene, 10 g PPO, and 0.25 g POPOP in dioxane to make 1 l.) The authors state: "The relative proportions of various radiolabeled metabolites (from the previous paragraph, apparently including ^{3}H labeled methiochlor) were determined by scraping 1 cm^2 or other appropriate sections of silica gel from developed TLC plates into 'cocktail D'" (Kapoor et al., 1970, p. 1148). From the 1971 Metcalf et al. paper, on the other hand, one is led to understand that the scintillation counting of ^{3}H labeled compounds removed from TLC plates was carried out in "^{3}H cocktail." Matters are made more confusing since, on the same page, it is stated: "The general methods for preparation and evaluation of radiolabeled samples have been described in detail by Kapoor et al. (1970)" (Metcalf et al., 1971, p. 710).

The Food Chains

The food chains involved in this microecosystem are described in two of the publications (Metcalf et al., 1971; and Metcalf et al., 1973). While at first perusal the proposed food chains appear similar, there is also an important discrepancy in these two descriptions. In the 1971 publication, the food chain pathways are listed as:

"(1) Sorghum → Estigmene (larva)
(2) Estigmene (excreta) → Odeogonium (algae)
(3) Odeogonium → Physa (snail)
(4) Estigmene (excreta) → Diatoms
(5) Diatoms → Plankton
(6) Plankton → Culex (larva)
(7) Culex → Gambusia (fish)"

(Metcalf et al., 1971, p. 711.)

In 1973, however, a modification is instituted which seems to indicate only two basic aquatic food chains: from Oedogonium to Physa; and from plankton to Daphnia to Culex to Gambusia. The later version is rather questionable, since it is highly improbable that mosquito larvae will consume Daphnia.

There is, in addition, one much more important problem with the presumed food chains in this system. In several of the publications it is stated that both Daphnia magna and Physa snails are introduced on day 1, or at the same time when the "few strands" of Oedogonium cardiacum and the "few ml" of old aquarium water are added to the aquatic portion. Under such conditions, it would seem rather unlikely that the Daphnia would survive, even without the presence of the pesticide (applied only after day 20), since they, like other mezoplanktonic forms, require up to five times their body weight in food per day (Hartman and Claus, 1971), and would certainly not obtain this from a few ml of old aquarium water containing microzoo- and phytoplankton. Furthermore, it seems unlikely that any substantial amounts of algae would grow in the presence of the 10 snails--animals consuming from 2 to 4 times their body weight in food under optimal conditions. This is particularly the case if the investigators were indeed working with Oedogonium cardiacum, since all members of this green algal genus are relatively slow-growing forms. In view of the fact that two of the diatoms mentioned as being present in the old aquarium water were obviously misidentified and also considering the rather curious fact that only diatoms were described as present in the water, one might suppose that the investigators were working with some other filamentous green alga exhibiting a faster growth rate. Given the voracious appetites of the snails, however, it is questionable that any filamentous green alga would produce enough biomass in 53 days to permit proper quantitation of the minor metabolites which they accumulated by the end of the experiment.

These doubts about the viability of the Daphnia and the appropriateness of the alga → snail food chain, led us to undertake some experiments designed to replicate as closely as possible the first aspects of the model ecosystem studies of Metcalf and his coworkers. These experiments, the results of which are reported below, tested the simple food chains of microplankton → Daphnia and filamentous or coenobial green algae → Planorbis.

Culture Experiments

The test containers consisted of 10 2 liter cylindrical glass beakers, Kimax(R) (13 cm diameter, 19 cm height). Carefully washed white quartz sand (1 kg) was placed into each of the beakers, and 1 l "standard reference water" of Freeman, as used by Metcalf et al. (1971) was added. (Constituents in mg/l: $MgSO_4$, 36.4; K_2SO_4, 0.135; $CaCl_2$, 14.0; $NaHCO_3$, 25.0; NH_4NO_3, 3.0; K_2HPO_4, 0.78; $CaCO_3$, 57.7; $NaSiO_3$, 23.6; $FeCl_3$, 0.81; prepared as 6 stock solutions. Solubilization of $CaCO_3$ was achieved by bubbling CO_2 through the stock, which also elevated the pH of the final "reference water" to 7.9.) After one day of equilibration, the film formed on the surface of the water was carefully removed with blotting paper. The water occupied an approximate 8 centimeter height in the beakers above the sand. These levels were marked and maintained throughout the experiment by adding "reference water" to compensate for loss by evaporation.

Each beaker was inoculated with 3 ml of "old aquarium water" and also with a 1 cm^2 scraping from the wall of the aquarium, containing periphyton. The weight of the microplankton in the aquarium water was established in the following manner: 10 ml of Millipore(R) (pore size 0.45 μ) filtered water was weighed in a beaker on a Mettler H30 analytical balance, and thereafter, 10 ml of aquarium water containing microplankton was filtered through a preweighed wet Millipore filter, as above, which was then added to the beaker, followed by another weighing. The weight difference, after subtracting that of the added Millipore filter, was less than 0.01 mg, which would indicate that in 1 ml of aquarium water, the weight of organisms is less than 0.001 mg. A quantitative cell count was performed on the aquarium water, using a Spencer(R) Neubauer Bright-Line hemocytometer, and the total number of cells per ml was established as ca. 980. Since the calculated average weight of a planktonic algal cell is about 1 X 10^{-9} g, 1000 cells/ml would weigh 0.001 mg, a figure in relatively good agreement with that obtained through the weighing method. The weight of a 1 cm^2 scraping of periphyton was established as 0.1_4 mg. Two beakers each were inoculated with the following green algae: Cladophora glomerata, Hydrodictyon reticulatum, Mougotia sp., Odeogonium fragile, and Ulothrix zonata. The algae were derived from the stocks of Carolina Biological Supply Co., Burlington, N.C.

Five of the beakers, each containing a different species of green algae under test, served as controls, while the other five were designated as the experimental containers. In the latter, Daphnia pulex and Planorbis sp. were added on day 1 in order to determine differences in algal productivity in the presence of grazers.

Cladophora glomerata: 20 large branched plants (up to 5 cm in length) harboring heavy growth of epiphytes were selected under a dissecting microscope and transferred into two beakers (10 in each) holding 10 ml of water, which had been previously weighed. After reweighing the beakers containing the plants, the weight of the 10 Cladophora in the two beakers was established as 8.3 and 7.8 mg, respectively. The plants were then placed into the experimental and control beakers containing sand, standard reference water, microplankton, and periphyton.

Hydrodictyon reticulatum: 20 nets, approximately 0.5 cm in length were selected under a dissecting microscope and 10 each were placed into the beakers containing the elements described above. The weight of the plants could not be determined directly; therefore they were calculated on the basis of average cell dimensions and the number of cells in the coenobium, using 30 μ length, 10 μ width, and approximately 6,000 cells in each net.

Mougotia sp.: 20 strands were separated under the dissecting microscope and the weights of the plants were calculated, using an average length for the filaments of 10,000 μ and a width of 12 μ. Ten filaments each were placed into the beakers as previously described.

The same procedures were carried out with Oedogonium fragile, where the average length of the filaments was established as 20,000 μ having a width of 10 μ and with Ulothrix zonata, which had an average length of 6,000 μ and a width of 8 μ.

Thirty Daphnia pulex were transferred into a beaker holding 1 ml of water which had been weighed. After reweighing the beaker with the Daphnia the weight of the cladocerans was established. This procedure was repeated five times, and the five experimental beakers containing algae and microplankton were then seeded with 30 Daphnia each.

Ten Planorbis sp. were placed into a beaker containing 10 ml of water which had been weighed and the weight of the snails established through reweighing the container. The snails were selected so that the total weight of the ten animals should come as close to two grams as possible. Again, the procedure was repeated five times, and ten snails were placed into each of the experimental beakers.

Both the Daphnia and the snails were purchased from a local aquarium supply store.

A list of the planktonic organisms together with the counts of the dominant forms, as well as lists of the periphytic and epiphytic forms, is given in Table 1. Where obvious periphytic forms were found among the plankton, they were enumerated only under the heading "periphytes." The zooplankton were exceedingly sparse, with the following organisms found in small numbers: Stylonichia pustulata, Oxytrycha sp., and Holophrya discolor. Among the periphyton, scattered individuals of Vampyrella lateritia, Tokophrya lemnarum, Vorticella sp., Stentor coeruleus, and Stephanoceros sp. were seen.

The five experimental and five control beakers were placed into a walk-in incubator kept at 26°C, and they were exposed to 12 hour illumination daily, with GroLight(R) fluorescent lamps of 5,000 lux. Each beaker was covered with an hour glass resting on a wire triangle and aerated with a Little Giant(R) air pump. From day 20 to the termination of the experiment on day 33, 20 mg daily of TetraMin(R) fish food was added to the water of both control and experimental beakers in order to simulate the organic enrichment originating from caterpillar excrement in the model ecosystem studies.

On the 33rd day, when the experiments were terminated, plankton counts were performed, and the weight of all surviving animals was either determined directly or through calculations. Concurrently, the filamentous algae were counted individually and their weight directly established, or, where they were too few in number, determined by calculations. After removal of the macroscopic organisms, the water from each beaker was filtered through a wet, pre-weighed Millipore(R) filter (0.45 μ pore size) and the weight of the plankton was measured where possible. In those cases where most of the microplankton had been consumed by the grazers, weights were calculated from the microscopic counts. The entire internal surface of each beaker was scraped with separate scalpels and the total weight of periphyton from each container was established. Since the water-exposed surface of the beakers could be calculated, the weight of periphyton could also be expressed in terms of mg/cm^2. Table 2 contains both the initial concentrations and weights of the organisms or groups studied and their concentrations and weights at the termination of the experiments.

Among the algae tested, only Cladophora yielded a biomas in the gram range, and that only in the control. In the test series, in the presence of grazers, neither the phytoplankton-periphyton complex nor the test plant itself gave yields above the 100 mg range even with Cladophora. In all of the experimental beakers, it was apparent that the grazers were starving. Only a few Daphnia survived, and only in those experiments where adequate epiphytic flora occurred on the test plants (Cladophora, Odeogonium, and Ulothrix) to provide nourishment for the cladocerans. Some snail mortality also took place--probably due to starvation--although it is recognized that snails are better able to tolerate long periods without adequate food supply than are the smaller invertebrates. Hydrodictyon had been virtually devoured by the snails by day 2, and this may account for the fact that the greatest loss of snails was observed in this experiment. In the Hydrodictyon, the Oedogonium, and the Mougotia experiments, the periphyton were also almost completely consumed by the snails. Relatively large numbers of Mougotia filaments were found in the experimental beaker at termination (13,000), perhaps reflecting the fact that this alga is not a preferred food organism for snails.

It is well known that small aquatic grazing invertebrates can eat, under optimal conditions, from 2 to 5 times their own body weight daily (Raymont, 1963). In none of these experiments was there sufficient food to nourish the animals adequately. The voracious appetite of the grazers was best demonstrated in the Cladophora experiment, where, at termination, the weight of the plants was 5,344 mg in the control as compared with 83.6 mg in the experimental beaker. Those Cladophora remaining in the experimental beaker showed scarce branching in comparison with the controls, having been badly damaged and partially eaten by the snails; hence their greatly reduced individual weights.

In the Oedogonium and the Ulothrix experiments, it seemed likely that the snails would have consumed all of the filaments before termination had they been able to locate them, since the animals were clearly without adequate nourishment. In no experimental series did the snails exhibit the gain in weight which would be expected after 33 days in an environment with an abundant food supply.

It should also be remarked that although these experiments were initiated using 10 plants of each test species on the assumption that the imprecise phrase "a few strands of algae" used by Metcalf and his coworkers should be interpreted as referring to a relatively small finite number, there would have been little difference in the quantities of algae obtained in 33 days, with the snails present from the beginning of the experiment, even had 100 filaments been used. The snails would most probably have consumed greater quantities of the initially added filaments, still leaving only a few plants able to reproduce during the course of the experimental period.

An additional comment should be made regarding the use of Oedogonium fragile rather than Oedogonium cardiacum in our growth experiments. It is recognized that the latter species is about 5 times as large as Oe. fragile. A substantial difference, however, between the two forms is that Oe. cardiacum is a dioecious form, whereas Oe. fragile is monoecious (Collins, 1928). With monoecious forms fertilization chances are far greater in a thinly populated culture than are those with dioecious forms under similar conditions. Therefore, differences in final biomass will not differ substantially between the two forms, since the faster sexual reproductive process in the monoecious form will compensate for the larger size of the dioecious organisms.

Although in the present culturing experiments beakers with only 1 liter of water were used, instead of aquaria containing 7 liters, this fact will not change the results with respect to final productivity, since these are expressed in terms of ratios: milligram of algae, or number of planktonic cells, per quantity of water.

On the basis of these culturing experiments, it seems rather questionable that the food chains postulated by Metcalf and his coworkers would be adequately supportive for the members of the higher trophic levels (Daphnia, Culex. Physa, and Gambusia) employed in their microecosystems. Furthermore, it seems even less likely that in any of their experiments, adequate quantities of algae would have been available at the end point of the studies for the investigators to separate, identify precisely, and quantitate minor metabolic products of the different pesticides. For these reasons, we wish to further scrutinize the techniques used and the findings reported by the Illinois group from their various experimental series.

Remarks on Radiotracer Techniques

Since no data are given regarding the efficiency of the scintillation counts it is necessary to turn to the published literature on radiotracer methods in order to gain some idea about the appropriateness of the "cocktails" used in the counting series and of the efficiencies involved in scraping portions of thin layer silica gel plates into scintillation vials. "Cocktail D" is a dioxane-based counting fluid which contains no wave shifter and no anti-freeze. "^{3}H cocktail" does have a wave shifter (POPOP), but it is also dioxane-based. Such fluids freeze at 12°C, and it seems therefore that counting must have been performed at or above this temperature. It is known that for every 10 degrees of temperature increase over 0°C an increase in "background noise level" of approximately a factor of 2 may be expected (Wang and Willis, 1965). Although the investigators mention the use of channels ratio technique for quench correction, the relatively high background noise in samples with low activities (to be discussed later) renders the accuracy of such quench correction curves questionable.

A second factor to be taken into account is that the silica gel with the radiolabeled compound adsorbed to it is scraped directly into the scintillation liquid. A nonhomogeneous system will thus be established. There is no reason to suppose that the parent compound and its metabolites will be equally solubilized by dioxane. Quite to the contrary, it is almost certain that only portions of the radiolabeled material will go into solution, while other portions will remain adsorbed on the solid support. Bransome and Grower (1970), using various solid supports and employing the channels ratio technique, demonstrated that ". . . beta spectra of (^{14}C), as well as (^{3}H), samples are shifted toward lower energies, and that external standard channels ratios are completely inadequate for quench correction" (Bransome and Grower, 1970, p. 404). Furthermore, as far as ^{3}H labeled compounds are concerned, they write: "Correction by CR for loss of (^{3}H) would obviously be statistically unreliable" (Ibid., p. 405). Indeed, in their samples, the severe quenching of the tritium spectrum caused by the presence of the solid support was such that most of their counts were below the detection threshold. In their conclusions they state: "The disappearance of most of the (^{3}H) spectrum below the detection threshold prevented any reliable quench correction by means of CR values, and made any assumption of constant efficiency very hazardous" (Ibid., p. 407).

McKenzie and Gholson confirmed these results, remarking in their introduction: "Partial and/or variable elution of the labeled material(s) in the vial can cause differences in the results obtained between duplicates of a given sample or when comparing chemically different compounds which may behave differently in the same systems" (McKenzie and Gholson, 1973, pp. 17-18). They tested a counting fluid which was far superior to those used by Kapoor et al. (1970)--one composed of 4 g PPO, 0.2 g POPOP, 400 ml absolute ethanol, and 600 ml of toluene per liter--which would not freeze at $0^{o}C$ and gives a higher counting efficiency than dioxane due to toluene's 30% greater excitation energy transfer. In spite of using this better "cocktail," they did not find the recovery rate of radioactive material from a silica gel support to be satisfactory. When they used a special formulation referred to as BBS-3 (Bio-Solv, Beckman Instruments, Inc.) in addition to their cocktail, they were able to achieve about 90% recovery with ^{14}C, but they still did not find satisfactory recovery of tritiated compounds under most conditions.

A further element of uncertainty in the experiments of Metcalf and his coworkers is added by the presence of the fluorescein marker in the silica gel. The emission wave length of fluorescein is 520 nm, and that of PPO is 380 nm; thus excitation of the fluorescein in the sample may interfere considerably with the final counting rate, acting in a manner similar to a secondary fluor.

Summarizing what we have stated concerning the scintillation counting methodology, the counting efficiency for the ^{14}C labeled samples is unlikely to be higher than ca. 40%, and that with tritium will certainly be below 10%, when such scintillation fluids as the investigators' "cocktail D" and "^{3}H cocktail" are employed.

Similar problems would arise if 1 ml aliquots of water were assayed in either "cocktail D" or "^{3}H cocktail," as was evidently the case in all of these experiments. The planktonic organisms present in the water will produce considerable quenching, quite like that introduced by the presence of a solid support.

An integral part of the radioassay techniques of these studies is the identification of the metabolic compounds through autoradiography. Knowing the amount of radioactivity in the starting material and calculating the equivalent dpm's in the metabolites, it is possible to gain an impression of the magnitude (or lack thereof) of the activities present. It is recognized that ". . . 10^{6} - 10^{8} beta particles must strike each square centimeter of X-ray film to produce optimal blackening. . ." and further that ". . . detectable blackening may occur as a result of 10^{5} - 10^{6} beta interactions per square centimeter" (Wang and Willis, 1965, p. 147).

When, for instance, some of the metabolites of methiochlor are represented (Kapoor et al., 1970), where it is unquestionable that a ^{3}H labeled compound was under test, it is possible to calculate the approximate exposure time required to produce even a faint image on the X-ray film. For some metabolites, necessary exposure is in the range of 700 days. It would be interesting to know the exposure times in these experiments, since they are not reported. Granting a two year exposure, the selection of Eastman Kodak's No-Screen(R) X-ray film still seems to be somewhat less than satisfactory, as this film has been described as having poor resolution and a high background sensitivity (Wang and Willis, 1965, p. 146).

The Dieldrin Experiment

Dieldrin has been selected from the 1973 publication of Metcalf et al., in which the results of model ecosystem studies of six different chlorinated hydrocarbon pesticides are reported, for three particular reasons. First, the specific activity of the original radiolabeled compound is rather low--1.03 mCi/mM. Secondly, a detailed list of metabolites in water and in the test organisms is given in the authors' Table 2. Thirdly, in an unpublished report by Metcalf and Kapoor (1972) treating the fate of aldrin and dieldrin in the model ecosystem, certain information is supplied which is missing from all of the published works.

As has been mentioned earlier, since the quantities used for extraction of water and organisms for further analysis are not specified, it is necessary to make certain assumptions in order to give some absolute value to the data reported in terms of ppm. It is assumed arbitrarily that 1 l of water was used for extraction purposes at the end point of the experiment. Although it is highly questionable that there could have been more than 10 mg of Oedogonium cardiacum present in the tank at termination, for these calculations we have granted a biomass of 100 mg of algae. We presume that the total weight of the snails is 2 g (200 mg each), even though the species is unidentified, and we further assume that the investigators extracted the whole 2 g. The average weight of Gambusia affinis is 2.1 g (Culley and Ferguson, 1969), and we assume that all three fish were homogenized and used; a total of 6 g. With these quantities, the conversion of the ppm values in Table 2 of Metcalf et al. (1973) to nCi or dpm's is possible. These numbers are compiled in Table 3. At 100% recovery and counting efficiency, several of the metabolites in the algae and even in the fish are below detection levels. Presuming a 40% efficiency, other figures will also represent cpm's below detection, or would require unrealistically long counting times--in the range of weeks rather than hours (Freedman and Anderson, 1952). The question must be raised why the investigators attempted to express these minor metabolites in terms suggesting precise quantification, rather than merely indicating trace amounts when they were counting at levels which were unquantifiable.

At the low specific activity employed, counting of 1 ml aliquots of water in "cocktail D" is also of questionable meaningfulness. The data from these periodic counts are not reported in the published papers. However, in the 1972 preliminary note of Metcalf and Kapoor on the aldrin and dieldrin series, the following sentence appears regarding dieldrin: "The radioactivity in the water phase rose to a maximum of 0.02 ppm by the 5th day and declined to about 0.005 ppm over the duration of the experiment" (Metcalf and Kapoor, 1972, p. 2). These values would indicate that on day 5, 54 pCi was detected and that later (presumably day 15 or day 28), only 13.5 pCi. Considering the relatively low counting efficiency and the unknown variation in the numbers of microplankton in 1 ml of water over the course of time, whether or not these figures have any true meaning cannot be assessed.

Returning to Table 2 of Metcalf et al. (1973), there is one further puzzle which applies equally to the reporting on the other pesticides tested in this series. In the aqueous phase, substantial portions of materials appear as unextractable residues. No methodology is described which would shed light on how the quantity of this fraction was determined. There is, however, a strong suggestion that rather than making independent determinations, the sum of the values for the parent compound and its metabolites was simply subtracted from the value given for total ^{14}C.

Concerning the dieldrin experiment, there are two further specific matters related to the behavior of the organisms for which the authors offer no explanation. It is stated: "The dieldrin application to the Sorghum was more toxic than aldrin and the salt marsh caterpillars Estigmene acrea, ate the plants with reluctance" (Metcalf and Kapoor, 1972, p. 2). Were it indeed the case that the caterpillar's "reluctance" to eat the dieldrin treated leaves reflected its greater toxicity over that of aldrin, this interesting observation should have been mentioned in the published version of this work and elaborated upon, since nothing in the literature suggests that dieldrin would have a higher toxicity to insects than aldrin. A more important problem reflecting directly on dieldrin toxicity is the discrepancy between the findings of the aldrin and the dieldrin series with respect to mosquito larvae mortality. In the dieldrin series, where its level in the water is given as 0.0014 ppm, a footnote indicates that all mosquitoes were killed throughout the experiment. On the other hand, in the aldrin series, where aldrin's breakdown product dieldrin is given as 0.0047 ppm, the mosquitoes not only did not die but managed to accumulate 1.1 ppm dieldrin. It seems most peculiar that in the aldrin experiment the larvae should have survived 3.3 times higher dieldrin concentrations.

Reproducibility

Among the strong claims made by the investigators respecting the value of their model ecosystem studies is the reproducibility of the results. They write: "The ultimate purpose of the model ecosystem is to be used as a single living unit for in-depth studies of environmental degradability. The question of reproducibility of results is of considerable importance as even this simple ecosystem is substantially more complex than any single experimental animal or groups of animals. This factor has been evaluated by two complete individual evaluations of the behavior of ^{14}C-labeled DDT in the model ecosystem with the results shown in Table II. The two studies gave remarkably similar results, both as to distribution and accumulation of total radioactivity in the components of the system and as to the quantitative biodegradability of DDT to DDE, DDD, and polar metabolites" (Metcalf et al., 1971, p. 711). There is absolutely no question that two completely different DDT model ecosystem studies were involved, since in Kapoor et al. (1970) the source of the radiolabeled DDT (specific activity 5.48 mCi/mM) was the World Health Organization and the volume of water employed in the aquarium was 12 liters; whereas in Metcalf et al. (1971) the ^{14}C-labeled DDT was supplied by the Radiochemical Centre, Amersham, England (specific activity 5.48 mCi/mM) but the aquarium contained only 7 liters of water. Table II in Metcalf et al. (1971) shows two separate experiments, with about 100% difference in total ^{14}C results. However, in Table III of the same publication, the DDT results clearly originate--not from the replicate experiment discussed--but rather from the earlier work of Kapoor et al. (1970). To the reader, this becomes evident only if the two publications are placed side by side and the figures of Table 6 from Kapoor et al. (1970) and those of Table 3 from Metcalf et al. (1971) are compared. The numbers are identical to the last decimal point. There seems to be no reason why the Metcalf et al. publication of 1971 should not contain detailed results of their replicate experiment, and there is no justification for reprinting the 1970 data in their Table III, without clearly designating it as such. Any reader looking only at the 1971 publication of Metcalf et al. would gain the definite impression that the results on DDT reported in Table III refer to the replication experiment of 1971. Furthermore, even from the scanty materials reported in Table II of the second publication, it is possible to question the authors' claim that the two studies gave "remarkably similar results," since in experiment I (1971) the accumulation of total ^{14}C in fish was 20.8 ppm, while in experiment II (1970), it was 54.2 ppm, giving a standard error of 23.6--well over 100% of the accumulation in the replicate experiment.

This matter of a 100% difference in the results of these two similar experiments using the model ecosystem approach to study the environmental fate of DDT is minor, however, compared with the markedly disparate findings between the 1970 publication of Kapoor et al. regarding excretion of DDT in mice (feeding experiments) with those of Kapoor et al. (1972) on the same subject, employing different radiotracer techniques. In this connection we cite two passages from the publications in question. In 1970, the authors write: "DDT is eliminated very slowly (1.02% in the first 24 hr.), while methiochlor (47.11%) and methoxychlor (98.3%) are eliminated rapidly. The degree of polarity of the excretory metabolites is indicated by the ratios of radioactivity in urine/feces which is 0.67 for DDT, 0.13 for methoxychlor, and 0.19 for methiochlor. Over a period of 11 days all of the methoxychlor and 86.69% of the methiochlor were eliminated, as compared to only 4.3% of the DDT" (Kapoor et al., 1970, p. 1150). The phraseology of the 1972 paper is notably similar, but the numbers are remarkably different. Here it is stated: "DDT was eliminated slowly (7.4% in the first 24 hr.), while methylchlor (43.7%) and ethoxychlor (99.0%) (sic, 69%?) were rapidly eliminated. However, over a period of 11 days, 90.8% DDT had been eliminated compared to 73.7% for methylchlor and 77.5% for ethoxychlor, thus indicating that although initially DDT has a much slower rate of elimination, it reaches the level of the other analogs within 6 days. The degree of polarity of the excretory metabolites is indicated by the urine/feces ratio, which is 0.47 for DDT, 0.69 for ethoxychlor, and 0.12 for methylchlor" (Kapoor et al., 1972, pp. 3-4).

The most notable numerical discrepancy is that between 4.3% DDT elimination in 1970 and 90.8% in 1972 after 11 days. These differences, which are undoubtedly due to the use of the "more efficient" O_2 flask combustion technique and to "N cocktail" (135 ml phenethylamine, 135 ml of methanol, 730 ml of toluene, 5 g of PPO, and 100 mg of POPOP), which is appropriate for CO_2 absorption and high efficiency liquid scintillation counting, are not emphasized by the authors. The fact remains, however, that the results after 11 days in the 1972 experiment indicate a 2,100% error in the 1970 findings, which were carried out by direct counting of diluted urine samples and water-acetone extracted feces in "cocktail D." These extreme differences in end results should have been pointed out by the authors and the investigators should have been alerted to the limitations of their earlier radiotracer techniques. Contrary to expectation, no mention is made of the irreproducibility of the first mouse excretion study and, in two publications appearing in 1973 (Metcalf et al., 1973; Kapoor et al., 1973), the techniques used by Kapoor et al. in 1970 are again described as the basic chemical and radioassay methodologies.

The real significance, however, of the 2,100% error in the mouse excretion studies goes beyond these experiments per se. It points to the probability that the radiotracer techniques applied in all of the model ecosystem studies--as we have suggested earlier--were highly deficient, and that the presented results are of doubtful validity. If the possibility of a 2,000% error is considered and the dieldrin table is reexamined, for instance, all dpm's which fall below the 10,000 level become questionable. The second importance of the findings of Kapoor et al., 1972, with respect in particular to DDT, is that by the 11th day after ingestion the results indicate DDT to have been more completely excreted than methylchlor, ethoxychlor, and methiochlor--compounds which the investigators, on the other hand, claim to be more biodegradable.

(Another indication that the 1972 publication of Kapoor et al. involved some improved techniques is the description of methods for isolating microsomal fractions to investigate enzymatic breakdown of radiolabeled compounds. In 1970, Kapoor et al. state that microsomal pellets were precipitated from fresh Swiss mouse liver at 114,000 - 140,000 X g. Such speeds are not appropriate for the separation of microsomes. In 1972, Kapoor et al. write: "The homogenate was centrifuged at 15,000 X g" (p. 3), a speed at which one might actually expect to find the microsomes still in the supernatant.)

Some Theoretical Concepts: "Biomagnification," "Ecological Magnification," "Bioconcentration," and "Biodegradability Index"

The terms mentioned in the subtitle have been used on and off since the first publication of Kapoor et al. in 1970, but only in Metcalf et al., 1973, the last of the series of publications under discussion, was an attempt made to delineate these terms. "Ecological magnification" (EM) is the magnification of pesticide storage through the ingestion of food chain organisms containing the pesticide. "Bioconcentration" (BC) is the accumulation of pesticide residues in an aquatic organism through direct uptake from water. "Biodegradibility index" (BI) is the ratio of polar products to nonpolar metabolites in the organisms. Unfortunately the attempt to define the terms does not actually result in a clear picture, especially as regards EM and biomagnification (BM). It would seem that biomagnification is composed of two factors, EM plus BC--that is, that a higher aquatic organism acquires its pesticide body burden both through food chain magnification and through direct uptake from water, the former being more important. On page 42, the authors write of "bioconcentration" which seems to refer definitely to direct uptake from water. On the other hand, in Table 8 on the same page, where results of studies of direct uptake from water are reported, the table is headed "biomagnification." In the following, we shall assume that BM indeed has two components: EM and BC.

The manner of arriving at the BI of any particular compound is clear. However, the biological significance of this concept is unclear. Supposedly, the smaller is the BI, the less biodegradable the compound. Since it is recognized that the means of eliminating nonpolar compounds is through transforming them into polar (i.e., water soluble) metabolites which will be rapidly excreted, it seems contrary to logic to measure the relatively small amount of polar compounds not yet excreted from an organism against the nonpolar fraction. A more realistic index of biodegradability would be to compare the nonpolar compounds within the organisms with the sum of the polar metabolites in their environment. The model ecosystem, however, is inadequate for such comparisons, because some of the water soluble metabolites may become further degraded and escape from the system is CO_2. Since the total recovery of radiolabeled materials does not exceed 8% in any of these experiments--a point to which we shall return later--there do seem to be indications of a number of metabolic routes which remove breakdown products from the system. Although there is great emphasis placed on the discussion of BI values for various pesticides in several of the publications, the problem of its biological meaningfulness is not confronted. A good example of the discrepancy between real numbers and the results of this calculated index may be drawn from the mirex data (Metcalf et al., 1973) referring to Physa and Gambusia. In snail, the BI for mirex is 0.006; whereas in fish it is 0.0145. This would seem to indicate that in fish mirex is 2.4 times more biodegradable than it is in snail. On the other hand, it is stated in the text that mirex was stored as unchanged parent compound in snail at 99.4% and at 98.6% in the fish, a difference of only 0.8%.

Regarding "bioconcentration," there is only one experiment (Metcalf et al., 1973) which deals specifically with these values. In attempting to ascertain the contribution of direct uptake from water (BC) to biomagnification (BM) by aquatic organisms, Daphnia, Culex, and Gambusia were exposed for from 24 to 72 hours in 1 l of standard reference water containing approximately from 1 to 3 ppb of radiolabeled pesticides. The results are presented in the authors' Table 8, where the concentrations of 7 organochlorine compounds are given in ppb and the BC is recorded for each of three days. As far as Daphnia is concerned, it is remarkable to note that the authors, when placing the organisms in water containing 2 ppb DDT, still recovered animals after 3 days, by which time the cladocerans had concentrated the pesticide by a factor of 1330, or, in other terms, had accumulated a total of 2.6 ppm DDT. One gathers that Metcalf and his coworkers regard Frear and Boyd as authorities on the sensitivity of Daphnia to pesticides, since they are so cited in Metcalf et al. (1971). They apparently did not compare their own results, however, with those of Frear and Boyd (1967) who found, without food and without pesticides, a 40% mortality of Daphnia after 77 hours in standard reference water, and whose data indicate that the LD_{30} of DDT for Daphnia is 2 ppb at 26 hours exposure. Of course, Metcalf et al. (1973) do not report either how many Daphnia they started with or how many they might have lost during this experiment. For all one knows from their table, the DDT levels on day 3 in this small experiment might have been in dead Daphnia, which would not be indicative of anything relating to bioconcentration. The main point of this three day experiment, however, was to demonstrate that the uptake of pesticide by Gambusia directly from water was less by factors of from 0.4 to 250 for the different pesticides than that of fish exposed in the model ecosystem.

By 1972, a number of publications in which various authors claimed that in aquatic environments direct uptake by organisms from the water plays a considerably more important role in accumulation of pesticides than does food chain magnification had appeared (among them: Epifanio, 1972; Reinert, 1972; Risebrough et al., 1972). Since Metcalf and his coworkers cite Hamelink et al. (1971) in nearly all of their publications, and the latter authors were among the first to propose that it is exchange equilibrium between water and the aquatic organisms which controls the degree of biomagnification of pesticides, it is not entirely clear why Metcalf and his coworkers seem to be attempting in 1973 to establish that "exposure to levels of pesticide contamination of the same general order of magnitude as found in the model ecosystem experiments does not produce levels of pesticide storage as high as those from ingestion of food chain organisms containing the pesticide" (Metcalf et al., 1973, p. 42).

Among the theoretical concepts under discussion, it is clearly the EM factor to which the most importance is attributed by the Illinois group. Although it is emphasized that ecological magnification takes place through the food chain, calculation of EM is defined as "ppm parent compound in organisms/parent compound in water" (Metcalf et al., 1973, p. 36). When the parent compound is known to break down rapidly--as is the case with aldrin, for instance--there seems to be no justification for establishing ratios between the parent compound in water and that in the organisms. This can be best illustrated by the differences between the BC of aldrin from water to algae, where the parent compound calculations show a magnification of 39,000 X, whereas when dieldrin is used as the parent compound, the magnification from water to algae is only 457 X.

The major problem with these supposed magnifications is the insufficient supply of food organisms, a fact which has been mentioned earlier. There does not seem to be any possibility that the snails could accumulate the quantities reported for any of these pesticides through the food chain; nor could the *Culex* derive their pesticide residues from grazing on planktonic organisms. To specify, using the dieldrin series, the snails are reported to have accumulated 86.32 ppm of the parent compound by the end of the experiment, presumably by feeding on algae containing 0.64 ppm of dieldrin. If we assume that the partition between EM and BC is approximately 4:1 in the case of dieldrin (unfortunately for dieldrin, no data are given for BC, but an extrapolation may be made between the aldrin and endrin values for an approximation), then ca. 69 ppm of dieldrin in snails should originate from the consumption of algae. This would correspond to 237.4g of algae (at the 0.64 ppm dieldrin level) eaten over the 30 day period of pesticide contamination of the system, or approximately 4 times the body weight for each snail daily, a figure in agreement with our earlier statement about the food requirement of grazers. However, since it should by now be clear that under no conditions could even 2 grams of *Oedogonium* be produced in 30 days in the presence of snails, much less 237 grams, and if we accept that the snails did indeed have the reported pesticide residues at the end point of the experiment, then we must assume that they ate something other than algae. The only choice within this limited test system would seem to be the dead caterpillar larvae and/or the leaf frass of the treated *Sorghum*. It should be obvious that were this the case, the whole presumed food chain from water to alga to snail is untenable.

Similar problems arise regarding the only other food chain for which at least some values are given--that is, water → plankton (values missing) → mosquito larvae → fish. In the DDT series (Kapoor et al., 1970) 0.00022 ppm DDT is present in the water at the termination of the experiment. Since no values are given for microplankton, we presume a 1000 fold magnification from water to the plankton. This can be justified on two bases: (1) that Metcalf et al. (1973) found the accumulation of various pesticides in algae from water to be between 400 X to 5000 X, with the higher values associated with more soluble compounds, and (2) that Södergren (1968), using similar starting concentrations in water, could not reach a 1000 fold accumulation of DDT in single-celled algae. Thus, even assuming a 1000 fold accumulation of the pesticide, the microplankton could not contain more than 0.22 ppm DDT. The cumulative value for mosquito larvae is given as 1.8 ppm. One mosquito larva weighs 1.2 mg (Metcalf and Flint, 1939), and the 300 larvae present in the system would have a total weight of 360 mg. In order for the 300 larvae to accumulate the 1.8 ppm body burden through ingesting the microplankton (a ratio of 90:1 EM:BC emerges from the data of Metcalf et al., 1973 and from that of Kapoor et al., 1970, therefore direct uptake from water is negligible), they would have to consume a total of 2.95 g of plankton during their 4 days in the aquarium, or 2.4 mg microplankton per mosquito larva per day. This last figure is exactly twice the body weight of the mosquito larva. On the other hand, the productivity of the microplankton in the aquarium would have to be about 100 mg/l/day, in order to sustain the mosquitoes and to permit the accumulation of the reported residues. This corresponds to approximately 100,000 cells per ml, a productivity level which, given the presence of 30 Daphnia introduced at the beginning of the experiment and reintroduced in cases when they died, could not be reached under any of the reported experimental conditions. Therefore, either the Culex could not accumulate the reported quantities or they must have, like the snails, fed on the disintegrating caterpillar carcasses.

The next step in the food chain--from Culex to Gambusia--is even more problematical, since these fish are not scavengers and their food was said to have been derived exclusively from mosquito larvae and Daphnia. It has already been mentioned that the accumulation of DDT in the mosquito larvae is reported as 1.8 ppm. That in the fish is 18.6 ppm. The EM:BC partition for fish is given as 250:1, indicating that the contribution from the water is negligible. The total quantity of radioactive DDT in the 250 mosquito larvae available for the fish would be 0.54 µg. That in the 30 Daphnia magna (total weight, after Reinert, 1972, 25 mg), which can accumulate a maximum of 2.6 ppm (Metcalf et al., 1973) would be 0.065 µg. The total contribution of radiolabeled DDT from 250 Culex and 30 Daphnia would thus be 0.605 µg. On the other hand, the 6 grams of fish should have contained 111.6 µg radiolabeled DDT. In order for the fish to accumulate this quantity through the food chain, they would have had to consume--not 250--but 51,666 mosquito larvae. In the case of the fish, it seems more than puzzling to establish where all this radioactivity might have come from.

Similar calculations could be undertaken for all those radiolabeled pesticides tested in the model ecosystem for which specific activities are given, and although the absolute quantities would be different in each case, analogous problems in explaining the reported magnification values would arise.

EM and Pesticide Solubility

In an attempt to explain differences in ecological magnification among chlorinated hydrocarbon pesticides, Metcalf et al. (1973) proposed that EM is inversely related to the solubility of the compound in water: that is, the less soluble a compound is, the higher will be its EM value. For this purpose the investigators calculated the logarithms of the water solubility of various compounds (in ppb) and plotted these against the logarithms of the EM values defined in fish. The line fitted by the least square method through 11 points (one aberrant point for hexochlorobenzene was disregarded) was claimed to show that the significance of the relationship is $p < 0.0005$. The solubility and the EM data for nine of the compounds are listed in Table 7 of Metcalf et al., 1973 (p. 41), and those for the three other chemicals can be found in Kapoor et al., 1973, Table 5 (p. 314). For three of the chemicals--aldrin, dieldrin and methoxychlor--incorrect solubilities were apparently used in the table. (Aldrin solubility is given as 0.20 ppm, dieldrin as 0.25 ppm, and methoxychlor as 0.62 ppm. According to Park and Bruce (1968) the solubility of aldrin is 0.027 ppm, that of dieldrin is 0.186 ppm, and of methoxychlor, 0.1 ppm.) Disregarding the matter of the accuracy of solubilities, however, one may also note that out of the 12 points plotted on the graph 5 are in the wrong position, even using the data of the investigators. These are: lindane, aldrin, endrin, methylchlor, and DDE. In Figure 1, we have reproduced the plot of Metcalf et al. (1973), adding to it three points corrected for solubility as well as the five points corrected from the data in the tables of Metcalf et al. (1973) and Kapoor et al. (1973).

Figure 2 shows the plot with the points corrected for both positions and solubility. If hexachlorobenzene is retained for the regression line, at the same time "disregarding" the DDT group as "obviously aberrant," then it may be seen that a line could be fitted through the remaining 9 points using the least square technique with a slope opposite to that of the authors, indicating that the more soluble a compound is in water, the greater will be its ecological magnification. We would not definitely state that this is the case, but it is difficult to imagine how such a simple problem as plotting 12 points on graph paper could lead to 7 incorrect positionings, which in turn still yielded a line with a relationship of exceedingly high statistical significance.

Extrapolations to Nature

In Metcalf et al. (1971) a rather strong claim is put forth regarding the usefulness of model ecosystem studies for predicting the behavior of pesticides in the natural environment. "Several years of study of the model ecosystem with a variety of radiolabeled insecticides have shown that this relatively simple method can be used to investigate the biodegradibility and ecological fate of candidate new compounds. The results obtained with DDT after one month in the food chains of the model system show remarkable approximations to conditions observed after many years in nature. The model ecosystem technique is precise and permits the observation and study of metabolic transformations of the pesticide in the various elements of the system" (Metcalf et al., 1971, p. 713, our emphasis). In view of the previous discussions, these statements seem to be somewhat exaggerated.

We still wish to make some comments on the claim that the results from the model ecosystem studies can be extrapolated to conditions in nature. Scrutiny of the data indicate that overall recovery of radioactivity in the water and the biomass ranges from less than 1% (methoxychlor) to a maximum of about 8% for DDT. If 92 - 99% of the originally applied compound disappears from the system in 33 days either through complete breakdown or through evaporative loss due to air bubbling of the water, it is difficult to accept that the system imitates nature. A further disturbing factor is that purified sand is used instead of soil. The rationale for this is the following: "The use of pure sand and water culture is not only much more reproducible than soil but also eliminates a large amount of organic materials which have uncertain effects and interfere with extraction and determination of radiolabeled products" (Ibid., p. 710). In nature, on the other hand, organochlorine pesticides are known to be adsorbed in large proportions to soil and its organic materials, and it is precisely soils or muds which are the principal sites for their bacterial degradation (Menzie, 1966). Cleaned quartz sand will not act as a good adsorbent, nor will it harbor the appropriate microbial flora for insecticide breakdown.

Finally, in view of the fact that the food chains described for the model ecosystem are, to say the least, questionable, extrapolation to conditions obtaining in nature seems to be rather far fetched.

Summary

An analysis of the reported materials on model ecosystem studies, as related to pesticides, by Metcalf and his coworkers has been carried out. Certain questions regarding the appropriateness and precision of the radiotracer techniques employed were raised, and it was shown that in at least one instance the authors themselves admit an error of 2,100% in replicate experiments. Our growth studies performed with different filamentous algae in the presence of Daphnia pulex and Planorbis sp. showed that in 33 days it is impossible to obtain quantities of algae sufficient for the food requirements of the fauna. It was also demonstrated that even without the fauna, with the exception of Cladophora glomerata, no filamentous alga tested would produce a large enough biomass to permit accurate determinations of metabolic products of radiolabeled pesticides with the techniques employed by Metcalf and his coworkers. The biomagnification values reported by these authors have been analyzed and it was concluded that they could not have been due to accumulations of pesticide body burdens through the food chain, since there was inadequate food within the system for all organisms. Nor could they be accounted for by direct uptake from water, according to the authors' own experiments. Total recoveries of radiolabeled compounds have been calculated and established as ranging from 1 to 8% for the different pesticides. In view of the methodological difficulties, inappropriate food chains, and exceedingly low overall recovery rates any attempt to extrapolate the results of these experiments to natural conditions seems exceedingly tenuous.

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TABLE 1. QUALITATIVE AND QUANTITATIVE COMPOSITION OF ALGAL FLORA

Plankton	No./ml	Periphyton	Epiphyton
Cyanophyta			
Synechocystis aquatilis	3	Pleurocapsa sp.	Clastidium sp.
Aphanocapsa montana		Oscillatoria terebriformis	Lyngbya minor
Dactylococcopsis rupestris	6	Phormidium foveolarum	Lyngbya kossinskaiae
Coelospherium kützingianum		Phormidium retzii	
Oscillatoria agardhii			
Oscillatoria tenuis			
Phormidium autumnale			
Euglenophyta			
Euglena gracilis			
Phacus pleuronectes			
Khawkinea sp.			
Astasia minor			
Peranema sp.	7		
Chrysophyta			
Synura uvella		Dinobryon sp.	Harpochitrium hyalothece
Bodo sp.	11	Tetraedron braunii	Achnanthes microcephala
Cyclotella meneghiniana	96	Tribonema sp.	Amphora ovalis
Melosira varians	64	Fragilaria fenestrata	Cymbella veneta
Synedra ulna		Cocconeis placentula	Gomphonema acuminatum
var. oxyrhyncha	47	Caloneis sp.	

TABLE 1. Continued

Plankton	No./ml	Periphyton	Epiphyton
Asterionella formosa	8	Cymbella veneta	
Achnanthes minutissima	58	Nitzschia cf. fontinalis	
Epithemia zebra			
Navicula pusilla	73		
Navicula bicephala	34		
Navicula cincta	14		
Nitzschia acicularis	86		
Nitzschia palea	112		
Hantzschia amphioxis	6		
Surirella sp.	3		
Chlorophyta			
Ankistrodesmus falcatus	32	Chlorococcum sp.	Cosmarium sp.
Scenedesmus brasiliensis	124	Prasiola sp.	
Pediastrum boryanum	108	Closterium ehrenbergii	
Staurastrum sp.	38		
Kirchneriella lunaris	56		
Total:	986		

TABLE 2. NUMBERS AND WEIGHTS OF ORGANISMS AT BEGINNING AND TERMINATION OF EXPERIMENTS

Test Cultures	Beginning of Experiment		Termination of Experiment		
	Nos.	Weight in mg	Numbers	Weight in mg	Total weight in beakers in mg
Cladophora glomerata					
Control (total plants)	10	8.3*	6,400	5,344.0*	5,344.0
Phytoplankton (per ml)	3	0.000003	1,240	0.0012	1.2*
Periphyton (per cm^2)	--	0.00033	---	0.146	44.6*
Experimental (total plants)	10	7.8*	160	83.6*	83.6
Phytoplankton (per ml)	3	0.000003	20	0.00002	0.02
Periphyton (per cm^2)	--	0.00033	---	0.011	11.3*
Daphnia pulex (total animals)	30	18.4*	6	3.7*	3.7
Planorbis sp. (total animals)	10	1,864.0*	10	2,158.0*	2,158.0
Hydrodictyon reticulatum					
Control (total coenobia)	10	0.244	12	4.0*	4.0
Phytoplankton (per ml)	3	0.000003	880	0.0009	0.9*
Periphyton (per cm^2)	--	0.00033	---	0.106	32.2*
Experimental (total coenobia)	10	0.244	0	0.0	0.0
Phytoplankton (per ml)	3	0.000003	750	0.0007	0.7*
Periphyton (per cm^2)	--	0.00033	---	0.005	1.4*
Daphnia pulex (total animals)	30	17.8*	0	0.0	0.0
Planorbis sp. (total animals)	10	1,926.0*	6	1,234.0*	1,234.0
Mougotia sp.					
Control (total filaments)	10	0.013	36,000	40.7*	40.7
Phytoplankton (per ml)	3	0.000003	1,160	0.0011	1.1*
Periphyton (per cm^2)	--	0.00033	---	0.093	28.2*
Experimental (total filaments)	10	0.013	13,000	14.7*	14.7
Phytoplankton (per ml)	3	0.000003	600	0.0006	0.6*
Periphyton (per cm^2)	--	0.00033	---	0.003	1.0*
Daphnia pulex (total animals)	30	17.6*	0	0.0	0.0
Planorbis sp. (total animals)	10	2,240.0*	8	1,766.0*	1,766.0

* Starred numbers are actual weights, others are calculated.

TABLE 2. Continued

Test Cultures	Beginning of Experiment		Termination of Experiment		
	Nos.	Weight in mg	Numbers	Weight in mg	Total weight in beakers in mg
Oedogonium fragile					
Control (total filaments)	10	0.023	39,200	90.2*	90.2
Phytoplankton (per ml)	3	0.000003	1,060	0.0011	1.1*
Periphyton (per cm^2)	--	0.00033	---	0.127	38.5*
Experimental (total filaments)	10	0.023	4,400	10.1*	10.1
Phytoplankton (per ml)	3	0.000003	35	0.00003	0.03
Periphyton (per cm^2)	--	0.00033	---	0.002	0.8*
Daphnia pulex (total animals)	30	17.2*	4	2.5*	2.5
Planorbis sp. (total animals)	10	2,070.0*	7	1,488.0*	1,488.0
Ulothrix zonata					
Control (total filaments)	10	0.003	538,000	161.4*	161.4
Phytoplankton (per ml)	3	0.000003	1,320	0.0013	1.3*
Periphyton (per cm^2)	--	0.00033	---	0.142	42.8*
Experimental (total filaments)	10	0.003	7,560	2.3*	2.3
Phytoplankton (per ml)	3	0.000003	280	0.0003	0.3*
Periphyton (per cm^2)	--	0.00033	---	0.008	2.5*
Daphnia pulex (total animals)	30	18.2*	1	0.6	0.6
Planorbis sp. (total animals)	10	1,895.0	10	2,040.0*	2,040.0

* Starred numbers are actual weights, others are calculated.

TABLE 3. RECOMPILATION OF DIELDRIN EXPERIMENTAL RESULTS OF METCALF ET AL. (1973)

	H_2O = 1 liter			Algae = 100 mg			Snail = 2 g			Fish = 6 g		
	ppm	nCi	dpm	ppm	nCi	dpm	ppm	nCi	dpm	ppm	nCi	dpm
Total ^{14}C	0.0039	10.5	23,000	0.73	0.197	433	90.09	486	1,069,200	3.96	64.3	141,460
Unknown 1	0.00009	0.24	534	0.033	0.009	19	0.83	4.5	9,900	0.01	0.16	352
Dieldrin	0.0014	3.8	8,360	0.64	0.173	380	86.32	467	1,027,400	3.78	61.3	134.860
Unknown 2	0.0009	2.4	5,340	0.012	0.003	6	0.98	5.3	11,660	0.04	0.54	1.188
9 OH Dieldrin	0.00009	0.24	534	0.03	0.008	18	0.51	2.8	6,160	0.07	1.13	2,486
9 CO Dieldrin	---	---	---	---	---	---	0.42	2.3	5,060	0.023	0.38	836
Unknown 3	---	---	---	---	---	---	0.32	1.7	3,800	---	---	---
Unknown 4	0.00012	0.32	704	---	---	---	---	---	---	---	---	---
Unknown 5	0.00038	1.0	2,200	0.0031	0.0008	1.8	0.09	0.5	1,100	0.0008	0.01	22
Polar	0.0002	0.54	1,188	0.001	0.0003	0.7	0.08	0.4	880	0.007	0.11	242
Unextractable	0.0013	3.5	7.722	---	---	---	---	---	---	---	---	---

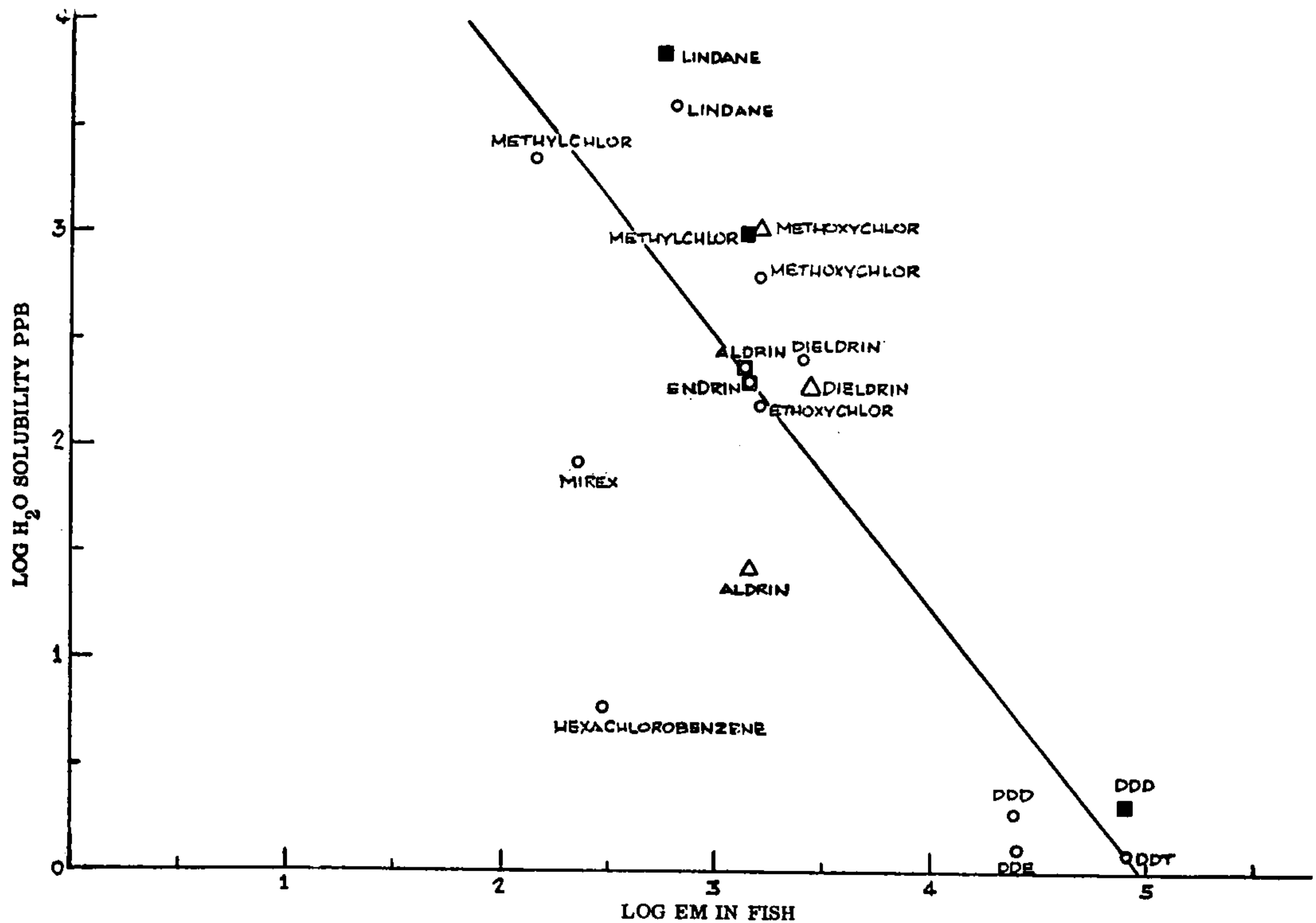

FIGURE 1. Reproduction of Figure 4 of Metcalf et al. (1973) together with points corrected for position and solubility. o original plots of Metcalf et al.; ■ corrected plots, according to their data, of points incorrectly placed; Δ plots of compounds with correct solubilities.

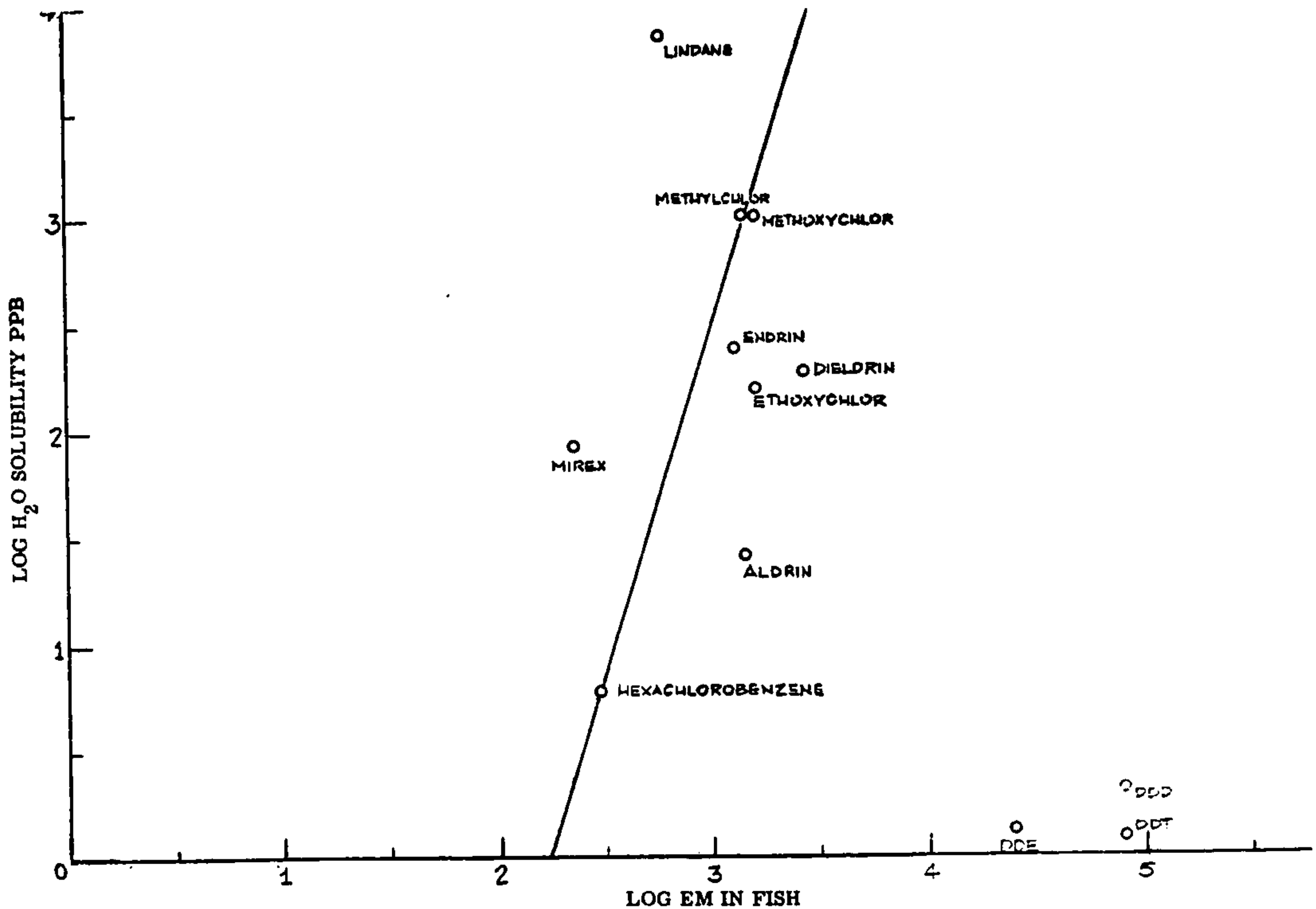

FIGURE 2. **Plot of water solubility of compound against EM in fish from data of** Metcalf et al. (1973) using **correct places and solubilities (DDT group considered aberrant),** line derived by least square **analysis.**

THE UTILIZATION OF INFORMATION ABOUT CONCOMITANCE OF WATER RESOURCES AND DEMANDS IN WATER RESOURCES DECISION MAKING

by

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1. THE PROBLEM

1.1 QUALIFICATION OF THE WATER MANAGEMENT BALANCE

The simplest tool of water resources management is the summarizing water management balance, widely used in Hungary even now. On the basis of this tool one can judge whether the water management situation of a given area is satisfactory; or if additional changes in water resources management are needed (E.C.E. 1972, Domokos 1972).

The basic principle of the summarizing water management balance is as follows: It is assumed that fluctuations of utilizable water resources can be characterized by a function R/t/ and the fluctuation of water demand can be characterized by a function D/t/. The domain of the functions R/t/ and D/t/ is T the reference period of the water balance.

It is assumed furthermore that there is measure γ of water shortage which:

- Depends on the functions R/t/ and D/t/;

- Can be expressed for T by a single value, failing analogous to a probability measure between 0 and 1;

- Has a monotonically increasing relationship to economic loss caused by water shortage;

- Is therefore helpful in the qualification of water balance as favorable, unfavorable or equilibrium.

Water balance is considered favorable--i.e. no measures to restore water management equilibrium are necessary--if the condition

$$\gamma//R/t/,\ D/t// \leq \gamma^* \qquad (1)$$

is satisfied, where γ^* is the upper limit of water shortage, or water shortage tolerance, prescribed on the basis of economic considerations (E.C.E. 1972).

If $\gamma//R/t/,\ D/t// \geq \gamma^*$, the water balance is unfavorable. Water management interventions--for example, the building of new storage reservoirs and water transfer facilities, the introduction of water recirculation, etc.--are needed.

There are several possible definitions of γ (Domokos, 1974). The appropriate choice depends primarily on such characteristics of the water users as, for example, the relationship between water shortage and economic losses. The most commonly used definitions are:

(a) The ratio of combined lengths of water shortage periods to the length of the reference period, or: the relative duration of water shortage:

$$\vartheta = \frac{1}{T} \int_{\substack{R/t/ < D/t/ \\ t \in T}} dt. \qquad (2)$$

The corresponding water shortage tolerance is ϑ^*. In Hungary this index has been used almost exclusively.

(b) The ratio of water shortage, water volume required during T, or the average relative water shortage. This can be defined mathematically in two ways:

$$\lambda_c = \frac{1}{T} \int_{\substack{R/t/ < D/t/ \\ t \in T}} \left[1 - \frac{R/t/}{D/t/}\right] dt \qquad (3a)$$

or

$$\lambda = \frac{\int_{R/t/ < D/t/} \left[D/t/ - R/t/\right] dt}{\int_T D/t/\, dt} \qquad (3b)$$

D/t/=const. (3a) and (3b) are equivalent: $\lambda_0 = \lambda.x$ - The corresponding water shortage tolerance indices are λ_0^* and λ^*. For most water users λ_0 and λ allow better founded decisions than the former used ϑ index did. Thus, their introduction into Hungarian water management is an urgent task.

When calculating the indices ϑ, λ_0 or λ, the water demand function is generally not used. Rather the equivalent water resource distribution function:

$$F/x/ = P/R/t/<x/ \qquad (4)$$

x/d/, the inverse of the water resources duration function:

$$d/x/ = 1 - F/x/ = P/R/t/\geq x/ \qquad (5)$$

is used. In practice it is also generally supposed, that T can be chosen so that the water demand function, D/t/, is a constant. For example T may be hononymous months considered over a series of years.

It can be proved (Domokos, 1974) that knowing the water resources distribution function F/x/, and the water demand value, D=const., water shortage indices may be calculated from the following formulae:

$$\vartheta = F/D/ \tag{6}$$

and

$$\lambda_0 = \lambda = \frac{1}{D}\int_0^D F/x/\ dx. \tag{7}$$

The conditions for a favorable water balance are in this case, according to (1):

$$F/D/ \leq \vartheta^* \tag{6a}$$

and

$$\frac{1}{D}\int_0^D F/x/\ dx \leq \lambda^* \tag{7a}$$

condition (6a) is often used in the more easily manageable form:

$$D \leq R/1-\vartheta^*/ \tag{6b}$$

where $R/1-\vartheta^*/$ is the ordinate belonging to the abscisse according to the $x/d/$ inverse expression of the $d/x/$ water resources duration function presented in (5).

The conditions for a favorable water balance are shown in Fig. 1.

1.2 THE PURPOSE OF THIS PAPER

The formulae (6b) and (7a) are simple in themselves, but well-grounded objections were often made concerning their use. The condition D=const., is a simplification which can no longer be accepted. According to this assumption, the two arms of water balance, utilizable water resources and water demands, are independent variables. It is well-known, however, that the period of lowest water availability often coincides with that of the highest water demand.

This study is an exploration of features characterizing the concomitance of water resources and water demand functions and application of these features to water resources decision making.

2. INTERPRETATION OF THE DEMAND-ARM OF THE SUMMARIZING WATER BALANCE

When compiling a summarizing water balance the D demand-arm is in actual practice the sum of the D_i values of all water users in the area. According to 1.2, each D_i is constant. Thus:

$$D = \sum_{i=1}^{m} D_i , \qquad (8)$$

where m is the number of water users.

This practice is disputable primarily because each D_i value actually is the critical (e.g. highest) value of the $D_i/t/$ function. Water users do not work continuously, and the coincidence of their critical demand values has a probability considerably smaller than 1.

As a finer approximation it is suitable to introduce an empirical coincidence factor (like that used in dimensioning municipal water supply networks). Thus, instead of the sum as per (8), some reduced sum

$$D = k_m \sum_{i=1}^{m} D_i \qquad (9)$$

would be utilized. The value of the coincidence factor k_m, falling between 0 and 1, would depend on the type and number of water users.

Obviously, calculation according to (9) is still rough. A better result might be expected from the following method: Knowing water demand time functions, some critical value of their sum function

$$D/t/ = \sum_{i=1}^{m} D_i/t/ \qquad (10)$$

should be used as the water demand.

Even this solution is rough, since the effects of synchronous water intakes at different points of the river basin do not appear at the same time in the lowest (exit) profile of the basin, to which the water balance is referred. Rather, the effect of the more distant intake appears later than that of the nearer one.

As a second approach, the water demand function, might be characterized by the "function of summarized effects" as follows:

$$D/t/ = \sum_{i=1}^{m} D/t- \Delta t_i/ \qquad (11)$$

Δt_i is the "average marching time," that is, the average time between water intake and its effect at the balance section. If the fluctuation of real marching times around this average value is small, such an approach can be accepted. Otherwise, the summarization according to (11) is still rough.

Things are complicated by the fact, that "negative flood waves" caused by water intakes reach the balance section not only with a certain delay, but also considerably distorted. It is a general experience that these negative waves decrease in volume and change their shapes by getting flatter. Because of these distortions the effect of a continuous, constant water intake far from the balance section may be impossible to investigate.

In order to take this into account, the following modification of (11) may be suggested:

$$D/t/ = \sum_{i=1}^{m} \alpha_i D_i/t- \Delta t_i/. \quad (12)$$

The empirical constants α_i (falling between 0 and 1) depend on the characteristics of the ith water user on his distance from the balance section, on the soil features of the river bed and the river basin, etc.

It is easily conceivable that when the effects of the Δt_i delays are negligible or they equalize each other, or concrete α_i values cannot be determined, the adoption of (9) may be suitable rather than (12). When adopting (9), k_m would express the resultant of all elementary effects.

Vituki (1972) discusses the interpretation of the demand-arm of water balance and deals with concomitance and superposition of water consumptions. Specific values of the coincidence factor, k_m of (9) are given.

3. GENERALITIES ABOUT HOW TO CHARACTERIZE THE CONCOMITANCE OF TWO RANDOM VARIABLES

The following ways of characterizing the relation between two random variables X and Y will be considered:

(a) The joint frequency or duration function

(b) The correlation coefficient and the REIMANN index,* both being measures of closeness of stochastic relation

(c) The functional relation $x=f/Y/$, and a measure of the reliability of function.

Observed data are $X_1, X_2, \ldots, X_s$ and $Y_1, Y_2, \ldots, Y_s$. Observations with the same i index $/X_i$ and $Y_i/$ form data-pairs.

Using previously introduced symbols, the enumerated ways of characterizing the relationship between X and Y are as follows:

3.1 THE JOINT FREQUENCY AND DISTRIBUTION FUNCTION

In order to produce the joint frequency table of the random variables X and Y, let us divide the intervals $[x_o, x_m]$ and $[y_o, y_n]$, each containing

*After Joseph Reimann, Hungarian mathematician (remark of the editor).

the entire value domain of the variable concerned; thus, $x_o \leq \min X_i$; $x_m \geq \max X_i$; $y_o \leq \min Y_i$; $y_n \geq \max Y_i$, equidistantly into a necessary number of $[x_o, x_1]$, $[x_1, x_2], \ldots, [x_{j-1}, x_j], \ldots, [x_{m-1}, x_m]$ and $[y_o, y_1]$, $[y_1, y_2], \ldots$, $[y_{k-1}, y_k]$, $\ldots, [y_{n-1}, y_n]$ partial intervals. Let us make a network (a table) consisting of m columns and n rows, the j-th column of which corresponds to the $[x_{j-1}, x_j]$ interval of the X variable, and the k-th row of which corresponds to the $[y_{k-1}, y_k]$ interval of the Y variable. Let us fill in this table so that into the field defined by the j-th column and the k-th row the a_{jk} number be written defining how many of the observed $/X_i, Y_i/$ data-pairs correspond to the conditions of the given field:

$$a_{jk} = \sum_{\substack{x_{j-1} \leq X_i < x_j \\ y_{k-1} \leq Y_i < y_k}} 1. \tag{13}$$

/Obviously, $\sum_{j,k} a_{jk} = s$./

The set of a_{jk} values is called the (joint) frequency function of variables X and Y or the (joint) frequency table. Its symbol is $h_o/x,y/$. An example of a joint frequency function is shown in Fig. 2.

Let us introduce two other symbols to be used later. The sums of the single columns and rows:

$$a_j = \sum_{k=1}^{n} a_{jk} \tag{14}$$

and

$$a_k = \sum_{j=1}^{m} a_{jk}. \tag{15}$$

The set of the a_j or a_k numbers, represents the frequency histogram of the X or Y random variable.

From the frequency table one can get the $h_o,/x,y/$ joint relative frequency table by changing each a_{jk} value to

$$f_{jk} = \frac{1}{s} a_{jk} \leq 1 \tag{16}$$

/where $\sum_{j,k} f_{jk}=1$/. Thus,

$$h/x,y/ = \frac{1}{s} h_0 /x,y/. \quad (17)$$

From the relative frequency table one gets a joint duration table by ordering to each $/x_j,y_k/$ network knot of the former the sum of the $f_{u,v}$ values written in the fields of the rectangle defined by $/x_j,y_k/$ and $/x_o,y_o/$:

$$d_{jk} = \sum_{\substack{1 \leq u < j \\ 1 \leq v < k}} f_{u,v} \quad (18)$$

Obviously, $d_{oo}=0$ and $d_{mn}=\sum_{u,v} f_{u,v}=1$, and $d/x,y/$ is a monotonically increasing function of both x and y.

The joint duration function (also called the joint empirical distribution function) $d/x,y/$ is the best estimate of the joint theoretical distribution function $F/x,y/$ of the variables X and Y, if the conditions of Glivenko's theorem are satisfied (Domokos, 1970):

$$d/x,y/ \sim F/x,y/ = P/X < x,\ Y < y/ \quad (19)$$

If necessary, a fitting function can be produced for the $d/x,y/$ duration function. This is often done in practice for univariate distribution functions.

3.2 THE CORRELATION COEFFICIENT AND THE REIMANN INDEX

Among the indices characterizing the closeness of stochastic relationship by one single number the correlation coefficient ρ, widely used in hydrological practice, is not very useful. The value of this index is 1 only if a linear relationship exists between the two variables. If there is any other kind of relationship, the absolute value of the correlation coefficient will be smaller than 1. Of course, if this relationship is known, transformation may be performed so that the correlation coefficient of the transformed variables will be a correlation coefficient of 0, indicates lack of correlation, but not necessarily independence. As a matter of fact, the correlation coefficient is scarcely usable as a measure of the closeness of the stochastic relationship between two variables because of its small information content.

More useful might be the index

$$r/X,Y/ = 1 - \frac{E/X \mid Y/}{E/X/} \quad (20)$$

introduced by J. Reimann. E is entropy, to be defined later. This index has the advantage being $r/X,Y/=1$ if there is a mutually unambiguous--but not necessarily linear or quasi-linear--relationship, and $r/X,Y/=0$, if X and Y are independent.

Now let us define E/X/, the entropy of the X variable. Let X posit the $x_1, x_2, \ldots, x_m$ values, by turns, with the probabilities $p_1, p_2, \ldots, p_m$--or, in approximation: let the X variable fall with p_1 frequency into the $[x_o, x_1]$ interval having the mean value X_1, ecc., and fall with p_m frequency into the interval $[x_{m-1}, x_m]$ having the mean value X_m, where:

$$p_j = \sum_{k=1}^{n} f_{jk} = \frac{a_j}{s}. \tag{21}$$

Then, entropy of the distribution of X is:

$$E/X/= - \sum_{j=1}^{m} p_j \overset{2}{\log} p_j = \overset{2}{\log} s - \frac{1}{s} \sum_{j=1}^{m} a_j \overset{2}{\log} a_j. \tag{22}$$

E/X|Y/ is, however, the entropy of the X variable conditioned by Y, that is:

$$E/X \Big| Y/ = \sum_{k=1}^{n} P/Y{=}Y_k/.E/X \Big| Y{=}Y_k/ =$$

$$= \sum_{k=1}^{n} \sum_{j=1}^{m} f_{jk} - \sum_{j=1}^{m} f_{jk}.\overset{2}{\log} f_{jk} \quad . \tag{23}$$

(23) is equivalent to the more easily manageable formula:

$$E/X \Big| Y/= \frac{\overset{2}{\log} s}{s^2} \sum_{k=1}^{n} a_k^2 - \frac{1}{s^2} \sum_{k=1}^{n} /a_k . \sum_{j=1}^{m} a_{jk} \overset{2}{\log} a_{jk}/. \tag{24}$$

Fig. 2 shows a numerical example of the calculation of the REIMANN index.

The single disadvantage of the information index of REIMANN is its sensitive dependence on the way of dividing the value domains of the two variables. One can always find a method of division, such that none of the a_{jk} values will be greater than 1. As a consequence, r/X,Y/ will be 0. This extreme condition does not mar the practical usefulness of r/X,Y/.

The following conclusions may be drawn from the value of r/X,Y/:

(a) If r/X,Y/=0, then X and Y are independent random variables. That is, their joint distribution function is the product of the distribution functions of the single variables: F/x,y/=F/x/.F/y/. In practice, the same can be said if the value of r/X,Y/ is approximately 0.

(b) If r/X,Y/=1, there is some deterministic functional relationship between X and Y. This relationship should be looked for and, if found, made use of in practice. The same can be said, if the value of r/X,Y/ is approximately 1.

(c) If r/X,Y/ falls within the [0,1] interval (say between 0.05 and 0.95), the relationship between X and Y can be properly characterized only by their joint frequency or distribution function.

3.3 DETERMINISTIC FUNCTION

In practice a deterministic functional relationship between the X and Y variables is accepted, if a simple Y=f/x/ function can be found such that the dispersion of data points around this curve is smaller than an empirical limit value given in advance. This limit value is determined depending on the purpose for which Y=f/x/ will be used and on the uncertainties of the observations. The more reliable the observations are, the smaller the deviation allowed.

If the value of the index r/X,Y/ is near 1 (say, it is greater than 0.95) it is worth looking for a Y=f/x/ function.

4. THE RELATIONSHIP BETWEEN WATER RESOURCES AND WATER DEMANDS IN A SPECIAL CASE

As an example, the concomitance of natural flow discharges and irrigation water demands in the Hungarian part of the Tisza river basin will be examined for June-August of six years (1964-69).

Among water resources data only natural flow discharge, Q is taken into account. The other quantitative components of utilizable water resources (additional water from reservoirs, the industrial water consumption, water withdrawals abroad, etc.) are negligible in this case.

As for water demands, only agricultural irrigation is taken into account because

- These are the only available data

- It seems very probable that water resources are closely related to irrigation demands. Both are dependent on climatic factors.

The discharge records of three gauge sections of the Tisza River (Polgár, Tiszabö and Szeged) are compared with water withdrawals by main irrigation water users. The major irrigation water intakes on the Hungarian part of the Tisza River and gauge sections and intakes are shown on Fig. 3. In addition, water demand curves have been calculated for each of the three sections according to (10), (11) and (12) (Fig. 4). Calculations are shown for the Tiszabo section.

4.1 THE INTERPRETATION OF REIMANN INDICES

For each section the concomitance of water resources and demands has been examined taking into account

(a) the whole data-pair series (6x3 months)

(b) the series representing single months (1 month)

(c) individual 3 months periods within each of several years (3 months) and

(d) the sets of hononymous months (6x1 months)

For each series the joint frequency table and r/Q,D/ REIMANN index were calculated. Value domains of both variables were divided into 15 intervals.

Data series and r/Q,D/ indices are presented in Table I. The following conclusions can be drawn from r/Q,D/ indices:

(a) The values of the 42 r/Q,D/ indices--calculated for 7 differently combined data series pairs and 6 differently defined periods--fluctuate between 0.57 and 0.88. Neither can independency be assumed, nor can a D=D/Q/ deterministic relation be hoped for. The concomitance of the examined data series has a stochastic character and can be characterized satisfactorily only by a joint frequency or duration function.

(b) Values of r/Q,I/ increase with the size of the area examined, thus with the number of water users. For a larger river basin than the Tisza, or for a basin with more water users an acceptable deterministic relation might be seen. In the case of considerably smaller water users than the irrigation system furnished by the Hungarian East Canal, a near independence between water resources and demands may exist.

(c) The tendency for r/Q,D/ to decrease as the period examination becomes longer, is less marked. This may be noted most sharply by comparing the r/Q,D/ values for 1 month periods (column 5) with those for 18 month periods (column 10). It may also be noted that r/Q,D/ values for periods of 6 hononymous months (columns 7-9) always surpass those of continuous three-months-periods of given years (column 6).

The latter fact supports Hungarian water balance practice, according to which hononymous months considered over a series of years has been considered as the reference period of the balance. (Domokos, 1974).

(d) Finally, it can be stated--as could have been anticipated from Fig. 4--that the effects of Δt marching times and α "flattening" factors on the values of r/Q,D/ indices are practically negligible.

4.2 THE SHAPING OF D/Q/ RELATIONS (Fig. 5.)

An attempt has been made to identify deterministic relationships in a graphical way for each of the 42 /Q,D/ data-series pairs as per Table I. 6 selected graphs from the 42 are shown in Fig. 5. The following conclusions can be drawn from these graphs:

(a) As was already expected from r/Q,D/ values, the observed points are widely scattered around the smoothing curve D/Q/. The standard deviation values, σ, are rather high: they fall between 0.1 and 0.3. The D/Q/ smoothing curves can be taken at best as rough approximations.

(b) Water demand is a monotonically decreasing function of flow discharge, Q.

(c) As noted in the interpretation of r/Q,D/ indices, deviation increases as the area examined increases. In this case, the relationship is not so definitive.

(d) Similarly, previously noted in the interpretation of r/Q,D/ indices, deviation increases with the length of the period examined and is less for periods consisting of hononymous months considered over a period of years for three month periods within single years.

5. CALCULATION OF WATER SHORTAGE USING CONCOMITANCE INFORMATION

The utilization of information concerning the concomitance of water resources and demands in compiling summarizing water balances, depends primarily on whether the concomitance of the R/t/ and D/t/ functions is stochastic or deterministic, that is, whether it can be determined by a joint frequency or duration function or by a deterministic function.

5.1 STARTING ASSUMPTIONS

Before giving details of the methods proposed, the utilizable water resources function, R/t/, and the water demand function, D/t/, are assumed to be known. D/t/ is not taken to be a single "critical" value as has been the practice until now.

Further, D/t/ is assumed to be a function of effects produced, according to formula (12). From the water balance functions the distribution functions

$$F/x/ = P/R < x/ \qquad (4)$$

and

$$G/y/ = P/D < y/ \qquad (25)$$

can be produced.

Note the following:

(a) The utilizable water resources functions, R/t/, are primarily determined by Q/t/ flow discharge functions. The latter are generally well known or can be calculated from hydrometric observations. The R/t/ functions themselves can be defined in several ways and are produced from Q/t/ functions by correction factors.

(b) The d/Q/ duration curves used for producing d/R/ duration curves or equivalent F/x/ distribution curves generally can be calculated from hydrometric measurements.

(c) There are few D/t/ functions available in practice. This is the reason for the use of D=const. in water balance investigations.

(d) Investigations of irrigation water users (David, 1971) lead to the conclusion, that their normed values generally have a normal distribution.

According to chapter 3.1, if R/t/ and D/t/ are known, the joint frequency function of the two balance arms, h/x,y/, can be calculated unambiguously.

It may happen that some deterministic function can be found to relate the two water balance arms. The existence of such a relation would be indicated by a value of the REIMANN index.

5.2 STOCHASTIC RELATION BETWEEN WATER RESOURCES AND WATER DEMAND

First let us consider the simpler case: There is no acceptable deterministic relation. The value of r/D,R/ does not approach 1. In this case the concomitance of D and R can be characterized either by the R/t/ and D/t/ curves, or by the joint distribution function produced from these curves.

Water shortage indices can be calculated from either the time functions or the joint distribution function. The first way is appropriate for computer use, the second for hand calculation.

(A) For the direct calculation from time functions definitions (2), (3a) and (3b) of water shortage indices should be adopted.

Since the R/t/ and D/t/ functions are given in practice not by continuous, but by step functions, the integrals of the last mentioned formulae become simple sums. Of course, the integrals can be replaced by sums, as an approach, even when continuous time functions are given.

The calculation of water balance indices directly from time functions by formulae (2), (3a) and (3b) is an exact and theoretically always possible way of considering the concomitance of water resources and demands. Its disadvantage in laboriousness is practically eliminated by the use of electronic computers.

(B) The formulae for calculating water shortage from the joint relative frequency function h/x,y/ are the following:

$$\vartheta = P/D < R/ = \iint_{x<y} h/x,y/ \, dx \, dy \qquad (26)$$

$$\lambda = \frac{\iint_{x<y} /y-x/ \, h/x,y/ \, dx \, dy}{\int_0^{\infty}\int_0^{\infty} y \, h/x,y/ \, dx \, dy} \qquad (27)$$

A similar formula for calculating λ_o from h/x,y/ is unknown as yet.

The formulae (26) and (27), however laboriously, are manageable by hand calculation. Instead of h/x,y/, the equivalent h_o/x,y/ function is simpler to use in calculations.

5.3 DETERMINISTIC FUNCTIONAL RELATION OF UNKNOWN FORM BUT KNOWN TENDENCY BETWEEN WATER RESOURCES AND WATER DEMAND

Let us consider the practice of compiling water balances according to (6b) and let us also assume, logically, that the so-called "critical" D constant on the left side of the formula is rarely surpassed value, that is, a value of small duration. Let us put for this small duration--with an arbitrary, but acceptable approach--the ϑ^* water shortage tolerance. With these assumptions, the (6b) condition for a favourable water balance might be written as follows:

$$D/\vartheta^*/ \leq R\ /1 - \vartheta^*/, \tag{28}$$

where $D/\vartheta^*/$ is the ordinate belonging to the abscissa $d=\vartheta^*$ according to the D/d/ inverse form of the

$$d/y/ = 1 - G/y/ \tag{29}$$

water demand duration function. In other words: $D/\vartheta^*/$ is the value of water demand surpassed with ϑ^* probability.

The assumption according to (28) has been generalized by Kovács (1963) and by Dávid (1971), who suggested plotting in a common coordinate system the water resources duration curve, R/d/ and D/1-d/, the mirror-image of the water demand duration curve D/d/ (Fig. 6). From this picture--called the stochastic water balance by Dávid--one can read, on one hand, the T_{crit} value, "characterizing the relative duration of the event that water resources are surpassed by water demand." With the symbols used in the present paper:

$$T_{crit} = \vartheta = \frac{1}{T} \int_{R/t/<D/t/} dt = \int_{d/R=D/}^{100\ \%} \partial d. \tag{30}$$

On the other hand, the hatched area A in the left lower corner of the diagram (called "water deficiency; unfavorable water balance") is in direct proportion to the λ index of the balance. Namely:

$$A = \frac{1}{T} \int_{R/t/<D/t/} \left[D/t/-R/t/\right] dt = \int_{d/R=D/}^{100\ \%} \left[D/1-d/-R/d/\right] \partial d. \tag{31}$$

At the same time, as per definition:

$$\lambda = \frac{\int\limits_{R/t/<D/t/} \left[D/t/-R/t/\right] dt}{\int\limits_{T} D/t/ \, dt} = \frac{\frac{1}{T} \int\limits_{R/t/<D/t/} \left[D/t/-R/t/\right] dt}{\frac{1}{T} \int\limits_{T} D/t/ \, dt} =$$

$$= \frac{\int\limits_{d/R=D/}^{100\,\%} \left[D/1-d/-R/d/\right] \partial d}{\int\limits_{d=0}^{100\,\%} D/d/ \, \partial d} = \frac{A}{\int\limits_{d=0}^{100\,\%} D/d/ \, \partial d} \tag{32}$$

Although not explicitly pointed out, Kovács and Dávid made an assumption when drawing the curves R/d/ and D/1-d/ in the same coordinate system and manipulating them in the described way that at an arbitrary moment, t_o within the reference period T, the relation

$$d/R/t_o// = 1-d/D/t_o// \tag{33}$$

is valid. That is, a deterministic relation is assumed to exist between R/t/ and D/t/.

Since this deterministic relation is a basic condition for this water balance, the title "stochastic water balance" is not fortunate at all.

Let us look now at what D/R/ functions satisfy condition (33). Obviously, each function in which D is a monotonic, non-increasing--function of R does so.

According to Fig. 5 a monotonic decreasing tendency generally characterizes the smoothing curves for the relation between irrigation water demand and flow discharges. Of course, the question of the acceptable level of deviation of observations from these curves remains open.

To sum it up: if it is sure that water demand is an acceptable deterministic monotone non-increasing function of water resources, the value of r/D,R/ being approximately 1, but the shape of this function is unknown, the compilation of water balance arms based on the duration curves of the two balance arms may be valid, and the water shortage indices ϑ and λ might be calculated according to (30) and (32). The qualification of the balance as favorable or unfavorable is obtained by comparing these indices with the tolerated limit values, ϑ^* and λ^*.

The advantage of the method is that it is simple and demonstrative. In most practical cases it may be helpful. However, before its use, the existence of a deterministic non-increasing function between the two balance arms must be proved.

5.4 DETERMINISTIC FUNCTION OF KNOWN FORM BETWEEN WATER RESOURCES AND WATER DEMAND

If there is an acceptable deterministic relationship between the two arms to be compared in water balance, then formulae can be found for the calculation of water shortage indices, at least for simpler relationships. Water shortage index is being calculated by these formulae and the qualification of water balance consists of the comparison of this actual (or expected) value with its tolerated limit value.

Three simple examples will be given. For each of them it will be assumed, that the distribution function of utilizable water resources and the ϑ^*, λ^*_o and λ^* tolerance indices are known.

(A) The simplest case of the D=f/R/ relationship is the trivial D=const. function, generally used in water balances. From this assumption the (6) and (7) formulae, or the (6a), (6b) and (7a) qualifications of water balance, can be deduced simply (Fig. 1) (Domokos, 1974).

Because it is more logical to use ourselves to a reliably estimated, "critical" D value, than relatively unreliable D/t/ functions or D/R/ functions, the use of D=const. is justified until considerable uncertainties are seen in this relationship.

(B) According to another assumption, a simple reciprocal relationship exists between the two variables. That is, during a given reference period the water demand of a water user is inversely proportional to the available water resources:

$$D/t/ = \frac{a}{R/t/}, \qquad (34)$$

where a is a constant, characterizing the water user and the catchment area furnishing water to the latter.

This assumption may probably be accepted as a good approach for irrigation water users supplied directly by natural water resources for suitably chosen periods.

If the (34) condition is valid, the λ_o water shortage index can be calculated by the following formula (Domokos, 1974):

$$\lambda_o = \frac{2}{a} \int_0^{\sqrt{a}} x \; F/x/ \; dx = \frac{2}{a} \int_0^{D_o} x \; F/x/ \; dx \qquad (35)$$

where $D_O=\sqrt{a}$ is the water demand value at the moment when water demand and water resources are equal.

It also can be shown easily that, in this case, the value of the ϑ water shortage is:

$$\vartheta = F / \sqrt{a} / = F/D_o/ \qquad (36)$$

The water shortage indicator function, u/t/ will be (Domokos, 1974):

$$u/t/ = \begin{cases} 1, \text{ if } R/t/ < \sqrt{a} \\ 0, \text{ if } R/t/ \geq \sqrt{a} \end{cases} \qquad (37)$$

The ϑ index can be calculated as the expected value of the u/t/ indicator function:

$$\vartheta = \int_0^{\infty} u/x/ \, dF/x/ = \int_0^{\sqrt{a}} dF/x/ = F/\sqrt{a}/ \qquad (38)$$

The ϑ-based condition (like (6a)) for a favorable water balance is:

$$F/\sqrt{a}/ \leq \vartheta^* \qquad (39)$$

For example, $\vartheta^*=15\%$, (39) can be written (patterned after (6b)) in the form:

$$\sqrt{a} < R\,/85\ \%/ \qquad (40)$$

On the right is the ordinate of the R/d/ water resources distribution function with the abscissa $1-\vartheta^*=85\%$.

Thus, if the condition (34) is valid and a ϑ-based water balance is to be compiled, it can be done formally according to (6b), by substituting $D_O=\sqrt{a}$ for D=const. The physical meaning of $\sqrt{a}$ is the value R/t/ and D/t/ at their intersection.

(C) Finally, let us assume

$$D/t/ = a - b\,R/t/ \quad \text{where} \qquad (41)$$

a and b are non-negative constants. In this case the common value of the time functions R/t/ and D/t/ at their intersection is:

$$D_o = \frac{a}{1+b}$$

Thus, after (40), the condition for a favorable water balance is:

$$\frac{a}{1+b} \leq R/1-\vartheta^*/ \qquad (42)$$

In this case no formula analogous to (35) can be deduced for the λ_o index.

In summary, from (6a), (40) and (42) the following conclusion can be drawn. If there is a known, deterministic monotonic, non-increasing D/R/ function relating R/t/ and D/t/ and D_o is the value at their intersection the condition for a favorable ϑ-based water balance is:

$$D_o \leq R/1-\vartheta^*/. \qquad (43)$$

For certain D/R/ relationships the λ_o index can be calculated by (3a) or (35).

Formula (43), generalizing (6b), points out, that until the ϑ-based qualification is used exclusively, it will be of no great importance whether the relationships between water resources and demands are known or not: When compiling ϑ-based balances, only one selected value of the water demand function is used--it might be called "critical water demand." No use is made of any other information included in the D/t/ function. This information would be used only if the λ index--or its generalizations (Domokos, 1974)--were adopted.

Obviously, the search for a deterministic relationship between simultaneous water resources and demand is justified if both variables strongly depend on the same factor. This may be characteristic for irrigation, especially if the area concerned is situated in the upper part of a river basin.

However, Table I and Fig. 5 show that the relationship between water resources and demand is rather loose even in this most favorable case. A considerably weaker relationship is to be expected between resources and demand in the cases of municipal and industrial water intakes.

5.5 OVERVIEW AND SIMPLIFIED EXAMPLE

Conditions and methods of utilization of the methods described in chapters 5.2-5.4 are summarizxed by Table II. Fig. 7 is an example of the calculation of water shortage indices where $D \neq 0$. For simplicity:

(a) The time series are short, concerning only 30 time units, e.g. days. (In practical cases the number of time units may be greater even by two or three orders of magnitude.)

(b) The water resources and demand are not given as continuous functions, but by series of daily average values. (As a consequence of the way of observing water resources and demand data, this is the general way of presenting functions.)

(c) An unambiguous deterministic relationship between water balance arms has been supposed to exist.

From chapter 5.4 and Table II. it is obvious that, if there is an acceptable D/R/ relationship, the simplest way of calculating water shortage indices is to use formulae, based on D/R/ and the water resources distribution function. In the example, water shortage indices ϑ, λ and λ_o have been calculated by each possible method to demonstrate numerical applications and to compare results obtained by different methods.

Discussing the lettered sections of Fig. 7:

(A) All water shortage indices can be calculated, on the basis of their definitions, directly from water resources and water demand functions. In this example the aim of these calculations is to produce values which can be compared with $\underline{\vartheta}$, $\underline{\lambda}$ and $\underline{\lambda_o}$ indices obtained by other methods. In the practical case of a longer and more varied time series this method is not suitable for hand calculation. However, it is the best method for computer calculation because of its simplicity.

(B) Instead of the joint relative frequency function, h/x,y/ the h_o/x,y/=s.h/x,y/ joint frequency function has been used for practical reasons. Because of the small amount of data used in the example, h_o/x,y/ has been calculated not as a set of a_{jk} frequency values ordered to fields, but as a set of ones ordered to discrete /D,R/ table points. The calculation of water shortage indices by this method has been shown only for the sake of completeness and comparison. In such a simple example the application of this method only makes the calculation unnecessarily complicated. In most practical cases--when the noncomitance of water resources and demand is stochastic--this is the best method for hand calculation.

(C) Shows water balance based on duration curve. Note its descriptiveness and the fact, that it can be used not only for D/R/ relationships which are known, but also for ones of unknown, but monotonically non-increasing form.

(D) Finally, the $\underline{\vartheta}$ and $\underline{\lambda_o}$ indices of water shortage could be calculated by simple formulae, because of the existence of an unambiguous D/R/ function. Formula (35) for index $\underline{\lambda_o}$ is valid only for the relationship D=a/R, according to (34). For the relationship D=(a/R)+b as exists in the example, it can be applied only as an approximation. Formula (30) for $\underline{\vartheta}$ is exact in the case of this example.

Fig. 8 shows a numerical example of a stochastic relationship between water resources and demand. In this case, water shortage indices can be calculated easily by hand only by use of the joint frequency function.

6. SUMMARY

One of the simplest ways of dimensioning and controlling water resources is by comparison of some water shortage index with an upper limit value, called water deficiency tolerance and based on economic considerations. The situation is considered satisfactory if water shortage is smaller than the limit value. Otherwise the dimensions and operating rules of system-elements (the volumes of storage reservoirs and water intakes, etc.).

Domokos (1974) showed several indices of water shortage and their calculation when water demand is a constant value and water resources are characterized by a probability distribution function. Tokar (1975) shows methods for the calculation of water shortage indices in this particular case.

This paper examines indices of water shortage, when water demand is not constant, but a stochastic or deterministic relation exists between water demand and resources.

Indices characterizing the concomitance of two arbitrary random variables are considered. Flow discharges and water consumptions of the Tisza basin (Table I, Figures 1, 4 and 5.) provide examples of their use.

The calculation of water shortage indices depends on relationship between resources and demands (Table II):

(a) If the relation between water resources and demand is stochastic, water shortage indices should be calculated either directly from the time functions of the two variables (by computer) or from their joint frequency function, by simple formulae.

(b) If there is a deterministic functional monotonic, non-increasing relationship of unknown form the water balance may be based on the duration functions of the two variables.

(c) Finally, if the relationship between water resources and demand is known, the water shortage index can be calculated from a simple formula and the distribution function of water resources.

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Table I. REIMANN indices r/Q,D/ characterizing the concomitance of irrigation water demand and flow discharges in the Tisza river system.

Serial number	Tisza section	Interpretation of data series of		r (Q,D) indices calculated from the daily data pairs of the period of					
		flow discharge	resulting water demand [2/3/]	June 1969	June/August 1968	June 1964-69	July 1964-69	August 1964-69	June/August 1964-69
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)
1.	Polgár	$Q(t)=Q_P(t)$	$D(t)=D_1(t)$	0,702 [1/]	0,586	0,732	0,764	0,655	0,568
2.	Tiszabő [4/]	$Q(t)=Q_T(t)$	$D(t)=\sum_{i=1}^{6} D_i(t)$	0,850	0,671	0,713	0,746	0,718	0,597
3.			$D(t)=\sum_{i=1}^{6} D_i(t-\Delta t_{i-T})$	0,850	0,690	0,721	0,748	0,730	0,604
4.			$D(t)=\sum_{i=1}^{6} \alpha_{i-T} D_i(t-\Delta t_{i-T})$	0,842	0,661	0,693	0,747	0,729	0,596
5.	Szeged	$Q(t)=Q_{Sz}(t)$	$D(t)=\sum_{i=1}^{12} D_i(t)$	0,873	0,790	0,788	0,827	0,762	0,762
6.			$D(t)=\sum_{i=1}^{12} D_i(t-\Delta t_{i-Sz})$	0,860	0,794	0,802	0,825	0,763	0,775
7.			$D(t)=\sum_{i=1}^{12} \alpha_{i-Sz} D_i(t-\Delta t_{i-Sz})$	0,872	0,774	0,828	0,825	0,781	0,761

Remarks:

1/ The calculation of $r(Q_p, D_1)$ is shown in Fig 2.

2/ Gauge sections and main water intakes are shown in Fig. 3.

3/ The Δt_{i-T} and Δt_{i-Sz} marching times and the assumed α_{i-T} and α_{i-Sz} „flattening factors" used for calculating resulting water demand alternatives are the following:

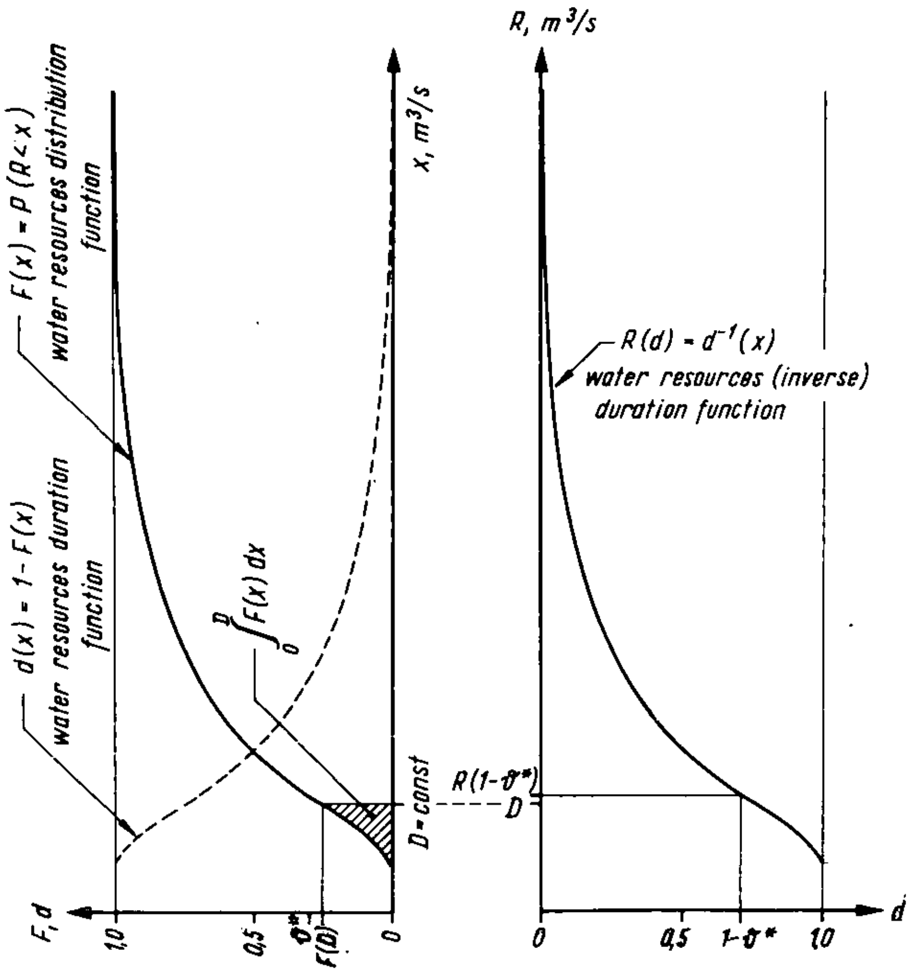
	Month	until Tiszabő						until Szeged											
		1-T	2-T	3-T	4-T	5-T	6-T	1-Sz	2-Sz	3-Sz	4-Sz	5-Sz	6-Sz	7-Sz	8-Sz	9-Sz	10-Sz	11-Sz	12-Sz
Δt_{i-T} and Δt_{i-Sz} (days)	June	2	1	1	–	–	–	6	4	4	3	3	3	1	1	–	–	–	–
	July	3	1	1	–	–	–	6	5	4	4	4	3	1	1	–	–	–	–
	August	3	1	1	–	–	–	7	5	5	4	4	4	1	1	1	–	–	–
α_{i-T} and α_{i-Sz}	June/August	0,7	0,9	1,0	1,0	1,0	1,0	0,5	0,7	0,7	0,7	0,7	0,7	0,9	0,9	1,0	1,0	1,0	1,0

4/ The production of resulting water demand time series for the Tiszabő section is shown in Fig. 4.

Table II. Utilization of information concerning the relationship between water resources and demand for the qualification of summarizing water balance.

Starting data about: water resources	water demand		joint distribution	Characteristics for the relationship between water resources and demand: REIMANN index $r(D,R)$	correlation coefficient $\rho(D,R)$	acceptable deterministic function $D-D(R)$	Functions to be used for compiling water balance	Conditions for a favourable water balance: on the basis of the ϑ index, with ϑ^* tolerance given in advance	on the basis of λ or λ_0 index, with λ^* and λ_0^* tolerance given in advance	Remarks
$R(t)$ and $F(x)$ or $R(d)$	$D(t)$	$G(y)$ or $D(d)$	$h(x,y)$							
known	D = const	unknown	unknown	—	—	—	$F(x)$, $R(d)$, D = const	$D \leq R(1-\vartheta^*)$	$\frac{1}{D}\int_0^D F(x)\,dx \leq \lambda^*$	Recent Hungarian practice (Fig. 1)
known	known	unknown	unknown	irrelevant	irrelevant	does not exist	$R(t)$, $D(t)$	ϑ, λ or λ_0 are calculated by using therier definitions, directly from time functions $R(t)$ and $D(t)$		Mainly for computer calculation
known				0 - 0,95	irrelevant	does not exist or is unknown	$h(x,y)$	$\iint_{x<y} h(x,y)\,dx\,dy \leq \vartheta^*$	$\frac{\iint_{x<y}(y-x)\,h(x,y)\,dx\,dy}{\int_0^\infty\int_0^\infty y\cdot h(x,y)\,dx\,dy} \leq \lambda^*$	Mainly for hand calculation
				0,95 - 1	< 0	has a known (monotone non-increasing) tendency	$R(d)$, $D(1-d)$	$T_{crit} = 1-d\,(R=D) \leq \vartheta^*$	$\frac{\int_{d(R=D)}^{1}[D(1-d)-R(d)]\,\partial d}{\int_0^1 D(d)\,\partial d} \leq \lambda^*$	Duration curve based water balance (Fig. 6)
					irrelevant	known	$F(x)$, $R(d)$, $D(R)$	$D_0 < R(1-\vartheta^*)$ [1]	The formula should be deduced for each type of $D(R)$ functions individually	Only if $D(R)$ is acceptable
						for example: $D = \frac{a}{R}$		$\sqrt{a} \leq R(1-\vartheta^*)$	$\frac{2}{a}\int_0^{\sqrt{a}} x\,F(x)\,dx \leq \lambda_0^*$	
						$D = a - bR$		$\frac{a}{1+b} \leq R(1-\vartheta^*)$	no simple formula	

[1] Definition of D_0 from $D(R)$ function: $D_0 = R(D_0)$



Conditions for a favourable water balance:

a, On the basis of the ϑ index, with ϑ^* tolerance given in advance:

$$F(D) \leq \vartheta^*$$

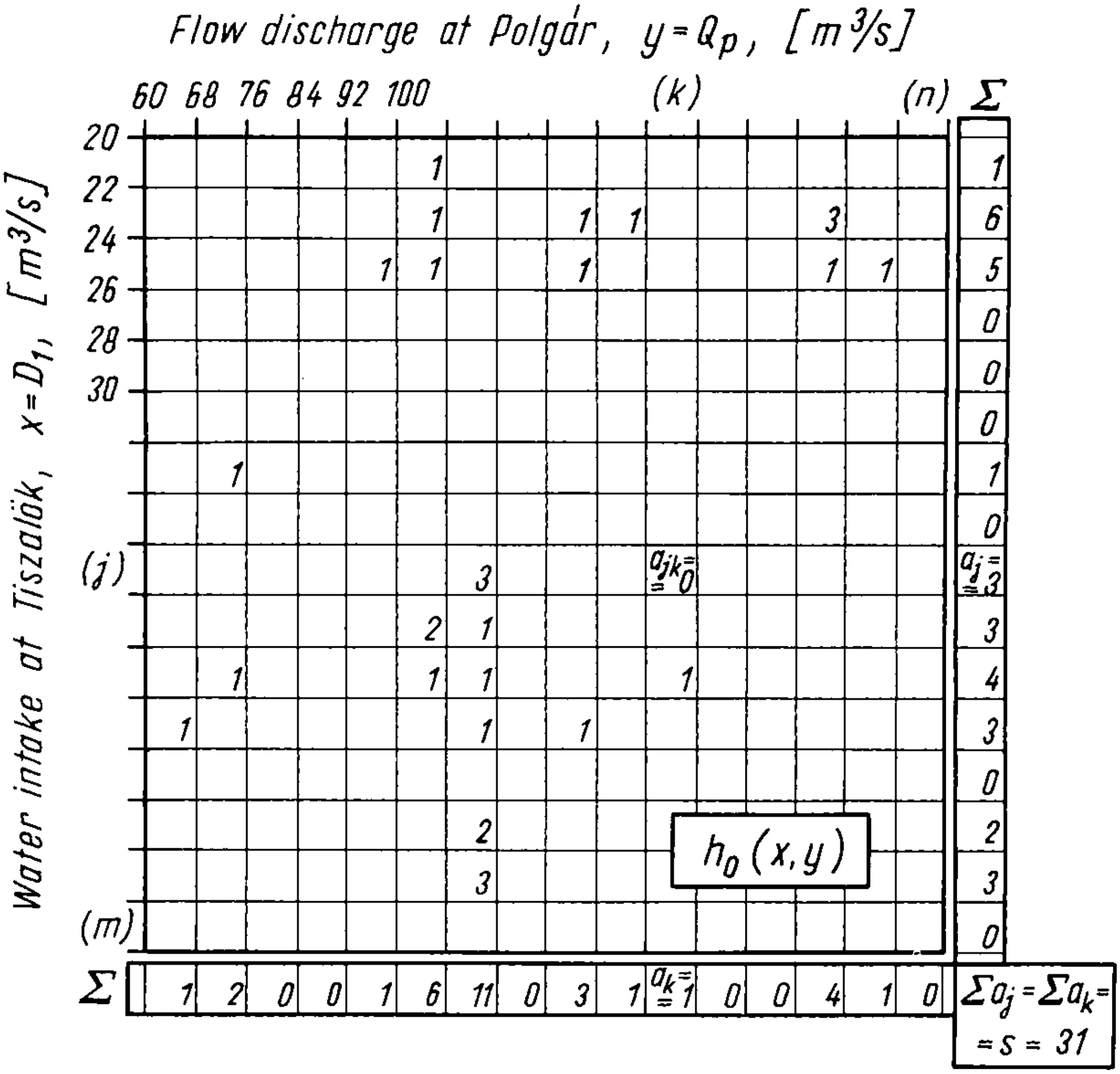
or

$$D \leq R(1-\vartheta^*).$$

b, On the basis of the λ index, with λ^* tolerance given in advance:

$$\frac{1}{D}\int_0^D F(x)\,dx \leq \lambda^*.$$

Figure 1. Qualification of summarizing water balance in the case D=const.



$$r(Q_p, D_1) = 1 - \frac{E(Q_p\,D_1)}{E(Q_p)} = 0{,}702$$

$$E(Q_p \mid D_1) = \frac{\log s}{s^2} \sum_{k=1}^{n} a_k^2 - \frac{1}{s^2} \sum_{k=1}^{n} \left(a_k \sum_{j=1}^{m} a_{jk} \log a_{jk} \right) = 0{,}247$$

$$E(Q_p) = \log s - \frac{1}{s} \sum_{k=1}^{m} a_k \log a_k = 0{,}828$$

Figure 2. Joint frequency function of water resources and water needs with the REIMANN index.

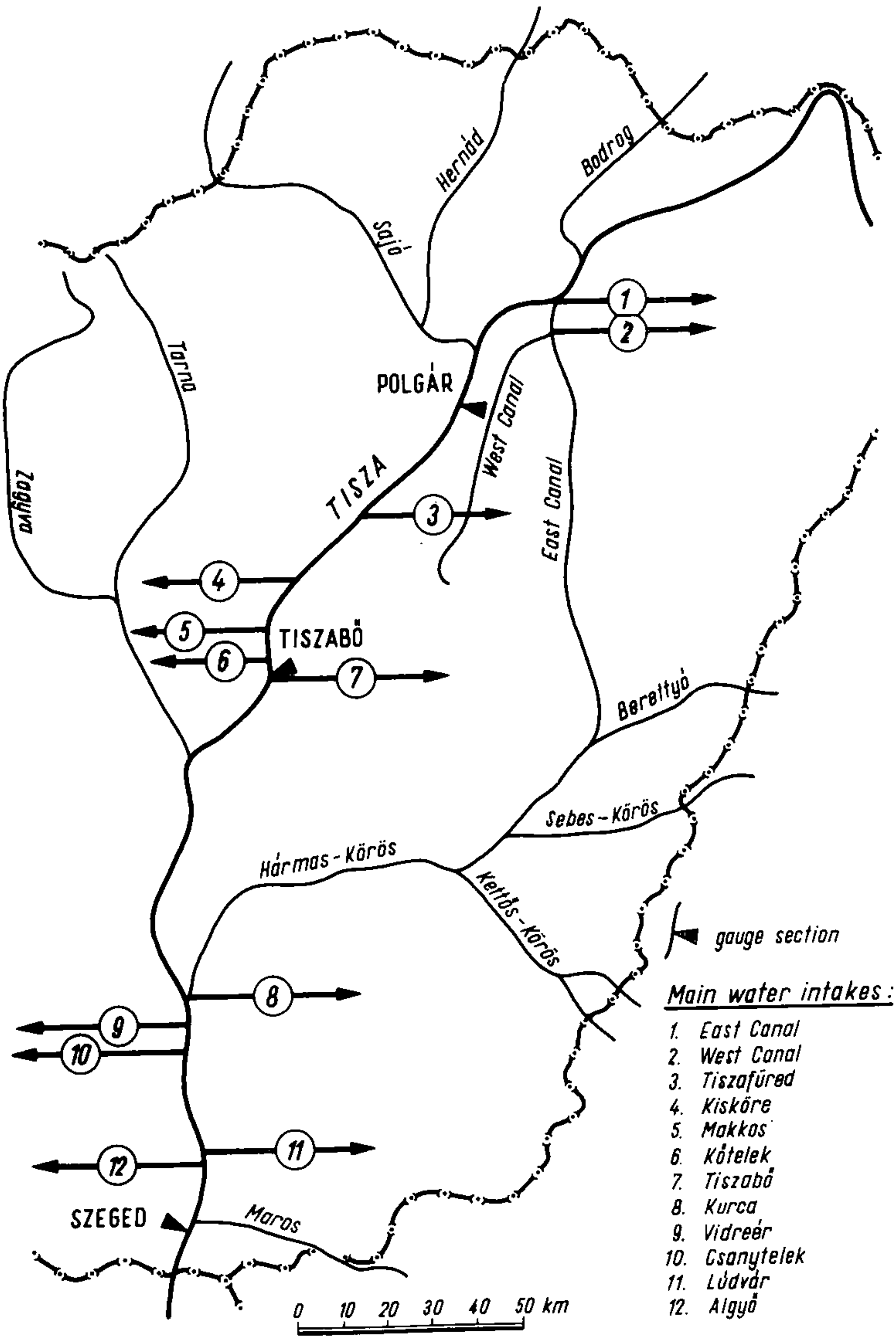


Figure 3. Sketch of the Hungarian part of the Tisza river basin with gauge stations and main water intakes.

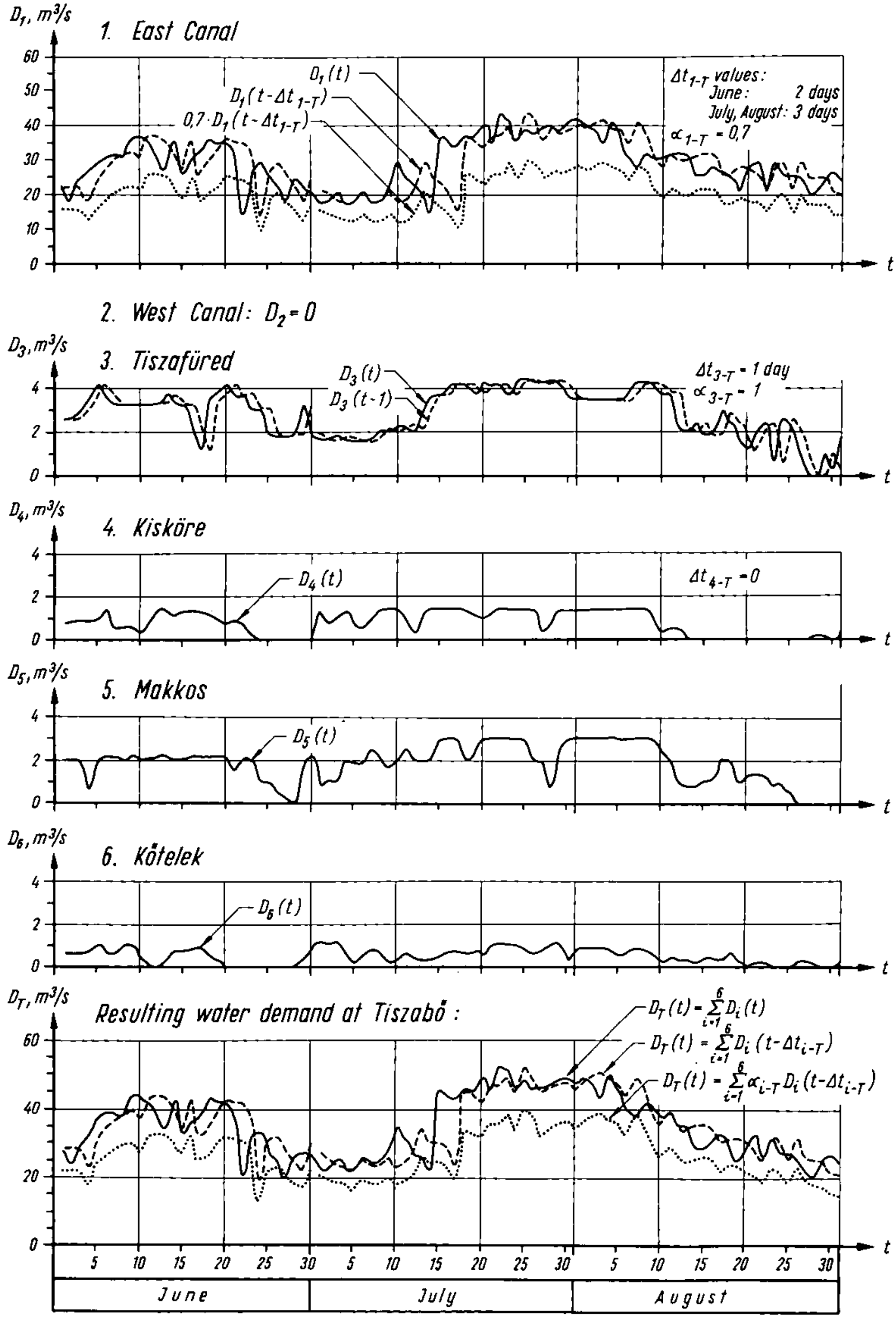


Figure 4. An example of determination of resulting water demand time function (Δt and α values are from Table I.)

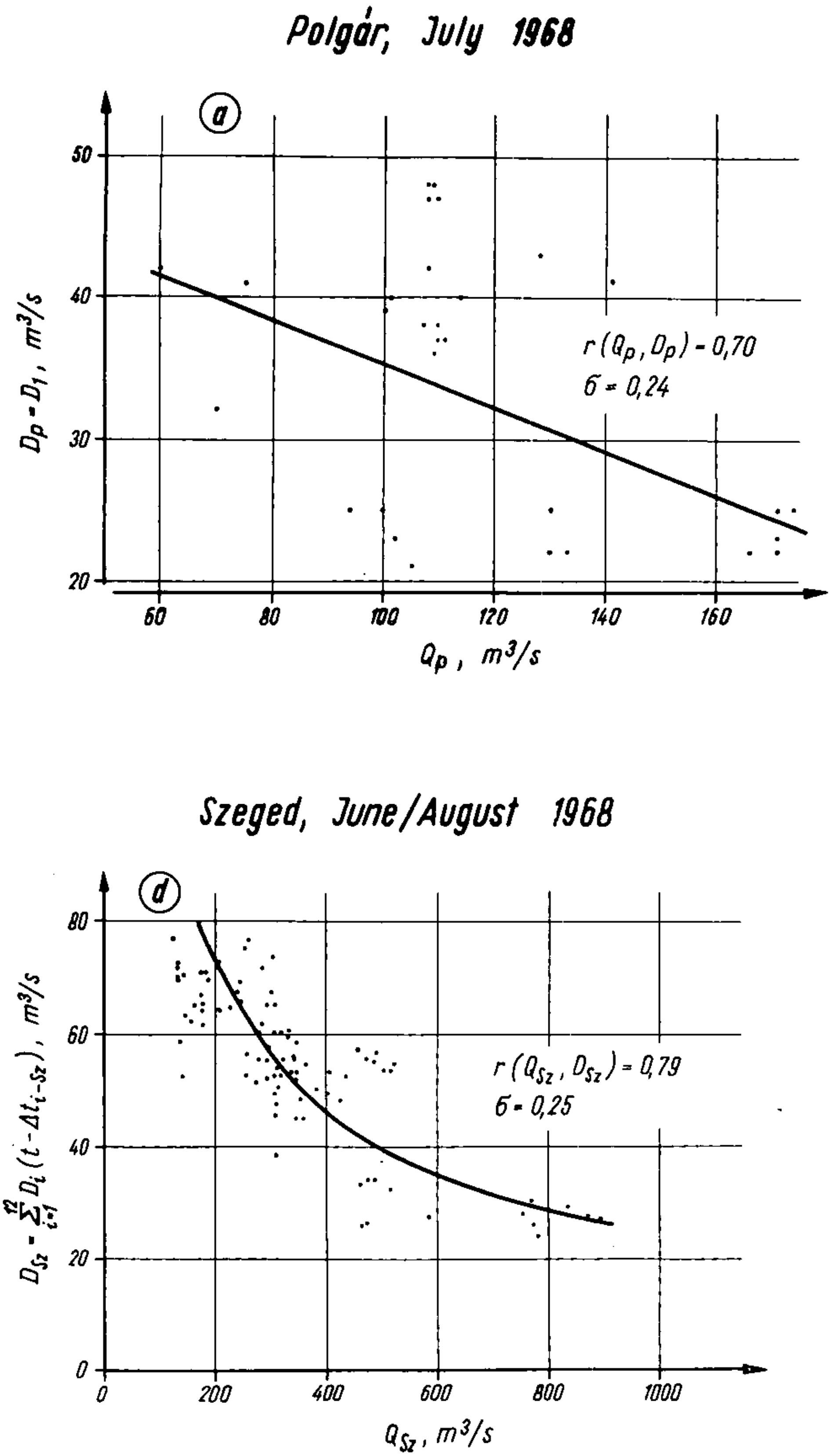
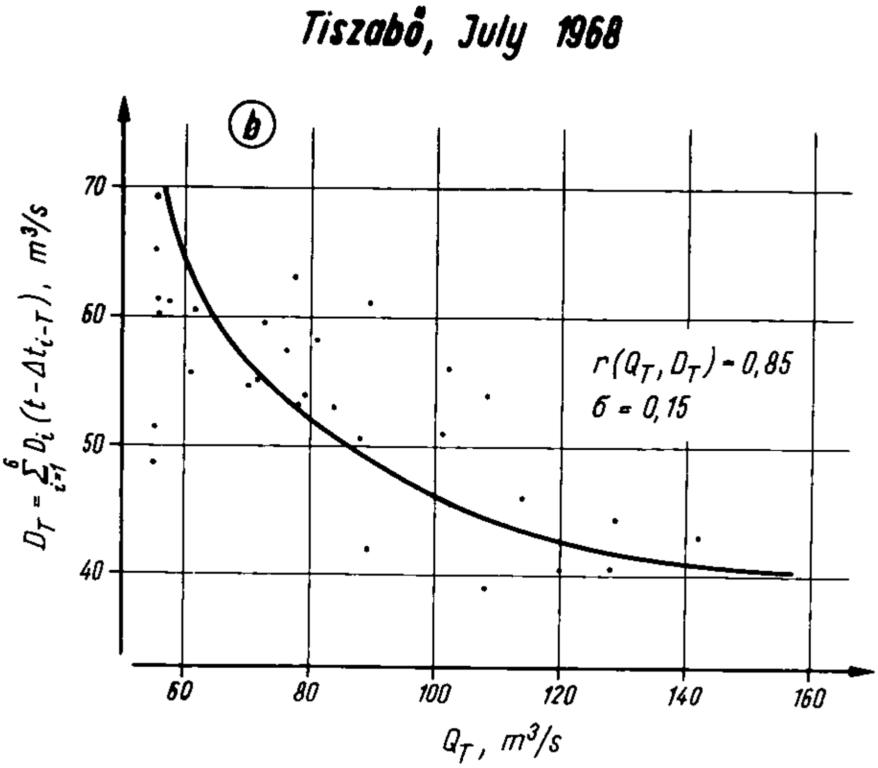


Figure 5. Relationships between irrigation water demands and flow discharges in the Tisza river system.



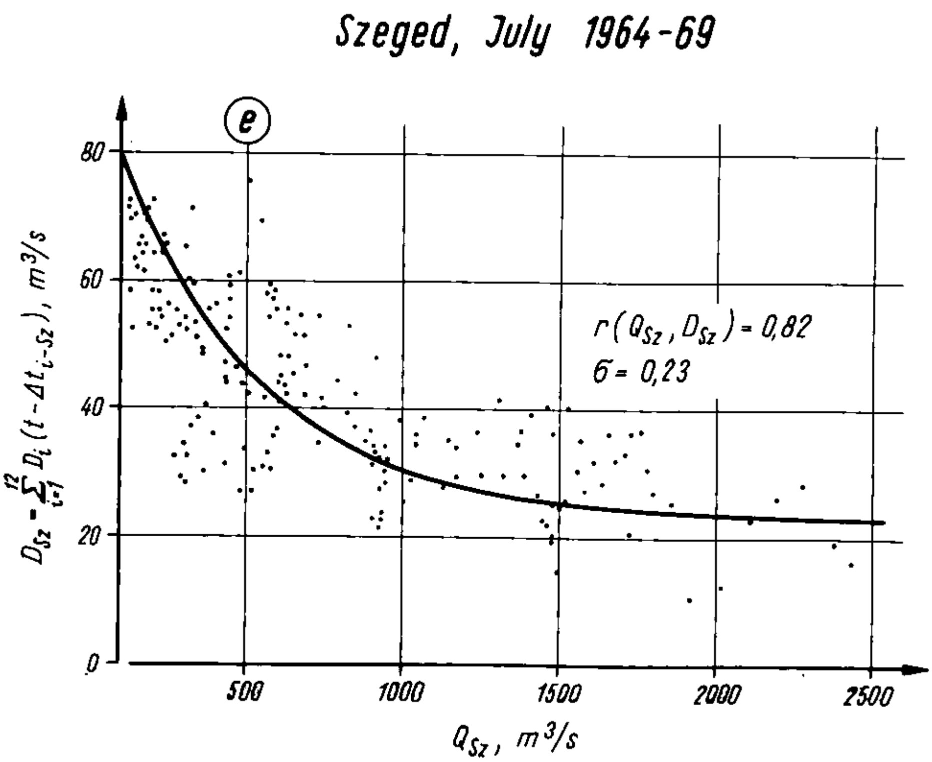
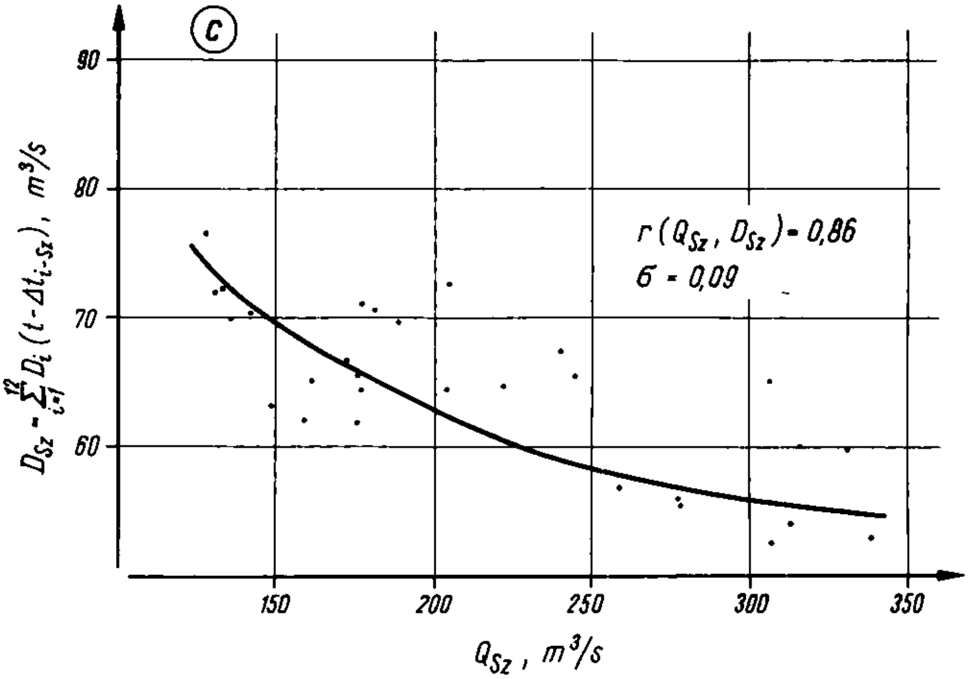


Figure 5--Continued.

Szeged, July 1968



Szeged, June/August 1964-69

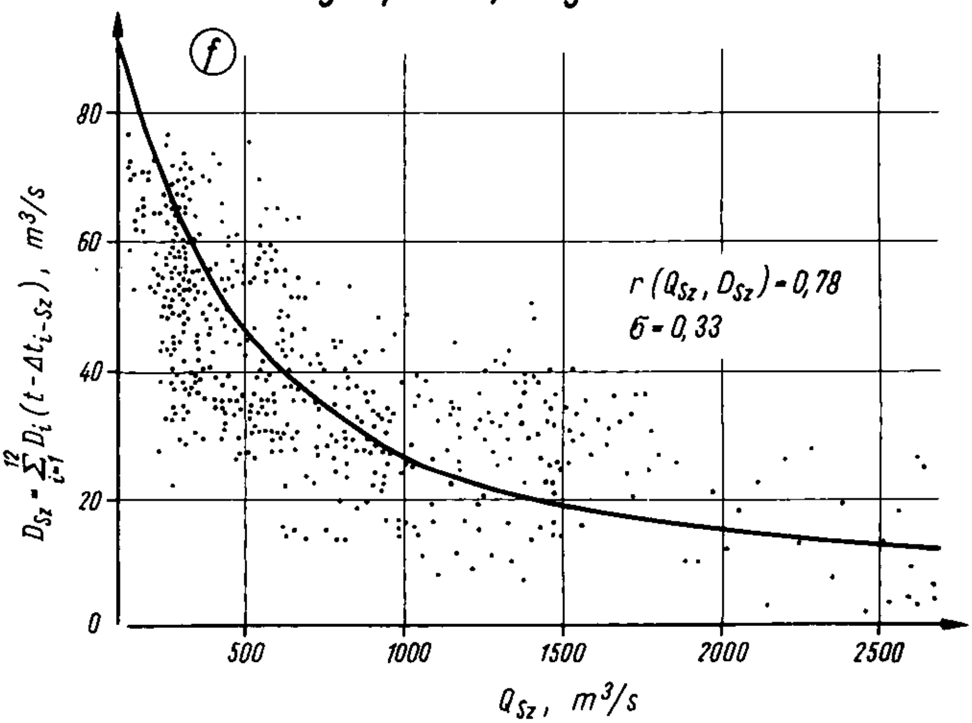


Figure 5--Continued.

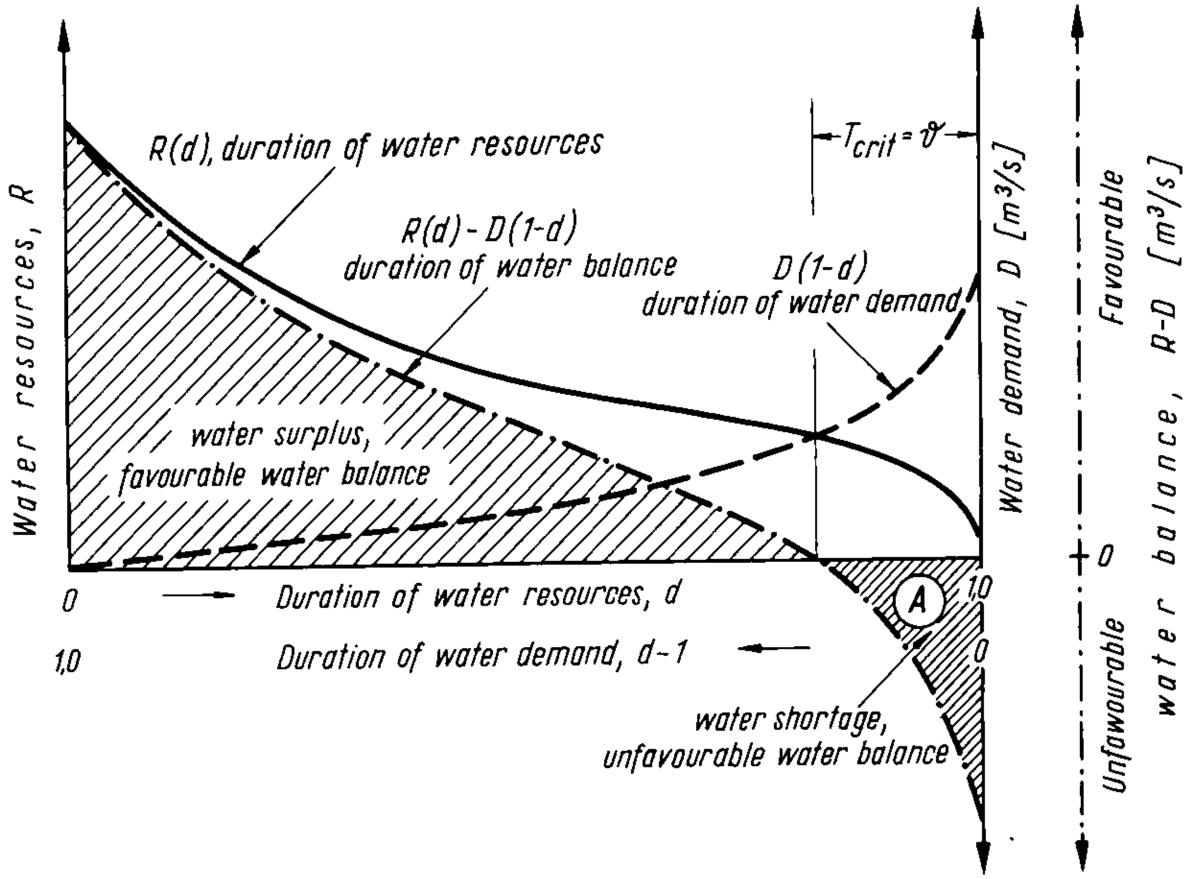


Figure 6. Water balance based on duration curves.

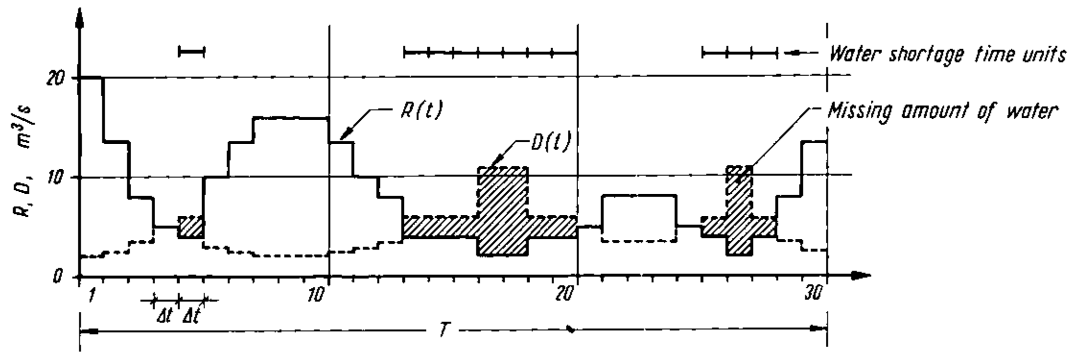
I. STARTING DATA

Serial number of time units:	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
R, water resources, m^3/s	20	13,5	8	5	4	10	13,5	16	16	16	13,5	10	8	4	4
D, water demand, m^3/s	2	2,5	3,5	5	6	3	2,5	2,25	2,25	2,25	2,5	3	3,5	6	6

Serial number of time units:	16	17	18	19	20	21	22	23	24	25	26	27	28	29	s=30
R, water resources, m^3/s	4	2	2	4	4	5	8	8	8	5	4	2	4	8	13,5
D, water demand, m^3/s	6	1	1	6	6	5	3,5	3,5	3,5	5	6	11	6	3,5	2,5

II. CALCULATION OF WATER SHORTAGE INDICES

(A) Directly, from time series:



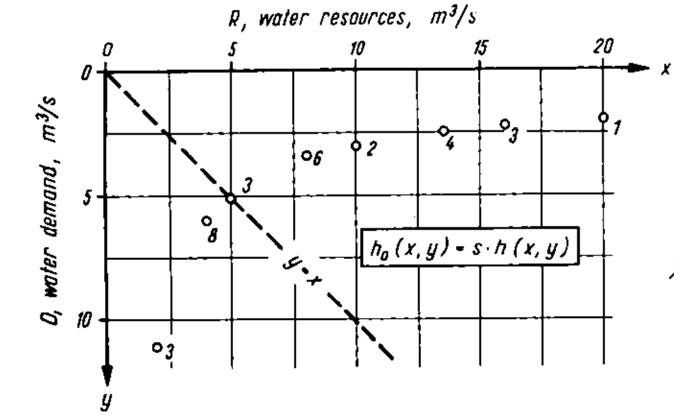
$$\vartheta = \frac{\text{number of water shortage time units}}{\text{number of all time units}} = \frac{11}{30} = 0,37$$

$$\lambda = \frac{\text{missing amount of water}}{\text{required amount of water}} = \frac{\Delta t \cdot [1 \cdot 2 + 3 \cdot 2 + 2 \cdot 9 + 2 \cdot 2 + 1 \cdot 2 + 1 \cdot 9 + 1 \cdot 2]}{\Delta t \cdot [2 + 2,5 + 3,5 + 5 + 6 + 3 + 2,5 + 2,25 + \cdots + 3,5 + 2,5]} = \frac{43}{142} = 0,30$$

$$\lambda_0 = \frac{1}{T} \int_{R(t)<D(t)} \left(1 - \frac{R(t)}{D(t)}\right) dt = \frac{\Delta t \left[11 - \left(\frac{6-4}{6} + 3\,\frac{11-2}{11}\right)\right]}{\Delta t \cdot 30} = \frac{6,88}{30} = 0,23$$

Figure 7. A simplified example of the use of information concerning concomitance of water resources and demands for summarizing water balance.

(B) From joint frequency function:

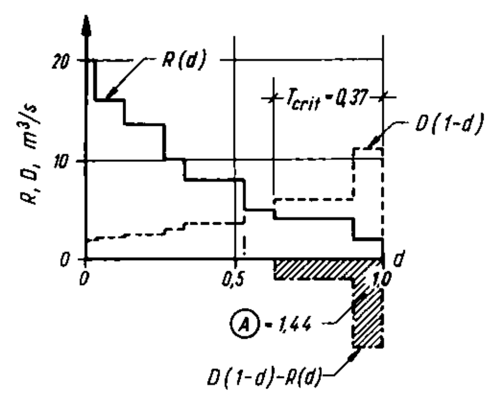


$$\vartheta = \frac{1}{s} \iint_{x<y} h_0(x,y)\,dx\,dy = \frac{1}{30}(3+8) \approx 0{,}37$$

$$\lambda = \frac{\frac{1}{s} \iint_{x<y} (y-x)\, h_0(x,y)\,dx\,dy}{\frac{1}{s} \int_0^{\infty}\!\int_0^{\infty} y\, h_0(x,y)\,dx\,dy} =$$

$$= \frac{(11-2)\cdot 3 + (6-4)\cdot 8}{11\cdot 3 + 8\cdot 3 + 3\cdot 5 + 6\cdot 3{,}5 + \cdots + 1\cdot 2} = \frac{43}{142} = 0{,}30$$

(C) With the help of duration curves:

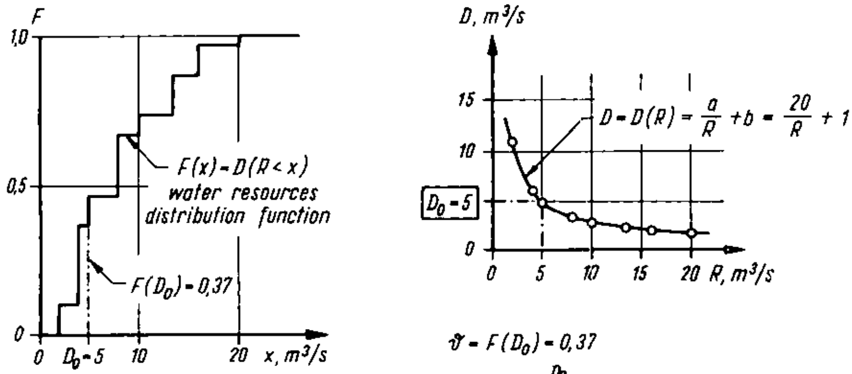


$$\vartheta = T_{crit} = 0{,}37$$

$$\lambda = \frac{(A)}{\int_{d=0}^{1} D(1-d)\,\partial d} = \frac{1{,}44}{4{,}72} = 0{,}30$$

Figure 7--Continued.

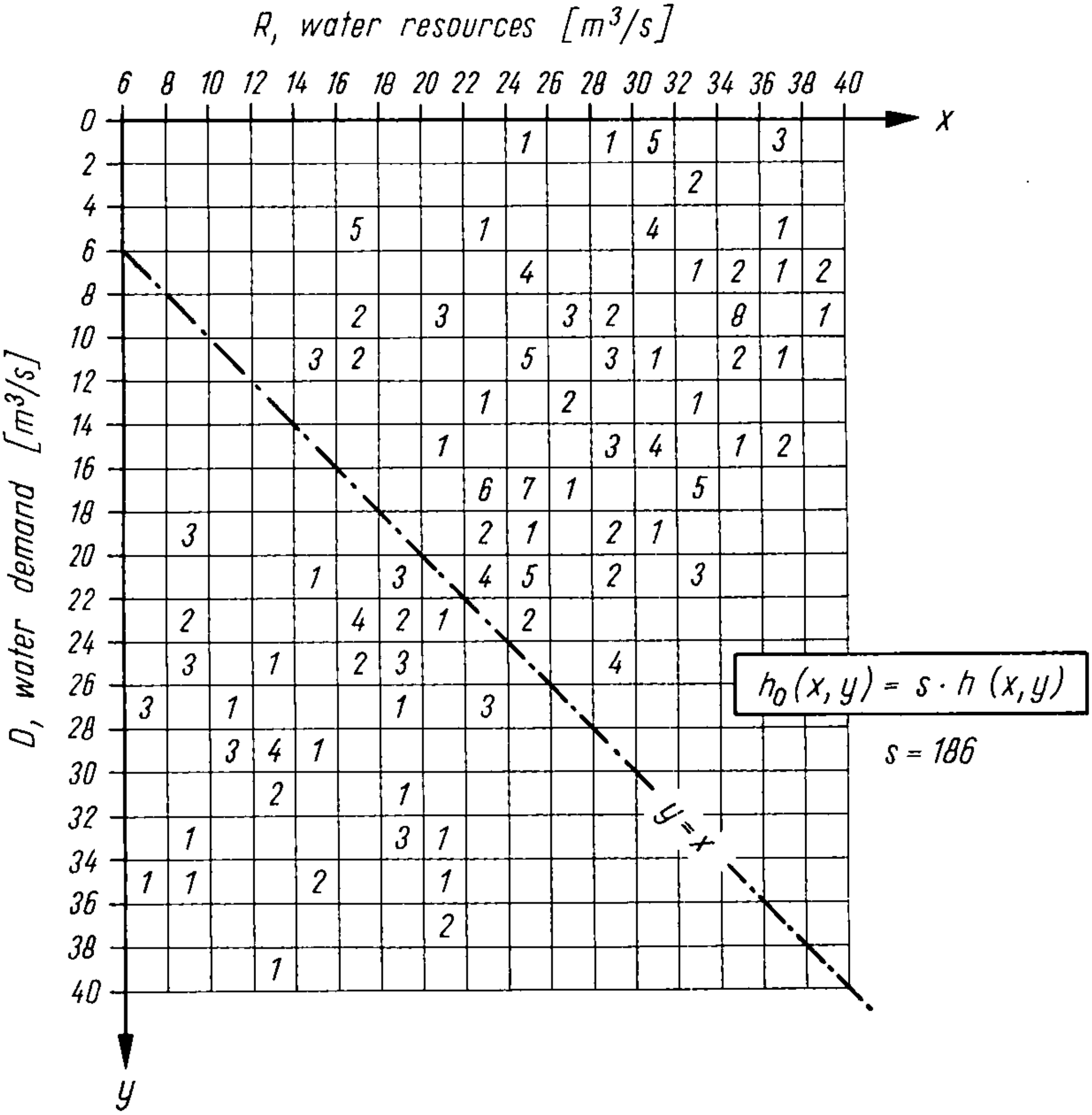
Ⓓ *By using the relation D(R):*



$\vartheta = F(D_0) = 0{,}37$

$\lambda_0 \simeq \frac{2}{a}\int_0^{D_0} x F(x)\,dx = \frac{2}{20}\,[3\cdot 0{,}10\cdot 2 + 4{,}5\cdot 0{,}37\cdot 1] = 0{,}23$

Figure 7--Continued.



$$\vartheta = \frac{1}{s}\iint_{y<x} h_0(x, y)\,dx\,dy = \frac{1}{s}\sum_{x_j<y_k}\sum a_{jk} = \frac{57}{186} = 0{,}306$$

$$\lambda = \frac{\frac{1}{s}\iint_{x<y}(y-x)\,h_0(x, y)\,dx\,dy}{\frac{1}{s}\int_0^\infty\int_0^\infty y\,h_0(x, y)\,dx, dy} = \frac{\frac{1}{s}\sum_{x_j<y_k}\sum a_{jk}(y_k - x_j)}{\frac{1}{s}\sum_j\sum_k a_{jk}\,y_k} = \frac{\frac{1}{s}\,737}{\frac{1}{s}\,3160} = 0{,}233$$

Figure 8. An example of the calculation of water shortage index in the case of stochastic relationship between water resources and demand.

A PHYSICAL APPROACH TO HYDROLOGIC PROBLEMS

by

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INTRODUCTION

My aim in this talk is to review for you the body of work relevant to hydrology which has been carried out in our laboratory. This work covers a time-span of 23 years. The present team includes about ten scientists, and the average complement over the 23-year period has been, perhaps, six or seven. During this time we have published well over 300 papers,* of which at least 200 have implications for hydrology. Obviously I can do no more here than attempt to convey something of the philosophy and the flavor of the work, and to identify in a broad way those lines which seem to me to have been the most important ones.

I must, at the outset, emphasize that our laboratory was not set up to work specifically on hydrology. We began in 1952 as the Agricultural Physics Section of the CSIRO Division of Plant Industry. (CSIRO stands for Commonwealth Scientific and Industrial Research Organization, and is the Australian Government institution for scientific research: the closest thing to it in North America is--or, at least, was--the National Research Council of Canada.) Consistent with the general philosophy of research administration in CSIRO, the terms of reference of our Agricultural Physics Section were quite broad: the application of mathematical and physical approaches and techniques to research problems in agriculture and plant biology. I am convinced that the fruitfulness of our work has depended quite centrally on the freedom we have had within CSIRO.

In the event, much of our early work dealt with problems arising in the context of irrigated agriculture--and this led us straightway into studies of water: water in the soil, water in plants, and water in the lower atmosphere. This early bias has persisted, so that we have contributed pretty well continuously over the years to studies of the movement of water (and other entities) through the soil, through vegetation, and through the lower atmosphere.

In 1971 there were some organizational changes, and our laboratory became an independent Division of CSIRO, the Division of Environmental Mechanics. The range of our concerns has thereby been formally extended from agriculture and plant biology to problems in the (more or less) natural environment as a whole. In fact, the content and character of our work has not really changed very much, since we had, in any case, been working essentially on the physics of transport processes in the natural environment.

WATER MOVEMENT IN UNSATURATED SOIL

The first broad area of our work which I shall discuss is that of water movement in unsaturated soil.

In its natural state the soil is normally unsaturated: that is, it contains both water and air. Most of the water involved in the hydrologic cycle is located in unsaturated soil between the time of its arrival as rain at the

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*The latest publication list (Anonymous, 1975) includes 328 papers and two books. Copies of the publication list and reprints of many of the papers are available on request.

soil surface and that of its return to the atmosphere. A small fraction of the precipitation does not enter the soil, but moves overland directly into streams or lakes; and a second small fraction percolates downward through the unsaturated 'zone of aeration' and joins the groundwater, i.e. the water in the deep, habitually-saturated strata of soil, alluvia, or rocks. In a dry country such as Australia, as much as 93% of the precipitation enters the soil; and, of this, 92% returns directly to the atmosphere, only about 1% reaching the groundwater (Nimmo, 1949; Philip, 1954).

The processes of water movement in unsaturated soil thus play a central part in the scientific study of the terrestrial sector of the hydrologic cycle and in the related problems of irrigated and dry-land agriculture, of plant ecology, and of the biology of soil flora and fauna. They are, in addition, of great significance in connection with the transport through the soil of materials in solution, such as natural salts, fertilizers, and urban and industrial wastes and pollutants. Scientific phenomena of great interest and importance include infiltration (the entry into the soil of water made available at its surface); drainage and retention of water in the soil strata; extraction of soil water by plant roots; and evaporation of water from the soil.

Some of these hydrologic processes, of course, do not involve the soil alone. It will be noted, for example, that the soil, the plant, and the atmosphere form a thermodynamic continuum for water transport, so that the proper study of natural evaporation from the earth's surface involves not only soil physics, but also micrometeorology and, in the case of vegetated surfaces, plant physiology. I shall say something about the soil-plant-atmosphere continuum at a later point.

My immediate theme, however, is the mathematical-physical analysis of water movement in unsaturated soil which has been developed in the last twenty years or so. Until the late 1950's the various phenomena of water movement in unsaturated soil tended to be studied separately and empirically and, it must be said, rather inconclusively. Since then, however, application of what is essentially the methodology of classical mathematical physics has made possible a unified approach: the study of water movement in unsaturated soils is now a reasonably coherent quantitative branch of physical science.

There are two basic ingredients in the now, more-or-less classical, analysis which has emerged.

1. Recognition that the conservative forces governing the equilibrium and movement of soil-water may be treated in terms of their associated scalar potentials. We then have, in appropriate units,

$$\Phi = \Psi(\theta) - z \qquad (1)$$

Here Φ is the total potential and Ψ, the moisture potential, is the potential of the forces arising from local interactions between soil and water: capillarity, adsorption, and electrical double layers may be involved. We do not need to know or to specify these forces in detail. It suffices that the relation between Ψ and θ, the volumetric moisture content, can be measured by well-established soil-physical techniques--so that $\Psi(\theta)$ is essentially an experimentally determinable functional characteristic of any particular soil. z, the gravitational potential, is simply the vertical ordinate, taken positive downward.

2. Recognition that Darcy's law holds for flow in unsaturated soils in a generalized form in which the permeability (hydraulic conductivity) is a function of θ:

$$v = - K(\theta)\nabla\Phi , \tag{2}$$

where v is the vector flow velocity, and K is the hydraulic conductivity. $K(\theta)$ is then a second experimentally determinable functional characteristic of the soil; and, as we shall see, the two functions $\Psi(\theta)$ and $K(\theta)$ constitute a necessary and sufficient characterization of the soil for the purpose of analyzing unsaturated flow phenomena. Typical $\Psi(\theta)$ and $K(\theta)$ functions are shown in Figures 1 and 2.

Combining (1) and (2) and taking the divergence, we obtain the general partial differential equation describing water movement in unsaturated soil:

$$\frac{\partial\theta}{\partial t} = \nabla.(D\nabla\theta) - \frac{dK}{d\theta} . \frac{\partial\theta}{\partial z} . \tag{3}$$

Here the moisture diffusivity $D = Kd\Psi/d\theta$ is a strongly varying function of θ; t denotes time. Figure 3 shows the $D(\theta)$ relation for the soil for which $\Psi(\theta)$ and $K(\theta)$ are given in Figures 1 and 2. It will be seen that $D(\theta)$ varies through some four decades over the θ-range. The second coefficient in equation (3), $dK/d\theta$, varies over several more. This very strong nonlinearity is typical.

It will be understood that the various phenomena mentioned earlier, such as infiltration, correspond to solutions of equation (3) subject to the appropriate initial and boundary conditions; so that (3) enables the integration of a seemingly disparate set of phenomena into one general theoretical structure. This is, of course, unsurprising to physicists, but was something of a novelty to soil scientists. Equation (3) is a nonlinear Fokker-Planck equation. The nonlinearity is very strong and cannot be ignored, so that progress with this work has depended quite centrally on the development of methods of solving (3) in all its nonlinearity. We note in passing that in horizontal systems and in other cases where gravity may be neglected, (3) reduces to

$$\frac{\partial\theta}{\partial t} = \nabla.(D\nabla\theta) , \tag{4}$$

so that we are also concerned with the nonlinear diffusion equation (4).

We have been able to establish a fair body of solutions of (3) and (4) (e.g., Philip, 1969; 1974); and these describe the experimental data fairly well (e.g., Philip, 1957; 1969).

Figure 4 shows a typical solution of the flow equation (3) corresponding to the process of infiltration into our illustrative soil with uniform initial moisture content θ_0 = 0.2376. The saturation moisture content θ_1 = 0.4950. It will be noted that the early stages are characterized by similarity behaviour, with the length scale of the wetting profile proportional to $t^{1/2}$. There is then a gradual transition until, for large t, a wetting front of essentially constant shape advances into the soil at constant velocity.

The present brief account necessarily passes over many complications and generalizations of this field of work: these include capillary hysteresis, the effects of entrapped air, water transport in the vapor phase, and temperature effects. Extensions to the work which are being actively pursued in our laboratory at present include the generalization to soils subject to volume change (e.g. Philip, 1973) and study of the hydrodynamic stability of flows in unsaturated soil (Philip, 1975a,b).

TRANSPORT OF WATER AND ENERGY IN THE LOWER ATMOSPHERE

Let me now say a little about our work on the transport of water and energy in the lower atmosphere.

The evaporation of water involves not only processes of transport of liquid water to, and of water vapor from, the evaporation site, but also the supply of energy (latent heat) needed for the phase change. A proper consideration of water transfer in the lower atmosphere therefore requires that we take cognizance not only of the transfer processes for water, but also for energy.

We have, in this connection, done a fair amount of work on the turbulent transport of water vapor and of heat in the lower atmosphere. When conditions are believed to be essentially constant in the horizontal, the problem may be taken to be one-dimensional and is relatively straight-forward, at least in the airlayers above any vegetation.

In the real world, however, conditions do not stay conveniently uniform in the horizontal. Some of the most obvious non-uniformities are due to man's intervention in the hydrological cycle, such as the development of an irrigation area, or the storage of water in a reservoir, in an arid region. In such circumstances we desire to know the answers to questions such as how evaporation (or evapotranspiration) and the microclimate vary as we move downwind of a change in surface conditions.

We have studied these questions both theoretically and experimentally. The theory is based on setting up simultaneous equations for the turbulent diffusion of water vapor and heat in the lower atmosphere and solving them subject to appropriate boundary conditions, including the energy balance at the ground surface. We have found that theory is at least adequate to predict the order of magnitude of the observed effects (Philip, 1959; Rider, Philip, and Bradley, 1963).

There are other problems connected with the transport of water vapor and other entities in the lowest part of the atmosphere: one is that of transport in the air layers within vegetation. In such regions the air flows and the patterns of turbulence are very complicated and all the surfaces of vegetation act quite differently as sources (or sinks) of the various entities of interest, such as momentum, sensible heat, and water vapor. Some progress has, however, been made with untangling these matters (e.g. Denmead, 1964;

Philip, 1964) so that progress is being made with the processes of vegetation-atmosphere interactions.

WATER TRANSPORT IN THE SOIL-PLANT-ATMOSPHERE CONTINUUM

Finally, a word about the matter of the whole continuum of the soil, vegetation, and the lower atmosphere as a vehicle for the transport of water. The system is clearly very complicated, and it might seem to be a hopeless undertaking to attempt to analyse the process in any detail.

Fortunately, thermodynamics provides a basis for treating the processes in these various regions in a unified way.

The energy state of water in the soil, the plant, and the atmosphere are all expressible in terms of a thermodynamic potential (in fact the partial volumetric Gibbs free energy) and it can be shown that water moves in all parts of the complicated soil-plant-atmosphere system down the gradient of this potential (Philip 1957d, 1966).

Water is taken up by the plant roots, and is transferred through the root tissues to the conducting vessels of the plant, and in these vessels to the mesophyll tissues of the leaves; it moves through these tissues to the evaporation sites, which are primarily the walls of the substomatal cavities. The final transfer of water from the substomatal cavities through the stomata of the leaves is a process of molecular diffusion of water vapor.

Schematically (Figure 5) one can look on the passage of water through the system as a flow through a sequence of resistances in series down a gradient of Φ. This concept gives a useful first picture, but it must be emphasized that for real plants the three-dimensional disposition of roots, leaves, and other plant parts makes for a more complicated hydraulic problem.

There is a whole body of work going on, involving soil physicists, micrometeorologists, and plant physiologists, devoted to improving methods of measuring the energy state of water in various parts of the soil-plant-atmosphere continuum and to measuring the rates of transfer of water through various parts of the system. Models of the soil-plant-atmosphere are becoming, in consequence, more accurate, more convincing and, one hopes, more useful.

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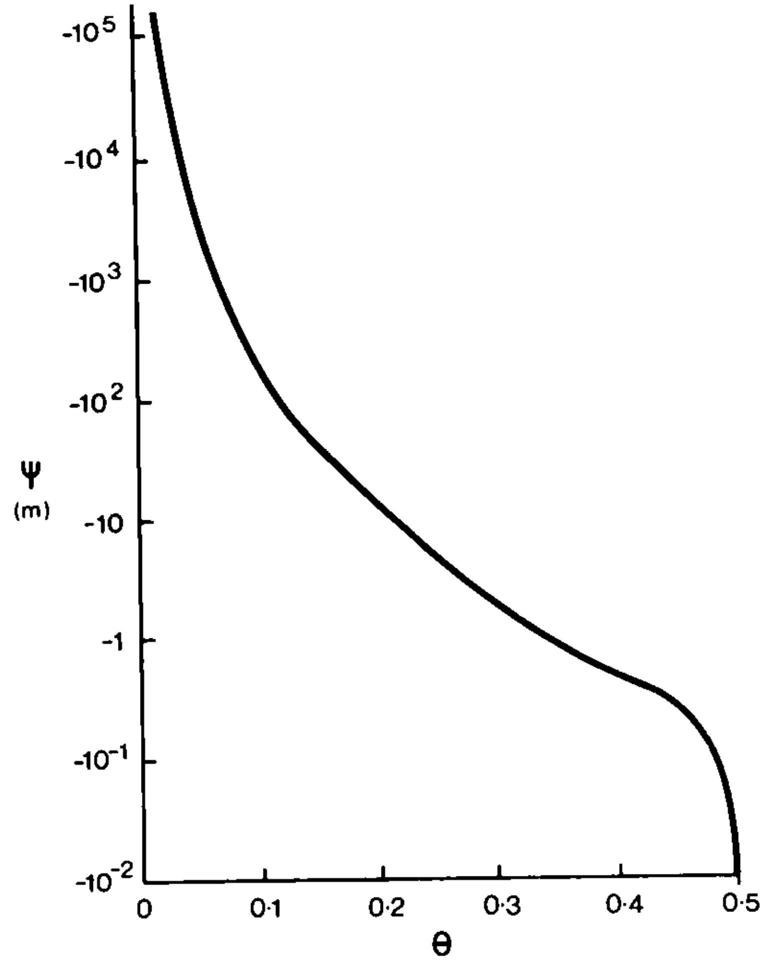

Figure 1. Dependence of moisture potential, Ψ, on moisture content, θ, for Yolo light clay (Moore, 1939).

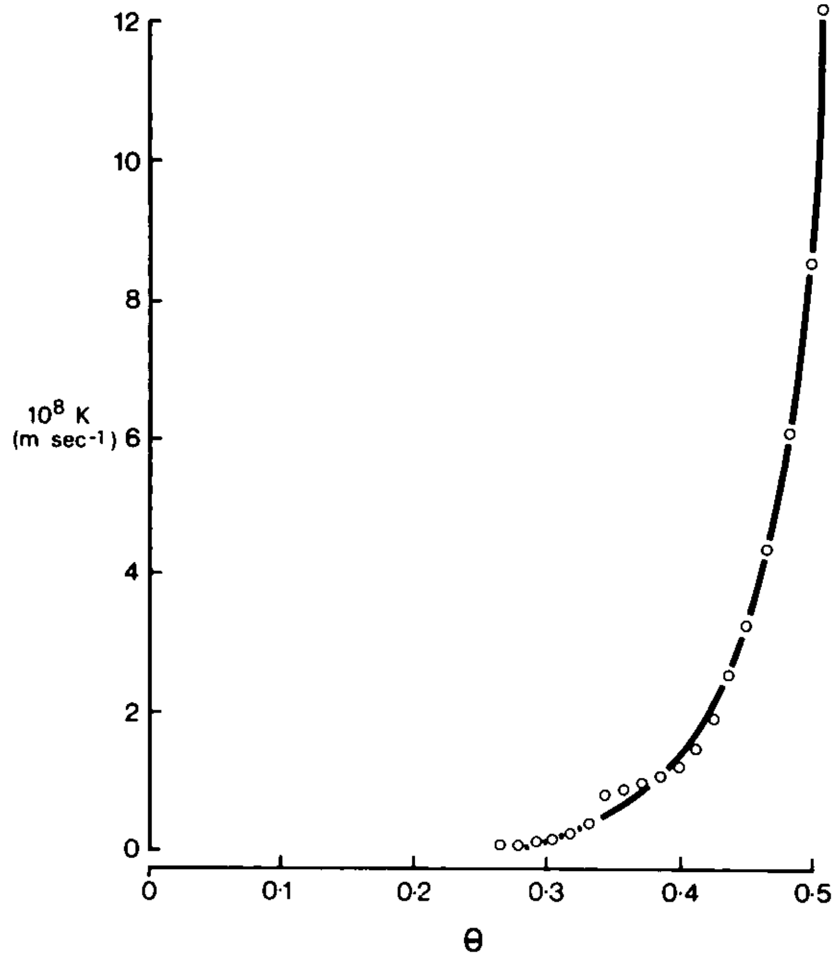

Figure 2. Dependence of hydraulic conductivity, K, on moisture content, θ, for Yolo light clay (Moore, 1939).

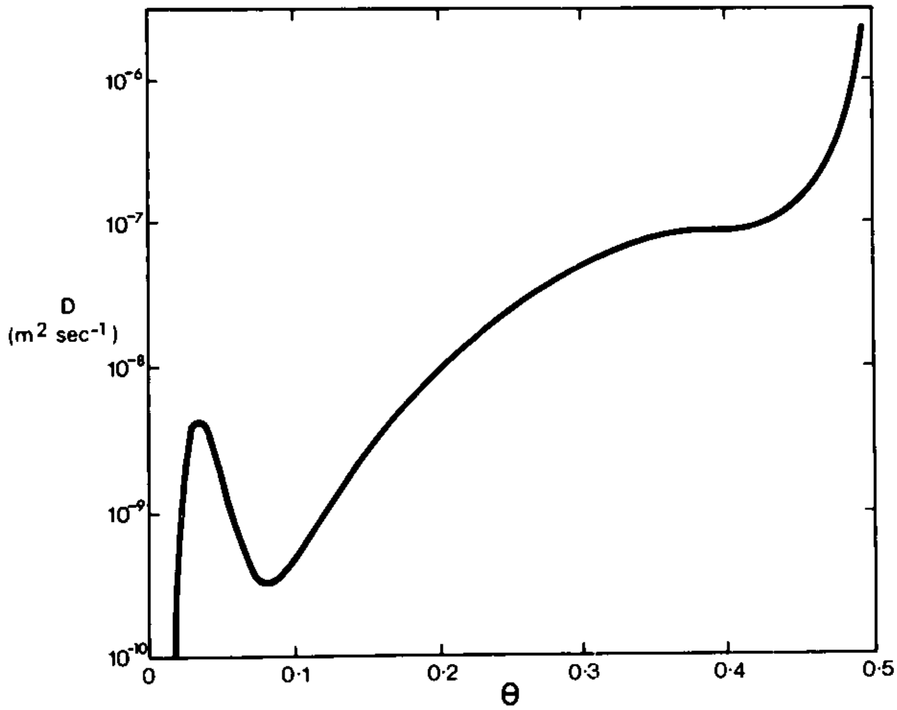

Figure 3. Relation between moisture diffusivity, D, and moisture content, θ, for Yolo light clay (Philip, 1955). For $\theta \leqslant 0.06$, D includes dominant contribution in vapor phase.

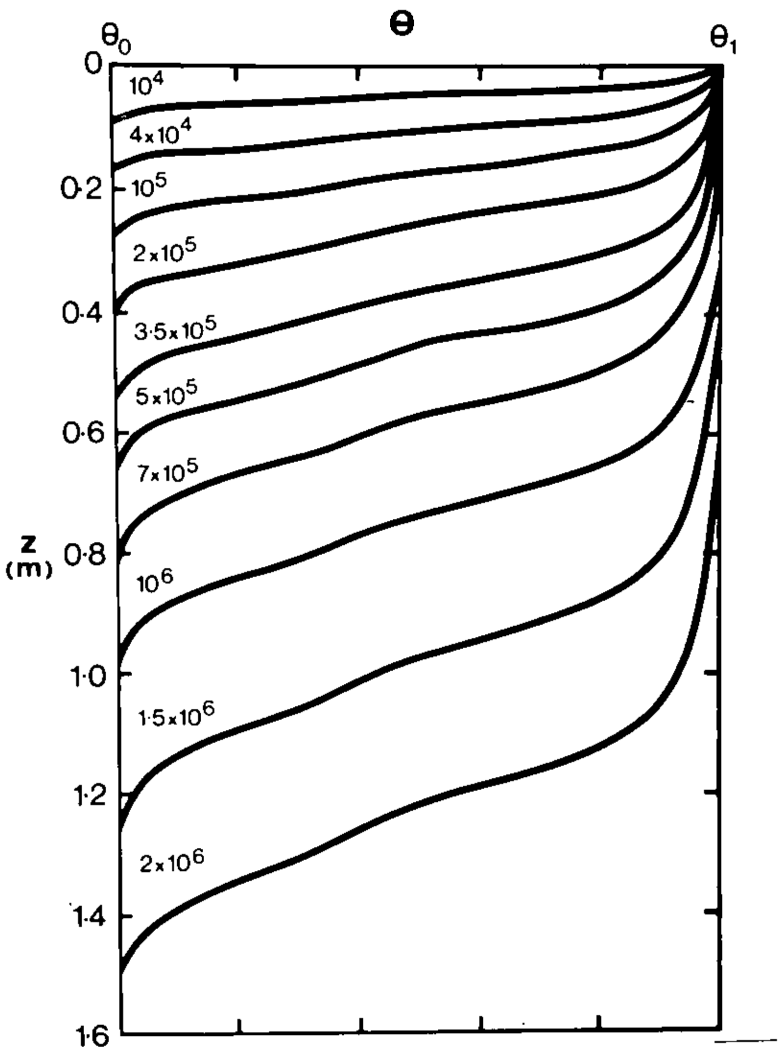

Figure 4. Computed moisture profiles for one-dimensional infiltration in Yolo light clay (Philip, 1954; 1957a,b). Numerals on each profile represent value of t (sec) at which profile is realized.

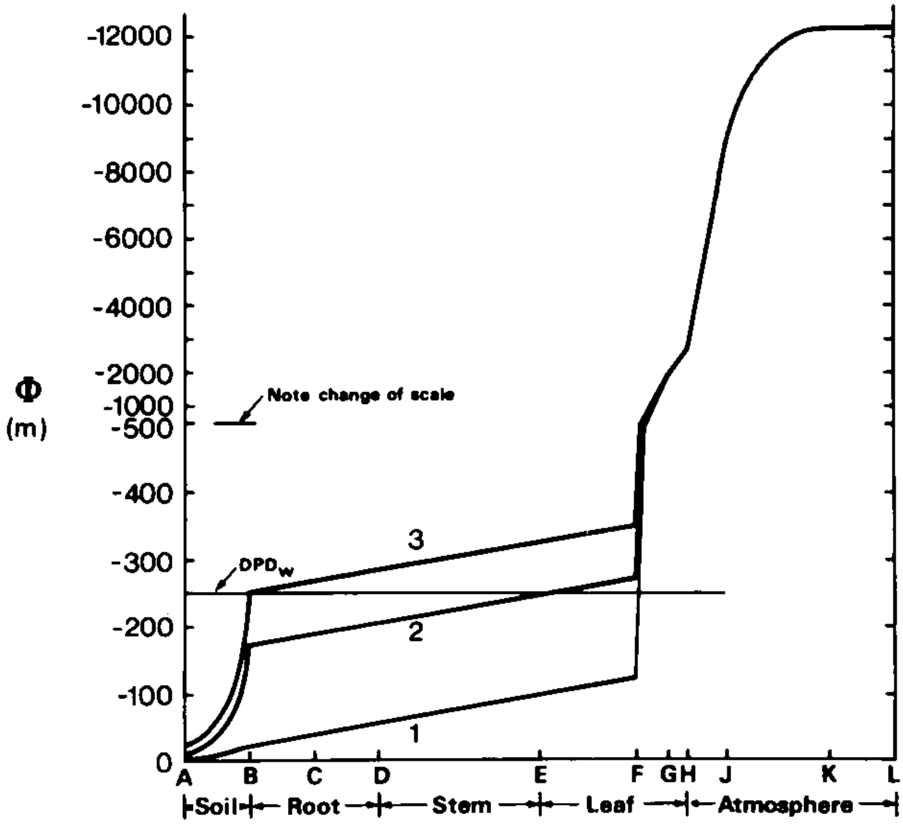

Figure 5. The soil-plant-atmosphere continuum showing profiles of total potential Φ: (1) during normal transpiration; (2) during temporary wilting; (3) at permanent wilting. Points of the transpiration path: A, soil (a definite distance from plant root); B, surface of root hairs and of absorbing epidermal cells; C, cortex; D, endodermis; DE, vessels and tracheids in xylem; E, leaf veins; F, mesophyll cells; FG, intercellular space and substomatal cavity; GH, stomatal pore; HJ, laminar sublayer if present; JK, turbulent boundary layer; KL, free atmosphere; DPD_W denotes Φ-value at incipient plasmolysis of root cells (after Philip, 1957d).

FACTOR ANALYSIS OF WATER QUALITY DATA IN NEW JERSEY:

EVALUATION OF ALTERNATIVE ROTATIONS

by

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ABSTRACT

A set of water quality data from the Passaic River Basin in New Jersey was factor analyzed. The data consisted of thirteen variables collected at semi-monthly to monthly intervals over a twenty-year period (1950-69). Using an eigenvalue cutoff of unity, varimax rotation resulted in three characteristic factors: 1) a flow-chemical factor (high loadings on discharge, pH, alkalinity, and chlorides); 2) an oxygen factor (high loadings on DO, saturation, and occasionally temperature); and 3) an appearance factor based on color and turbidity. To see if alternative rotations would affect factor structure, the same sets of data were factor analyzed using another type of orthogonal rotation (quartimax) and four types of oblique rotation (covarimin, biquartimin, quartimin, and direct quartimin). The results indicate that alternative rotations had only a minimal effect on factor structure output. The low to moderate factor correlation coefficients on most of the oblique rotations suggest that the initial choice of the varimax orthogonal solution was reasonable.

INTRODUCTION

Factor analysis is one form of multivariate analysis wherein a set of intercorrelated variables are collapsed to form a smaller number of composite variables, or factors (13, 17). These factors may then be rotated to yield a set of independent, uncorrelated factors. Thus, factor analysis may assist in the interpretation of variable relationships.

Although the application of factor analysis to problems in the social and behavioral sciences is far more extensive than in the field of hydrology, a fair-sized literature exists. For example, Wallis (19) used factor analysis in a study of the agents that contribute to soil erosion and stream sedimentation in northern California. Dawdy and Feth (4) applied factor analysis to results of chemical analyses of ground water samples from the Mohave River Valley in California. Matalas and Reiher (15) felt that factor analysis was technically underdeveloped, a view seconded by Wallis (20) who also felt, however, that the technique was a powerful tool for screening variables. Rice (16) suggested varimax rotation as an aid in rationally interpreting factors resulting from a study of hydrologic relationships. Eiselstein (7) used a principal component regression analysis with varimax rotation of the factor weight matrix as a means of synthesizing flow records for small ungaged watersheds. Annual precipitation and runoff data from fourteen watersheds in Ohio and seven watersheds in Texas were subjected to principal component and factor analysis by Diaz, Sewell, and Shelton (5) in an attempt to identify the factors affecting the water yield of the basins. Knisel (14) used factor analysis on thirteen variables for five reservoirs in Texas to determine which variables were significant for estimating reservoir losses on the fissured limestone terrain. Morphometric data consisting of five parameters from five landscapes in eastern Australia were factor analyzed by Abrahams (1) in an attempt to associate departures from topological randomness with the evolutionary decline of relief. Jackson (12) used factor analysis to study the relationship between variations in shoreline physiography and water level fluctuation as perceived by reservoir recreation users.

The first purpose of this paper is to examine the temporal changes in water quality in the Passaic River Basin in New Jersey during 1950-69, using factor analysis as a tool to extract the major sets of information from the data. The period in question included a major period of suburbanization and, in turn, a major impact on watershed quality, and periodic events such as the record drought of 1962-66. It was hoped that the relative effects of these trends and events could be isolated by factor analysis.

A second purpose is to test the impact of alternative factor analytic rotations on the information that is extracted from the raw data. The goal is to see the effect of varying rotations on the factor structure output.

METHODOLOGY

The factor analyses discussed in this paper were calculated with a number of conservative assumptions regarding the degree of information covariance. First, the communality was estimated by using the square of the multiple correlation coefficient (R^2) between each variable and all other variables in the data set. These communalities would appear along the principal diagonal of the correlation matrix. Alternative estimates of the communality could have been chosen; for example, ones could be inserted in the principal diagonal. This procedure then assumes that all of the variance of each variable is related to the common factors of the data set. The true communality presumably lies between the R^2 and unity estimates; thus, the R^2 estimate is probably more realistic.

The BMDO8M factor analysis program (6) extracts a set of factors by the principal components method. In order to increase the interpretability of the resulting factor loading patterns, the unrotated factor loadings are rotated. The first rotation used was the varimax solution, which involves a series of orthogonal transformations of factor pairs. The varimax orthogonal routine is the most commonly used form of rotation.

Another type of orthogonal rotation is the quartimax solution. However, it is less commonly used, inasmuch as it tends to load more variance on the first factor.[1]

The second conservative assumption followed was that rotations were to be performed on factors only if the eigenvalues exceeded unity. In almost all cases, this arbitrary rule ensured that all factors accounted for at least as much as one of the original variables. In order to maintain uniformity among factor structures on some data sets, a few analyses were repeated with a stipulated number of factors to be rotated.

At this point, a methodological question arises: to what extent are we producing an artifactual bias in our output by forcing the data to yield a set of independent, uncorrelated factors? Perhaps data from the real world are inextricably interrelated, especially as the size of the observation unit decreases. Two recent studies by Hughes and Carey (10) and Greenberg and

[1]See Rummel (Ref. 17, footnote 1, pp. 390-91) for a fuller discussion of this point.

Hughes (8) discuss the validity of the orthogonal model and the resulting possibility of biased output.

To help resolve this matter, a variety of oblique rotations can be performed. In addition to the usual output of factor loadings and scores, oblique rotation yields a set of factor correlations which can indicate the degree of departure from orthogonality and zero correlation. The oblique rotations used in this study include the direct quartimin (utilizes a structure matrix), the quartimin (favors high factor correlations), the covarimin (favors low factor correlations), and the biquartimin (compromises between the biases of the quartimin and covarimin).

APPLICATION OF FACTOR ANALYSIS TO WATER QUALITY DATA PASSAIC RIVER BASIN, NEW JERSEY

The data consist of thirteen water quality variables collected at semimonthly to monthly intervals over a twenty-year period from 1950 to 1969 (see Table 1). The sampling site on the main stem of the Passaic River in New Jersey just above the confluence with the Pompton River is part of a network of surveillance stations maintained by the Passaic River Water Commission at its own expense. Previous investigation by Carey, et al (3) had indicated that some of the best water quality information in New Jersey was routinely collected by large water supply agencies.

The nearly 5,000 pieces of information were grouped into six time periods (1950-53, 1954-56, 1957-59, 1960-63, 1964-66, and 1967-69) so as to maintain a favorable ratio of cases to variables.[2] Fortunately, the groupings tended to coincide with periods of above-normal, normal and below-normal precipitation totals for northern New Jersey as discussed by Anderson and Faust (2). This situation is desirable, as precipitation obviously influences discharge which is a very important variable in water quality studies. Thus, a certain degree of homogeneity within each time period was imparted to the study.

ORTHOGONAL ROTATION

The conservative eigenvalue cutoff of unity resulted in three factors being rotated for five of the six time periods; the remaining 1957-59 period was rerun so as to yield three factors. Ranked in order of importance, the three characteristic factors resulting from varimax rotation were as follows: 1) a flow-chemical factor exemplified by high loadings on discharge, pH, alkalinity, and chlorides; 2) an oxygen factor (high loadings on DO, saturation, and occasionally temperature); and 3) an appearance factor based on color and turbidity.

Somewhat similar results were obtained from the quartimax rotation, but the structures were not as clear since the solution favors high loadings on the first factor. In Table 2, which shows the rotated orthogonal factor

[2] A rough rule of thumb in factor analysis is that the ratio of the number of cases to variables should be at least 2:1. In this study, the ratio ranged from 2.8:1 to 5.5:1.

loadings for a sample time period, note how the first factor for the quartimax solution accounts for 41.6 percent of the total variance, as compared to 30.0 percent for the varimax solution. Also, although temperature in the varimax solution is shown to have a high inverse loading with DO and saturation, the relationship is not clear during the other time periods (Table 2). In particular, the temperature-DO relationship broke down during the 1950's, as indicated by the two variables not loading highly together in the same factor. The relationship improved during the three time periods of the 1960's.

The cumulative percentage of total variance explained (which does not change with the type of rotation) ranged from 57 percent in 1950-53 to 71 percent in 1967-69, averaging 65 percent for the two decades. Surprisingly, the degree of explanation offered by the factor analytic model was quite stable during the study period, even rising during 1967-69. This stands in sharp contrast to similar studies on the Raritan River in New Jersey, wherein the explanation decreased noticeably during the 1960's (9).

The interbasin differences can be attributed to several factors. First, the data set for the Raritan consisted of nine water quality variables as compared to the thirteen available for the Passaic. Second, since the Raritan data was collected (by the Elizabethtown Water Co., another large water supply agency) at weekly intervals, the information could be grouped into an annual series. Thus, the particular assemblage of variables and the different groupings of time periods could explain part of the interbasin variations in behavior. At any rate, the factor analytic model appears to detect changes in instream interactions among the variables over time. Perhaps the secular increase or decrease in the cumulative degree of explanation can be attributed to perturbations of the steady state caused by land use changes within the basin and varying effluent loading patterns. At this point, it is unclear why the explanation should be increasing for the Passaic basin while the Raritan basin experiences a decline, since both data sets are internally consistent (i.e., the variables within each set are the same from time period to time period).

OBLIQUE ROTATION

As previously mentioned, oblique rotation yields a set of correlation coefficients among the factors. Different factor correlations are obtained for each of the time periods for each of the four types of oblique rotations (Table 3). As expected, the factor correlations varied from the covarimin set of low coefficients (averaging .08) to the quartimin set of high coefficients (averaging .40), with the biquartimin ranging in between (.13). The direct quartimin coefficients (.15) were similar to those of the biquartimin. If we accept the last type of oblique rotation as a compromise solution, we can then conclude that most factor correlations are below .25; thus, the orthogonal solution should not be very different from several of the oblique solutions.

This assumption of similar factor structures is borne out by examining the output from the oblique rotations. Three characteristic factors emerge from all rotations (flow-chemical, oxygen, and appearance), albeit with slightly different factor loadings (Tables 4 and 5 show the output for a sample time period). The quartimin rotation presents special problems, inasmuch as the rotated factor loadings may exceed unity. Indeed, during 1964-66 when factor correlations averaged .98 (see Table 3), several factor loadings on the quartimin exceeded 5.0. Obviously, interpretation of the loadings under these circumstances becomes quite difficult. Note that 1964-66 marked a drought period of unprecedented severity.

DISCUSSION

The results of this study suggest that the use of alternative rotations on the water quality data from a downstream station on the Passaic River does not unduly affect factor structure interpretation. Perhaps this result is not unexpected, inasmuch as factor correlations were generally moderate. Thus, the assumption of orthogonality in the factor model is reasonable in this instance.

Of all the rotations, the varimax orthogonal rotation is probably the most desirable one to use for the following reasons:

1) The orthogonal solution yields a set of uncorrelated factor scores which can be later used as independent variables in a multiple regression problem.

2) Factor structures can be quantitatively compared by using a computer program called RELATE as long as the data are rotated orthogonally. As discussed by Veldman (18), the program accepts as input the factor loading matrices that were obtained from an orthogonal factor analysis of identical sets of variables. The factor axes are then rotated until maximum overlap between corresponding test vectors in the two structures is attained. The degree of rotation required is expressed as the cosine of the angle between the factor axes. These cosines may be interpreted as correlations between the factor variables, thereby facilitating quantitative factor structure comparisons.

3) The percent of total variance explained by each rotated factor is available with orthogonal rotation, whereas only the sum of squares for each factor can be provided with oblique rotation. Thus, the orthogonal solution allows one to rank more accurately the rotated factors in terms of statistical explanation and importance.

Given the advantages of the varimax rotation, one would prefer not to use the other types of rotation. However, the interpretation of the factor structure output may be biased unless the extent of departure from orthogonality is assessed. Therefore, the following procedures are recommended for the analysis of new sets of data.

First, use the biquartimin rotation as a compromise between the high and low factor correlation biases of the quartimin and covarimin to test for covariance among the factors. The quartimin should be avoided because it may yield factor loadings greatly exceeding unity. The output from this study suggests that the direct quartimin should give results similar to those of the biquartimin and is therefore redundant.

Second, if the factor correlations from the biquartimin or direct quartimin are .25 or less, the factors may be considered operationally independent and the orthogonal solution may be used. In that case, it is preferable to use the varimax rotation, since the quartimax orthogonal solution loads most of the variance on the first factor, an undesirable trait with respect to clarity of interpretation.

The procedures described above appear to be in accord with the views of Hunter (11), who suggests that only method-independent factors be treated as important substantive findings. A method-independent factor is defined as a factor which has similar loading patterns in both the orthogonal and oblique rotations.

CONCLUSIONS

A set of water quality data from the Passaic River Basin of New Jersey was factor analyzed and then subjected to six different types of rotation. The data set consisted of thirteen variables collected at semi-monthly to monthly intervals from 1950 through 1969. The twenty years of record were divided into six time periods of three to four years each.

Although there was some variation, the two types of orthogonal rotation (varimax and quartimax) and the four types of oblique rotation (covarimin, biquartimin, quartimin, and direct quartimin) yielded similar factor structures for each of the time periods. Using an eigenvalue cutoff of unity for rotation, three characteristic factors emerged: 1) a flow-chemical factor (high loadings on discharge, pH, alkalinity, and chlorides); 2) an oxygen factor (high loadings on DO, saturation, and occasionally temperature); and 3) appearance factor based on color and turbidity.

The output from the oblique rotations includes a set of factor correlations which dimension the degree of factor independence. The covarimin and quartimin rotations are biased towards low and high factor correlations, respectively, whereas the biquartimin and direct quartimin represent compromise solutions. The factor correlations for the biquartimin and direct quartimin average .14 in this study. Thus, the assumption of orthogonality in the factor analytic model is reasonable and the varimax orthogonal solution, which has many advantages, may be employed with greater confidence. These findings are important because the orthogonality of the factors supports the contention that some water quality parameters may be modeled independently of the effects of others, while other indicators of water quality may be used as surrogates for a larger set of interdependent indicators.

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TABLE 1. PVWC - WATER QUALITY SAMPLING VARIABLES.[a]

1. Stream Discharge
2. Temperature, Water
3. Turbidity
4. Color
5. pH

6. Alkalinity
7. CO_2, Free
8. Chlorides
9. DO - Dissolved Oxygen
10. Saturation, Percent

11. BOD - Biochemical Oxygen Demand
12. Bacteria - Plate Count on Agar at 35.5 C
13. Coliforms - MPN/100 ml

[a] PVWC - Passaic Valley Water Commission

TABLE 2. ROTATED ORTHOGONAL FACTOR LOADINGS, 1967-69 [a,b]

		Varimax			Quartimax		
		1	2	3	1	2	3
1.	Discharge	-64	43	13	(-76)	01	15
2.	Temperature	-01	(-86)	25	48	(-71)	24
3.	Turbidity	04	24	(84)	-08	23	(84)
4.	Color	-19	-18	(88)	-04	-25	(88)
5.	pH	(88)	-25	-01	(87)	29	-03
6.	Alkalinity	(81)	-52	03	(96)	02	01
7.	CO_2	60	-48	-07	(76)	-06	-09
8.	Chlorides	(94)	-15	-07	(86)	40	-10
9.	DO	-26	(95)	07	(-74)	64	08
10.	Saturation	-29	(87)	23	(-72)	56	24
11.	BOD	(70)	33	03	40	66	02
12.	Bacteria	35	-33	19	48	-08	18
13.	Coliforms	26	-27	29	37	-08	28
Percent Total Variance		30.0	27.2	13.6	41.6	15.8	13.4

[a] Decimals omitted from all factor loadings. All loadings greater than or equal to /0.70/ are indicated in parentheses.

[b] PVWC Station No. 1051.

TABLE 3. FACTOR CORRELATIONS[a,b]

FACTORS		Direct Quartimin			Quartimin			Biquartimin			Covarimin		
		1	2	3	1	2	3	1	2	3	1	2	3
1950-53	1	100	-03	-33	100	11	70	100	-03	-32	100	07	20
	2		100	03		100	-07		100	-03		100	04
	3			100			100			100			100
1954-56	1	100	-12	-06	100	-26	-14	100	-14	-06	100	01	09
	2		100	-13		100	-29		100	-13		100	06
	3			100			100			100			100
1957-59	1	100	07	-25	100	13	53	100	24	22	100	10	15
	2		100	-28		100	49		100	08		100	16
	3			100			100			100			100
1960-63	1	100	11	-27	100	20	-52	100	12	-22	100	01	10
	2		100	-05		100	-10		100	01		100	09
	3			100			100			100			100
1964-66	1	100	-08	-44	100	97	99	100	32	-04	100	11	11
	2		100	-09		100	98		100	06		100	09
	3			100			100			100			100
1967-69	1	100	28	02	100	57	06	100	28	01	100	-10	03
	2		100	06		100	15		100	06		100	-03
	3			100			100			100			100

[a] Decimals omitted from all correlation coefficients.

[b] PVWC Station No. 1051.

TABLE 4. ROTATED OBLIQUE FACTOR LOADINGS, 1967-69[a,b]

	Quartimin			Biquartimin			Covarimin		
	1	2	3	1	2	3	1	2	3
1. Discharge	-57	-29	14	-62	-31	14	-66	-47	13
2. Temperature	-32	(97)	22	-07	(86)	23	02	(86)	26
3. Turbidity	16	-41	(86)	06	-29	(85)	02	-23	(84)
4. Color	-27	16	(88)	-21	19	(87)	-20	18	(88)
5. pH	(93)	-02	-01	(89)	07	-01	(89)	30	-02
6. Alkalinity	(75)	32	02	(80)	36	02	(83)	57	03
7. CO_2	51	35	-08	58	36	-08	62	51	-07
8. Chlorides	(103)	-15	-07	(96)	-04	-08	(95)	20	-09
9. DO	06	(-103)	10	-19	(-92)	09	-29	(-96)	06
10. Saturation	-01	(-94)	25	-23	(-84)	24	-33	(-89)	22
11. BOD	(93)	-64	05	(75)	-48	04	69	-29	02
12. Bacteria	29	24	19	34	26	19	36	36	19
13. Coliforms	20	19	28	25	21	28	26	29	29
Sum of Squares	4.26	3.91	1.78	3.97	3.12	1.74	4.11	3.77	1.74

[a] Decimals omitted from all factor loadings. All loadings greater than or equal to /0.70/ are indicated in parentheses.

[b] PVWC Station No. 1051.

TABLE 5. DIRECT QUARTIMIN ROTATED FACTOR LOADINGS, 1967-69[a,b]

	1	2	3
1. Discharge	-64	-30	13
2. Temperature	06	(86)	24
3. Turbidity	06	-30	(84)
4. Color	-21	18	(87)
5. pH	(90)	05	-01
6. Alkalinity	(81)	34	02
7. CO_2	59	35	-08
8. Chlorides	(96)	-06	-08
9. DO	-20	(-91)	08
10. Saturation	-25	(-83)	24
11. BOD	(75)	-50	04
12. Bacteria	34	25	19
13. Coliforms	25	20	28
Sum of Squares	4.05	3.06	1.74

[a] Decimals omitted from all factor loadings. All loadings greater than or equal to /0.70/ are indicated in parentheses.

[b] PVWC Station No. 1051.

POLLUTION CRUNCH IN JAPAN

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Ten years ago, no one worried much about pollution or the protection of the environment in Japan. But public concern has grown steadily since that time. This is evidenced by the fact that during one month in 1971, one Japanese newspaper carried no less than 124 articles about various aspects of the pollution problem. Some sensational incidents have attracted widespread attention and anxiety. I will mention some of these incidents.

▷1.→ The Minamata disease. This is a form of methyl mercury poisoning, which was identified in 1956 in the coastal areas of Minamata Bay and in 1964 along the drainage basin of the Agano River. It is caused by the long-term consumption of sea-foods with a high content of methyl mercury compounds. Its symptoms include difficulties in walking and hearing, impairment of speech and various sensory disturbances. More than 450 victims were found in the Minamata Bay area, of whom 71 have died. In the Agano River basin more than 300 victims have been found, of whom 13 have died.

2. The Itai-itai disease. This is a form of cadmium poisoning, which impairs the functioning of the kidneys and softens bone tissue. It was identified in the Jinzu River basin in Toyama prefecture, where wells and irrigation water for rice paddies had been contaminated by effluents from a mine belonging to a company of the Mitsui group. More than 120 victims have been identified, of whom 42 have died. As the result of a suit brought against the mining company, damages amounting to $450,000 have been awarded to 34 of the victims. The surviving victims of this disease and of the Minamata disease are receiving special benefits under the law concerning Special Measures for the Relief of Pollution-related Patients.

3. Polychlorinated Biphenyls (PCB). In 1968 a number of people in different parts of Japan suffered attacks of acute poisoning as the result of eating a brand of rice bran oil. It was discovered that PCB (a chloride used in heat conductors, condensers, carbonless copy paper and electrical insulating materials) had been used as a heating medium in manufacturing the rice bran oil, and had leaked into the oil through a hole in a corroded pipe. Since then PCBs have also been found in soil, in sea foods, in birds and in human milk in Western Japan.

4. Pollution of the Seto Inland Sea. The so-called "Red Tide" -- due to rapid proliferation of plankton which colours the water red -- was twenty years ago a local phenomenon of limited importance in two small areas, only sporadically occurring. The incidence of this phenomenon has grown steadily over the years, and it now affects practically the whole of the Seto Inland Sea, an area designated in 1934 as a national park, and widely known as a treasure-house of marine resources. Not only has the scenic beauty of these waters been marred, but as the result of the red tide the fishing industry has suffered heavy losses. While scientists do not yet completely understand how this phenomenon develops, the studies that have been made would seem to show that it is the result of the manifold pollutants which flow into the sea, which include effluents from such industries as paper and pulp mills and vast quantities of raw sewage. The Inland Sea has also been polluted by oil from ocean-going ships. Finally, special problems are posed by the dumping of plastic wastes, which not only affect fishing grounds, but also block up the engine cooling water intakes of ships.

5. Urban smog. This is the most obvious and most frequently experienced kind of pollution for the largest number of people. Mount Fuji, which once could be seen from Tokyo one day in every three, is now visible only one day in seven. In 1971 nearly 50,000 people in and around the big cities of Western Japan suffered eye, throat or lung irritation from photochemical smog. Public attention was caught by an incident in July 1970 when 43 girls at a high school playground in Tokyo suddenly became nauseated and fainted.

All these incidents and developments have been widely reported and aroused much public concern and anxiety. Thousands of complaints and petitions have been received from both urban and rural districts in all parts of the country. The largest proportion of these complaints (over 33%) is concerned with noise and vibration; offensive odors follow with nearly 24%; third comes air pollution with about 18%. The total number of such complaints accepted by regional public bodies in 1971 was more than 75,000.

An idea of the cost of pollution to the nation can be obtained from estimates made for 1970. No attempt was made to quantify the costs of damage to health, but the loss of production in agriculture and fisheries was estimated at over 38 billion yen. Domestic expenses, such as additional laundry costs and new paint, were estimated to be over 410 billion yen. Costs incurred by industry for pollution prevention and control were 780 billion yen. (Large scale industry has recently been spending about 10% of its total investment funds on pollution control.) Government spending for protection of the environment totaled over 300 billion yen. The total cost per citizen had risen from 2,000 yen in 1960 to 4,500 yen in 1965 and 15,000 yen in 1970 - almost 8 times in 10 years.

Appropriations by ministries and agencies for pollution control and conservation of the natural environment rose from 111 billion yen in 1971 to 169 billion yen in 1972 and 273 billion yen in 1973. Treasury investment and loans relating to pollution control increased from 170 billion yen in 1971 to 263 billion yen in 1972 and 430 billion yen in 1973.

The foregoing paragraphs give a general idea of the magnitude of the pollution problem in Japan, and of its serious effects on the citizen and the economy. It may now be interesting to consider how the problem has arisen, and what has been done about it.

Japan's drive to modernize its economy dates from the beginning of the Meiji era in 1868. Economic development has been rapid, and the pace of development has accelerated very much since the end of the second world war. As the result, Japan is today one of the leading industrial countries of the world. However, investment in social capital has lagged behind. For example, in 1965 only 15% of the population was served by sewer systems, and by 1971 the proportion had only risen to 22%. This compares with 90% in England (1963) and 71% in the U. S. A. (1968).

Moreover, the Japanese economy is so structured that it tends to produce more pollution than the type of economic structure in other industrialized countries. For instance, a French type of economic structure would generate about 40% less sulphur oxides, an American type 20% less and an English or West German type 10% less. The same kind of pattern applies to BOD, particulates and industrial waste.

The spectacular Japanese economic development took place in a country where population and industrial density have now almost reached an upper limit. Annual production valued at $200 billion must be supported by only 10,000 km^2 of level land. Already twenty years ago gross national product per equal area of level land was more than twice as much in Japan as in the U. S. A. Today it is more than eleven times as much. The visitor to Japan is struck by the fact that wherever he travels in the country, he is never out of sight of the mountains -- but this reflects the fact that there is only 30 m^2 of level land per person -- and this exiguous amount of level land includes the roads, the railroads and the rice paddies. No wonder that terraced fields ascend every little mountain valley and cover every side of many hills. New steel plants and many other new industrial facilities have to be constructed on land reclaimed from the sea.

The number of automobiles in use has increased dramatically. Between 1959 and 1969 the number of automobiles per 1,000 hectares of level land rose ten times, from 130 to 1,300. This means that in 1969 the number of automobiles per hectare of level land was no less than 8 times the corresponding figure for the U. S. A. in that year, and that on the average in Japan more than one automobile was driven within each hectare of level land. It is clear, therefore, that air pollution from exhaust gas, noise and vibration have a much greater impact in Japan than in other countries.

Pollution problems are aggravated because population and industry are concentrated in a few areas. Two of these -- the so-called Pacific Belt and the northern part of Kyushu -- cover only about one quarter of the land area, but in 1964 they were responsible for 75% of the biochemical oxygen demand and for nearly 70% of the total emission of sulphur oxides.

Pollution of rivers and streams flowing through urban areas is acute and becoming worse rapidly, on account of the increase in untreated domestic sewage. The problem of garbage disposal is a serious one -- the total output of garbage in 1970 was 35 million tons. Traffic congestion, with its accompanying noise, vibration and air pollution is universal in all the crowded urban and suburban areas.

Part of the pollution problem flows from the fact that industrial growth has been concentrated in such industries as electric power, iron and steel, paper and pulp, chemicals and ceramics. In 1970 these industries accounted for over 80% of sulphur discharge. Paper and pulp, food industries, chemicals and textiles were responsible for over 95% of the biochemical oxygen demand in the same year.

Energy consumption per hectare of level land in 1969 was ten times that in the U. S. A. World energy consumption just about doubled in the years from 1955 to 1970, while in the same period in Japan per capita energy consumption increased more than 200% and absolute energy consumption 250%. Moreover, during the last twenty years there has been a remarkable change in the sources from which Japan obtains its energy. In 1955 thermal plants produced 25.7% of all electricity. By 1970 the proportion had risen to 76.4% of a very much larger total. Thermal plants burn mostly oil imported from the Near and Middle East, with a large sulphur content, which aggravates the air pollution problem.

Industrial water usage has also increased rapidly. In 1962 it accounted for only 35% of total water usage; by 1969 it was already more than half total usage. The three largest producers of biochemical oxygen demand load -- paper and pulp, food industries and chemicals -- used 60% of total industrial water. The paper and pulp industry has expanded at a particularly rapid rate -- the Japanese people are almost 100% literate and voracious readers -- and was responsible in 1970 for almost 50% of the biochemical oxygen demand load.

During the last twenty years, while total industrial production has grown at a spectacular rate, the share of basic production goods has steadily increased, and that of basic consumption goods has decreased. This partly reflects the continuing and increasing investment in capital equipment and construction and partly the need to increase exports to pay for imported raw materials and fuel, which coincided with a very strong world demand for chemical products and for steel.

The economy has however grown so fast that even though the share of consumption goods in total production has lagged behind that of production goods, there has been a very large absolute increase in the production of consumption goods, and especially in that of durable consumption goods. Parallel with this goes an increasing problem in the disposal of discarded products of this kind.

For instance, ownership of television sets skyrocketed in a few years. In 1958 only about 14% of the population owned a television set; five years later the figure was over 90%. Less than 10% owned a refrigerator in 1958; ten years later the figure was over 80%. Ownership of cars, air conditioners and color television sets have all been rising rapidly. The use of disposable packaging (non-returnable containers and plastic packaging) aggravates the problem of solid waste disposal. Plastic waste disposal poses a special problem. Production shot up from about 10,000 tons in 1960 to 5 million tons in 1970. Plastic waste material was reported to be 1 to 3 million tons in 1970. One result of these developments is that solid refuse collected in Tokyo has been increasing about twice as fast as the population of the city.

Although the ownership of automobiles has risen rapidly -- from 1.5 million in 1955 to 19 million in 1970 -- the rise has been so recent that the problem of disposal of junked automobiles is not yet serious, though it certainly will be in the future. The air pollution problem from automobile exhaust, on the other hand, is already very serious. In Tokyo alone -- the most recent figures available are for 1967 -- exhaust gases released 850,000 tons of carbon monoxide, 170,000 tons of hydrocarbons and 3,500 tons of nitrogen oxides into the air.

The various sensational incidents, the consequent public concern, the ubiquitous evidence of pollution and the volume of complaints received have all combined to make the protection of the environment an urgent political issue. In consequence, many laws have been passed and many regulations imposed to cope with the many different aspects of the problem.

A basic Law of Environmental Pollution Control was passed in 1967. This law was strengthened in 1970. The budget for expenditures for environment protection increased nearly five times from 1967 to 1972, and the figure for 1973 is more than 50% above the 1972 level.

Expenditure on research has grown rapidly and in 1972 the environmental agency decided to coordinate the research activities of all other government agencies in the field of environmental preservation, and to unify budget expenditures for testing and research institutes belonging to other government agencies, and for contracts with private organizations that are mainly devoted to pollution control. In 1972 this unified budget for testing amounted to 2,300 million yen. In addition about 6,400 million yen was appropriated for research and surveys by government agencies relating to pollution countermeasures.

It is interesting to compare these figures with the more than $300 million spent in 1970 by the U. S. Government for pollution control research. However, Japanese industry -- especially paper and pulp, iron and steel, electricity and automobiles - stimulated by emission and effluent standard targets established by government, is making a major effort to develop pollution control technology. The automobile industry, for instance, spent almost $100 million for this kind of research in 1972. But for industry as a whole, expenditure for pollution control research and development is still less than 10% of total research expenditures.

An important step was taken by the government in 1971, when the Environment Agency was established and made responsible for laying down standards and for coordinating action over the whole field of environment protection. The following paragraphs give a general idea of the action taken to cope with the most important threats to the environment.

Air Pollution

As of March 1973 environmental standards have been established with respect to sulphur oxides, carbon monoxide and suspended particulate matter. Similar standards for lead and nitrogen oxides are being considered. Air pollution controls have been extended over the whole country. Emission standards for soot and dust have been applied in 29 designated areas. Uniform emission standards for the whole country have been fixed for cadmium, chlorine, hydrogen chloride, fluoride and silicon fluoride and lead. Emergency measures are in force for special meteorological conditions.

Automobile exhaust standards have been established. The maximum permissible amount of lead in gasoline has been laid down. Steps have been taken to reduce the sulphur content of heavy oil and stack smoke.

A national Air Pollution Monitoring Network has been constructed with 15 stations. Some of these stations, in the Tokyo and Osaka areas, are linked by telemetric information exchange systems. The 1973 budget included funds for construction of an additional two stations.

Water Pollution

Environmental standards were established in 1970, covering over 500 different types of production, with penalties for violation of effluent standards. A special Water Pollution Control Law was passed in 1971. Strict control has been established over effluents from mines and smelting plants.

A new sewerage law became effective in 1971, and a third five year sewerage plan, beginning in that year, is designed to increase the proportion of urban areas served by sewer systems from 22.8% (of 5,945 rm^2) in 1970 to 38% (of 8,490 rm^2) in 1975. This would allow the proportion of urban population served to rise from 34.7% (of 62.8 million) in 1970 to 55% (of 75.4 million) in 1975. This program will involve a total investment of 2,600 billion yen, and in view of the urgency of the situation, expenditure is proceeding ahead of the original schedule.

Dams are being built to reduce fluctuations in river flow, which otherwise may be very marked in a country where rivers are relatively short and rapid.

A system of monitoring the condition of public waters is being installed.

A Marine Pollution Control Law was passed in 1970, which regulates the drainage of oil and waste products from ships. Waste oil disposal facilities are being constructed in port areas. High speed patrol boats and helicopters are being used to maintain a system of marine surveillance.

Human Health

Areas in which the air is highly polluted have been designated as eligible for aid under the 1969 law concerning Special Measures for the Relief of Pollution-related Patients. By the end of March 1973 over 8,700 patients affected by air pollution had been found eligible to receive financial aid to meet their medical expenses. They were suffering from chronic bronchitis (22.9%), bronchial asthma (34.8%), asthmic bronchitis (41%) and emphysema (1.3%). Half of these patients were children under 9 years old; 20% were over 60 years old.

Similar aid was being given to victims of the Minamata and Itai-itai diseases and to victims of PCB poisoning.

Nature Conservation

Various areas of natural beauty, green belts on the border of urban areas, etc. have been protected by making any proposed alteration to the state of nature subject to special permission.

It is interesting to note that 13.5% of the total land surface of Japan consists of publicly-owned parks. In these areas there is strict control of trees and gravel mining.

These parks were visited by nearly 540 million people during 1971, an increase of 60% over the 330 million visitors in 1966. Now public facilities are being constructed to handle the garbage problem caused by the large number of visitors, which seems likely to continue to grow.

Noise and Vibration

Standards were established in 1971 to cover noise and vibration caused by factories, at construction sites, and by traffic on highways, super-express trains and jet aircraft. Take-offs and landings of jet aircraft at Tokyo and Osaka airports have been restricted within designated hours of the day.

Offensive Odors

An Offensive Odor Control Law, which became effective in 1972, has given prefectural governors the responsibility and authority to control the emission by industry of substances causing offensive odors.

Polychlorinated Biphenyls

The manufacture of PCB's, the production of which had grown from 5,000 tons in 1968 to 11,000 tons in 1970, decreased from then on and completely stopped in 1972. In September of that year practically all importation of PCB's was forbidden. In August 1972 provisional permissible levels were laid down for PCB content of human and animal food.

Agricultural Chemicals

An Agricultural Chemical Control Law was passed in 1970, resulting in a complete ban on the use of DDT and similar compounds and the strict regulation of the use of many other agricultural chemicals. Standards of Safe Use have been established.

Administration

The Environment Agency was established in 1971 to formulate the basic principles for the conservation of the environment and to coordinate measures taken by the various ministries and agencies active in the field. In that year nine ministries and six agencies received appropriations for environmental control and research.

The Environment Agency issues guidelines for pollution control programs, and all proposed programs must be submitted to it for approval. It establishes environmental and emission standards. It enforces the various pollution control laws and supervises the work of the Environment Pollution Control Service Corporation. It initiates and controls research programs and studies.

Pollution Control Programs are being worked out for strategic areas.

A Central Board and various Prefectural Commissions have been established to deal with pollution-related disputes.

Many prefectures and municipalities have established special pollution control sections. By the end of 1971 there were over 1,300 such sections in the country.

Financing Pollution Prevention Works

Loans are available from the Environmental Pollution Control Service Corporation for the installation of anti-pollution facilities. The amount available for such loans increased from 45 billion yen in 1972 to 55 billion yen in 1973. The Japan Development Bank also makes loans for such purposes; 35 billion yen was available in 1972 and 65 billion yen in 1973.

Investment in pollution control facilities benefits from special tax provision. Owners of pollution control equipment are permitted to write off 50% of the cost in the first year. A special depreciation system allows one-third of the cost of pollution-free manufacturing equipment to be written off for tax purposes in the initial year. Similar arrangements reduce the impact of local taxes.

The Small Business Finance Corporation and The People's Finance Corporation also lend money for pollution control for facilitating changes from polluting industries to non-polluting ones and for relocation of industries away from over-congested areas.

Settlement of Pollution-Based Disputes

A law concerning the Settlement of Environmental Pollution Disputes was enacted in 1970, providing for government intervention to mediate and arbitrate such disputes. Late in 1970 a Central Pollution-based Disputes Examination Board was established, and Local Pollution-based Disputes Examination Commissions have been set up in the prefectures. Grievance counselors are stationed in large cities and in each of the prefectures to deal with complaints, to mediate between parties where possible, and to advise the competent offices of complaints received. By July 1972 there were over 2,300 of these counselors.

The Central Board has since been replaced by a Pollution Coordination Committee, and now the plaintiff in a dispute may have recourse to any of the different types of semi-judicial administrative relief as an alternative to seeking help in the complaints. These four are:

(1) Arbitration by the Pollution Coordination Committee.

(2) Mediation by the same committee.

(3) Mediation by the Prefectural Pollution Examination Board, and

(4) Reconciliation by that Board.

The Outlook

A recent study by the Economic Planning Agency of the government concludes that if the present rate of migration from the rural areas to the cities were to be maintained, living conditions would become intolerable by 1985. By that year, Tokyo would have about 38 million inhabitants, and the Nagoya-Osaka area about 30 million. Monumental traffic jams would be chronic. Garbage would pile up in the streets with no way of disposal. The demand for housing, schools and transportation could probably not be met. Water supply would fall short of demand by about four billion tons a year. There would be no prospect of sufficient electricity on present estimates. It would be impossible to supply so many people with perishable food-stuffs. City life would simply collapse.

Faced with this appalling prospect within twelve years, the study concludes that the only way to guarantee decent urban living conditions would be not just to halt the migration from rural to urban areas, but actively to reverse the flow of population.

The government intends to formulate by 1975 a new land use and development policy which hopefully will carry the nation through at least till the end of the century.

Source: The Environment Agency, Tokyo.

SIMULATION MODELING OF STREAMS FOR WATER QUALITY STUDIES[1]

by

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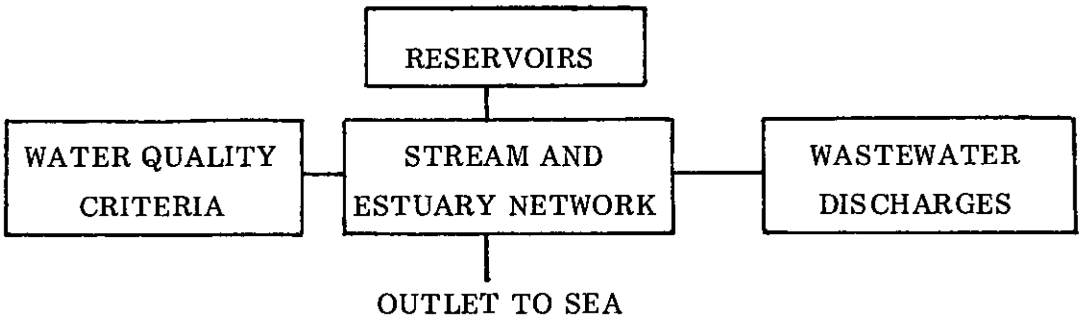
[1]Presented at Seminar on Pollution and Water Resources, Columbia University, October 16, 1974.

INTRODUCTION

The planning methodologies discussed in this paper concern the problems of water quality in the stream environment. The stream's physical, chemical, and bacteriological characteristics are modified by waste water discharges, diversions, in situ uses, and natural runoff. To meet requirements for water quality, it is necessary to determine the stream's natural purification capabilities, and to limit the organic loadings on the stream resulting from man's activities. The elements of the stream system are shown schematically in the following figure.



The water quality of the stream and estuary network is affected by the discharges of treated and untreated waste water to the receiving waters. The water quality is compared with specified water quality criteria, or is made to conform to these criteria by changing the levels of waste water treatment. The flows in the streams may be unregulated, or they may be modified by the operations of one or more upstream reservoirs. The flow pattern may be assumed to be a repetition of historical events, or the investigator may generate synthetic hydrology. The system may be studied for one or more critical low flow high temperature periods, or wide ranges of operation may be considered in which attention is directed to the stochastic nature of input and/or output data.

Mathematical models are used to describe the systems to be investigated, and the simulation is programmed for processing data with the aid of a computer. Both steady--state and time--variable models have been studied for a variety of problems including:

(1) Determination of reservoir releases to maintain specified water quality.

(2) Determination of optimum set of treatment plants (usually least-cost system) to maintain specified water quality.

(3) Estimate of allowable organic loadings to stream reaches, consistent with specified water quality.

(4) Investigation of the sensitivity of stream parameters.

STEADY STATE MODEL OF STREAM SYSTEM

A configuration based on the Buffalo River Basin in New York State, with hypothetical locations for water-based recreation, water supply and treated sewage discharge, is shown on Figure 1. The following flow and water quality characteristics were evaluated for this model.

(1) Stream flow, mgd

(2) Time of travel from upstream location, days

(3) BOD, ppm (mg/l)

(4) Dissolved oxygen deficit, ppm

(5) Coliform count, MPN/100 ml.

(6) Chlorides, ppm

(7) Water quality index for water supply

(8) Water quality index for recreation

The water quality indexes (items (7) and (8)) were based on weightings of various water quality parameters. A portion of the results for one simulation is shown for Buffalo Creek on Figure 2. Straight lines are used in this figure to connect the values that were computed.

DISSOLVED OXYGEN VARIATIONS

The most important water quality parameter in these studies is dissolved oxygen, or dissolved oxygen deficit related to the saturation value. Factors causing variations in dissolved oxygen include the following:

(1) Organic (BOD) loadings from communities, industries, and agricultural activities

(2) Stream flow

(3) Temperature

(4) Deoxygenation rate

(5) Reaeration rate

(6) Settling and resuspension of BOD

(7) Benthal demands on oxygen resources

(8) Algal activity

(9) Sunlight, nutrients (potassium, nitrates, and phosphates), and possibly other environmental parameters affecting algal activity.

Most of the factors are included in the following expanded forms of the Streeter-Phelps formulas for changes of BOD and Dissolved Oxygen Deficit in a stream reach between locations "a" and "b".

$$L_b = \left[L_a - \frac{p}{2.3(k_1+k_3)} \right] 10^{-(k_1+k_3)\,t} + \frac{p}{2.3(k_1+k_3)}$$

in which L_a and L_b are BOD's (ppm)

- t is the time of flow (days)
- k_1 is the deoxygenation rate constant ($days^{-1}$)
- k_3 is the rate constant for settling out of BOD to bottom deposits (days-1)
- p is the rate of addition of BOD to the overlying water from bottom deposits (ppm per day)

$$D_b = \frac{k_1}{k_2-k_1-k_3} \left[L_a - \frac{p}{2.3(k_1+k_3)} \right] \left[10^{-(k_1+k_3)t} - 10^{-k_2 t} \right] - \frac{k_1}{k_2} \left[\frac{p}{2.3(k_1+k_3)} - \frac{a}{2.3\,k_1} \right] (1-10^{-k_2 t}) + D_a \cdot 10^{-k_2 t}$$

in which D_a and D_b are DO deficits (ppm)

- k_2 is the atmospheric reaeration rate constant ($days^{-1}$)
- $\underline{a}$ is the rate of production of DO by algae through photosynthesis (ppm per day)

In the above formulas, the parameters may be determined by laboratory testing methods, equations of various investigators, or fitting of computed and observed BOD and DO profiles.

WASTEWATER TREATMENT OPTIMIZATION

Optimization techniques for steady state assumptions were developed using a 50 mile reach of the Merrimack River in Massachusetts as a basis. Nine communities with 300,000 persons would theoretically use the river reach for water supply, wastewater disposal, and recreation. Parameters in the formulas for BOD and DO deficit were estimated by Federal and State agencies. The computerized simulation provided output on 8 flow and quality characteristics for each of 62 river sections, and 31 water related characteristics for each of the 9 communities. For the community and river model, as a whole, the simulation determined the total investment and annual costs for water treatment, sewage treatment, and recreation facilities, and the total annual benefits from these facilities.

Graphed river characteristics for three different flow patterns, with secondary treatment employed by all sewage treatment plants, are shown in

Figure 3. Note that the DO deficit for the basic design flow (solid line) ranges from 3 ppm to 0 ppm.

An optimizing routine was developed utilizing the operations research technique of "steepest ascent," by which successive computer cycles made efficient changes in treatment plant levels (in terms of BOD removal) to meet specified DO deficits at minimum cost. For assumptions that the maximum DO deficit is 3 ppm and that levels of sewage treatment are permitted to range from primary to tertiary treatment, the results of the optimization are shown on Figure 4. In 1965 dollars, the optimum treatment and all secondary treatment alternatives would involve investment costs in sewage treatment programs of $34.5 million and $61.0 million, respectively.

Current Federal regulations require a minimum of secondary treatment but, conceptually, the optimizing routine can handle problems with treatment levels ranging upwards from secondary treatment. It is noted that other methods have also been utilized to determine optimum sewage treatment programs. In addition to simulation, operations research techniques for this purpose have included linear programming and dynamic programming. These techniques have also been used to plan wastewater collection systems, components of wastewater treatment plants, and construction programs.

ALLOWABLE ORGANIC LOADINGS

In 1973 and 1974, the author assisted a firm of consulting engineers in a study of the Chemung River Basin in New York. The program of investigations included both field surveys and data analyses. There were two periods of field work. October 8-19 and November 8-16, 1973. The total length of stream studied was 102 miles.

The following were the principal elements of the field surveys:

(1) Field reconnaissance and selection of stations for field measurements and for taking samples. Samples were collected at all significant domestic and industrial wastewater outlets and at observation stations on the streams.

(2) Selection of times for field measurements and sampling, prior to each day's work. Progress of biochemical oxygen demand and dissolved oxygen (DO) in each stream reach was based on one-dimensional, slug flow, and steady state assumptions.

(3) Field determinations of flow, temperature, pH and DO. Collection of 2-hour composite samples for laboratory testing. Testing to determine diurnal variations in DO due to photosynthetic oxygen production and algal respiration.

(4) Laboratory determinations of pH, COD, BOD, phosphates, chlorides, turbidity, alkalinity, and nitrogen forms (ammonia, nitrite, nitrate, and Kjeldahl).

(5) Examination of BOD_5 and DO results after completion of Survey 1. This assisted in determining the program for Survey 2, including the selection of portions of the streams that could be omitted from further study because they were unpolluted.

The following were the elements of data analyses:

(1) Selection of appropriate formulas for stream purification dynamics, and refinement of a computerized mathematical model for the stream reaches studied.

(2) Determination of laboratory deoxygenation constants and first-stage (carbonaceous) BOD's. Interpretation of these estimates and laboratory results to determine the general nature of the wastewaters and stream reaches involved.

(3) Reproduction of BOD and DO sag curves for Surveys 1 and 2, consistent with stream quality data and estimates of deoxygenation and reaeration constants.

(4) Prediction of DO conditions for MA7CD10YR conditions with existing waste loads.

(5) Examination of State standards for water quality in reaches studied and develpment of methodology for determining allowable waste loading in pounds of BOD_5 per day.

(6) Determination of allowable waste loads in terms of pounds/day of BOD_5, and comparisons with existing and known potential waste loads.

(7) Sensitivity analyses to determine water quality estimates with different deoxygenation and reaeration constants.

(8) Studies of nitrogenous and total oxygen demands, and nutrients.

(9) Recommendations for additional surveys and analyses, and monitoring.

The analyses of field data were made for the purpose of obtaining estimates of deoxygenation and reaeration for predictive purposes, that is for minimum average 7 day continuous discharge with 10 year return interval and maximum BOD loading consistent with specified water quality. In this work, it is desirable to perform the field work when stream conditions are near to design conditions. Because this was not possible for this study, the field data analyses were hampered by the following:

(1) Temperatures during the surveys, particularly Survey 2, were much lower than expected MA7CD10YR values;

(2) Heavy rainfall between Surveys 1 and 2 resulted in flooding that affected stream conditions to such an extent that it was not feasible to correlate the results of the two surveys;

(3) Stream flows during the surveys were very much higher than MA7CD10YR values, in fact from 5 to 9 times these values; and

(4) Diurnal variations in DO, particularly during Survey 1, were very large compared to the variations measured or estimated to have occurred from oxygen sags due to pollution. Diurnal variations in one stream reach that was unusually affected by algae activity are shown on Figure 5.

For this work, the original simple forms of the Streeter-Phelps formulas were used, as follows:

$$L_b = L_a \, . 10^{-k_1 t}$$

$$D_b = \frac{k_1 \quad L_a}{k_2 - k_1} \left[10^{-k_1 t} - 10^{-k_2 t} \right] + D_a \, . \, 10^{-k_2 t}$$

The values of k_1 were determined to be appropriate for reproducing the BOD profiles observed in the field. The k_2 values were determined by using Tsivoglou's formula, as follows:

$$K_2 = c \frac{\Delta h}{t}$$

In this formula, Δh is the drop in water surface elevation (feet) in time t (hours) and c is a constant selected in accordance with the recommendations of Tsivoglou.

Tsivoglou recommends the use of the following "escape coefficient" c values for 25°C.

High pollution	BOD = 30 mg/l, c = .030
Average pollution	BOD = 15 mg/l, c = .054
Low pollution	BOD = 2 mg/l, c = .085

The K_2 values are for base e computations. For base 10 computations with k_2, K_2 is divided by 2.3 and adjusted for $days^{-1}$ units.

With the k_1 and k_2 values determined, and with upstream BOD and DO deficit known, the profile of the dissolved oxygen profile was computed. Measured values of dissolved oxygen were compared with the DO profile ("sag curve") and the profile was accepted if the measured values were within the ranges indicated by the diurnal DO variations.

To determine the allowable organic load in terms of BOD for a reach, various values of this load were assumed and the oxygen sag curves were computed until the load caused a critical sag meeting the specifications for minimum dissolved oxygen.

SENSITIVITY ANALYSIS

Of particular interest is the effect of stream purification parameter in determining the results of the analysis. For example, for the Chemung River Survey discussed above, Figure 6 shows that for an organic loading determined for a design k_1 from Survey 1 and a design k_2 from Tsivoglou's formula, the minimum DO would be 3 mg/l corresponding to the State specification. For other values of k_1 and k_2, the resulting minimum DO's would range above and below the 3 mg/l value. The implications in terms of unacceptable water quality or uneconomic sewage treatment plant construction are obvious.

With respect to the latter concept, the following table shows the range of investment costs in 1965 dollars required depending upon the stream parameter values chosen for the Merrimack River, discussed earlier.

Range of Investment Costs

Parameter	Million $	% of $33.1 Million	% of Difference
k_1	30.5-39.5	92-120	8-20
k_2	30.5-36.5	92-110	8-10
k_3	32.4-35.6	98-108	2-8
p	33.1-36.0	100-109	0-9
a	30.5-43.0	92-130	8-30

TIME VARIABLE MODELS

For important streams with existing or potential trouble areas with respect to water quality, a model based on the steady state may not provide a sufficiently adequate simulation of conditions when stream flow and environmental factors vary substantially over a period of operation.

A stream reach may have a number of designated stations where quality determinations are to be made. The modeling consists of two principal steps. In the first step, the flows are routed to completely define the time-variable flow regimen of the stream. The quality in terms of BOD, DO, coliforms, and chlorides are then mapped to yield a record of these parameters at any specified station in the stream. Principal factors affecting the quality characteristics are water temperature, solar radiation, and stream flow. Figure 7 shows these input factors varying with time, while the output water quality characteristics are obtained.

Unsteady state models can be used to investigate the effectiveness of an assumed configuration of treatment plants, in terms of compliance with stream quality criteria, while a stream's assimilative capacity changes with distance and time. A simulation showing the variation of quality with distance and time can also be used to study the suitability of the stream for fish propagation or other specific purpose.

CLOSING REMARKS

This paper has shown a number of different ways in which steady-state and time-variable simulations can be used in a water quality management program. Considering the informal nature of the Columbia seminar setting and the limitations of time, this paper has not provided any working details of the methodologies presented. The references following this paper are selected from publications of the author, but acknowledgment should be made of the other investigators in this field.

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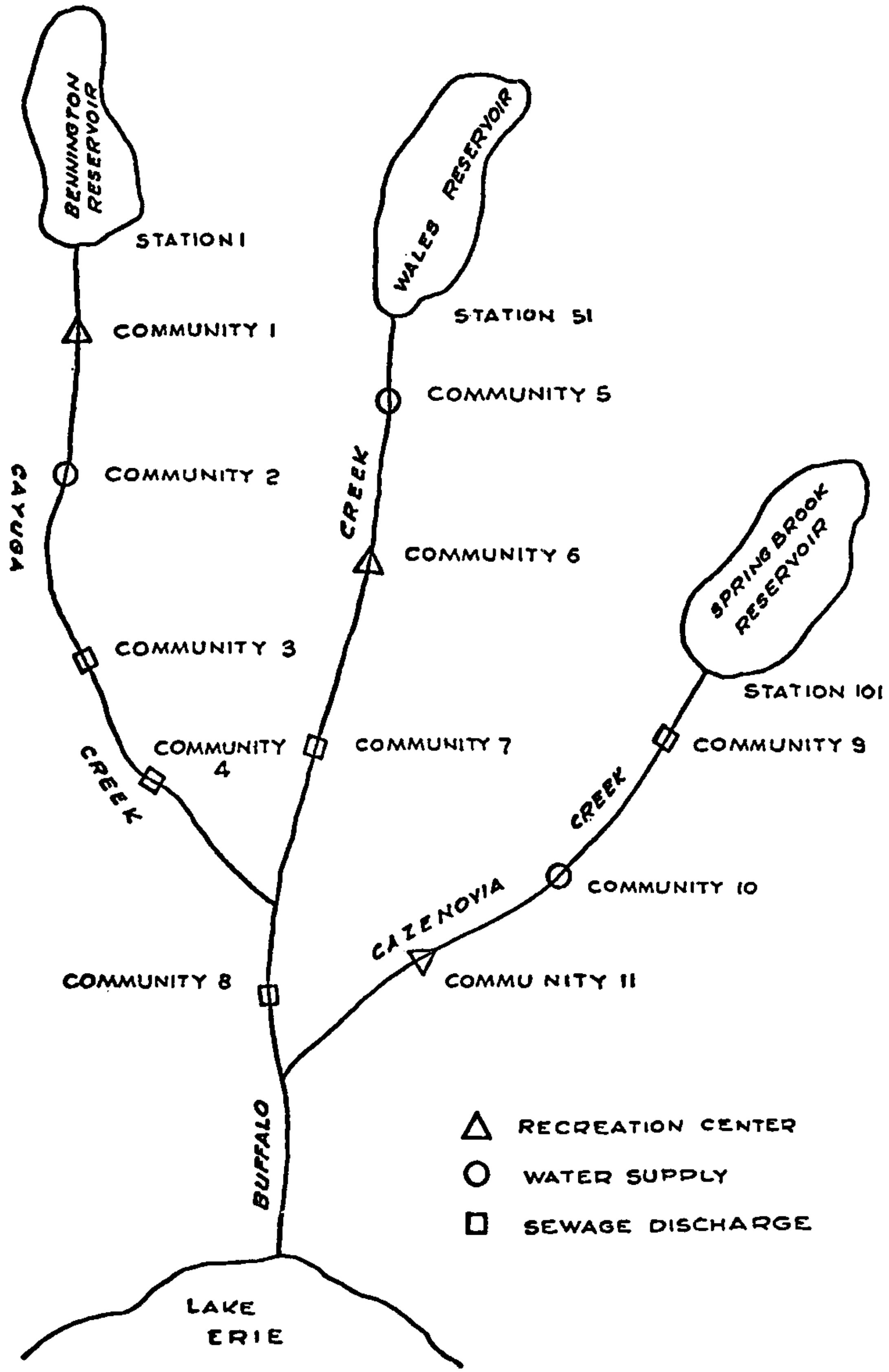

Figure 1. Configuration based on Buffalo River System in New York State.

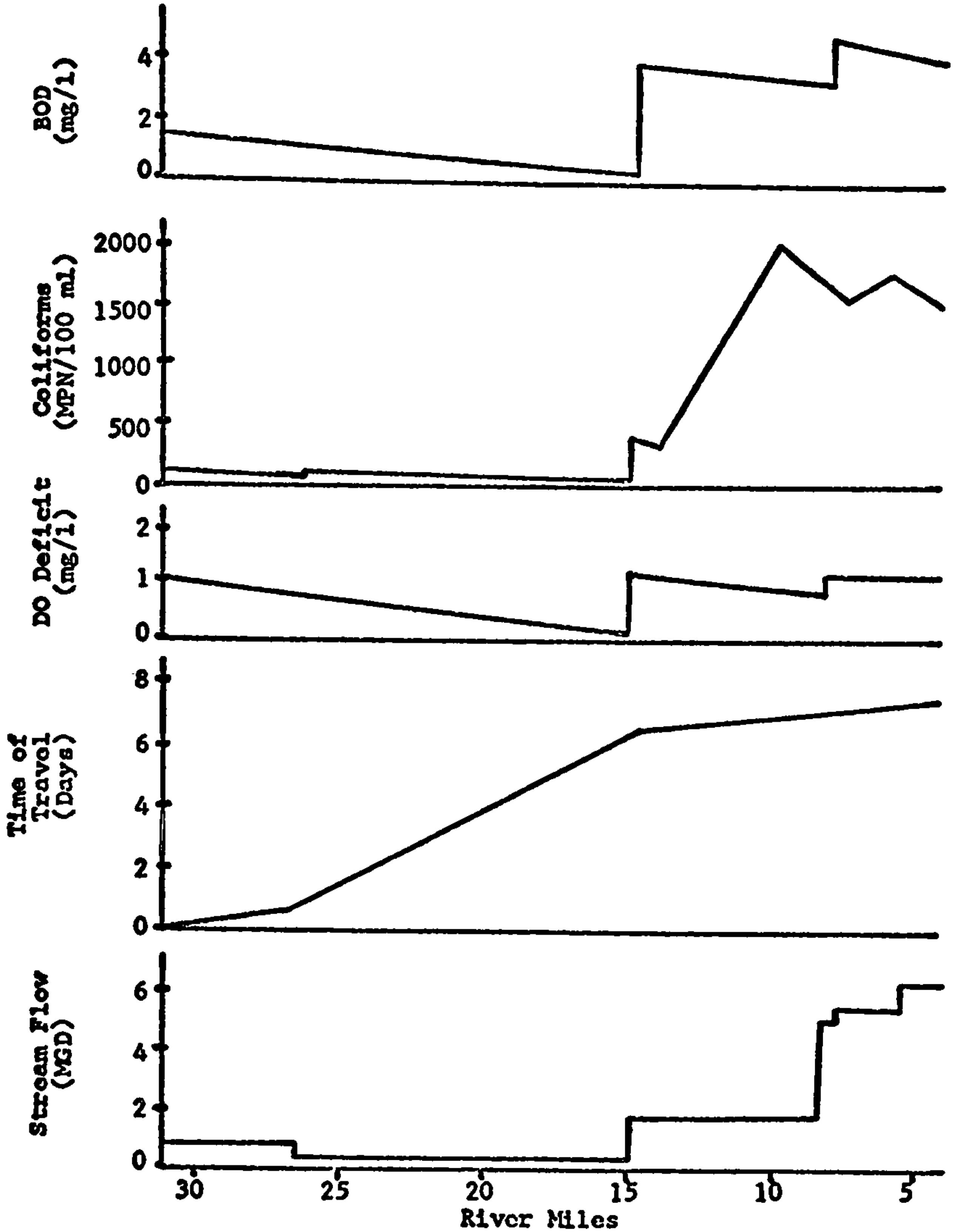

Figure 2. Results of one simulation for Buffalo Creek.

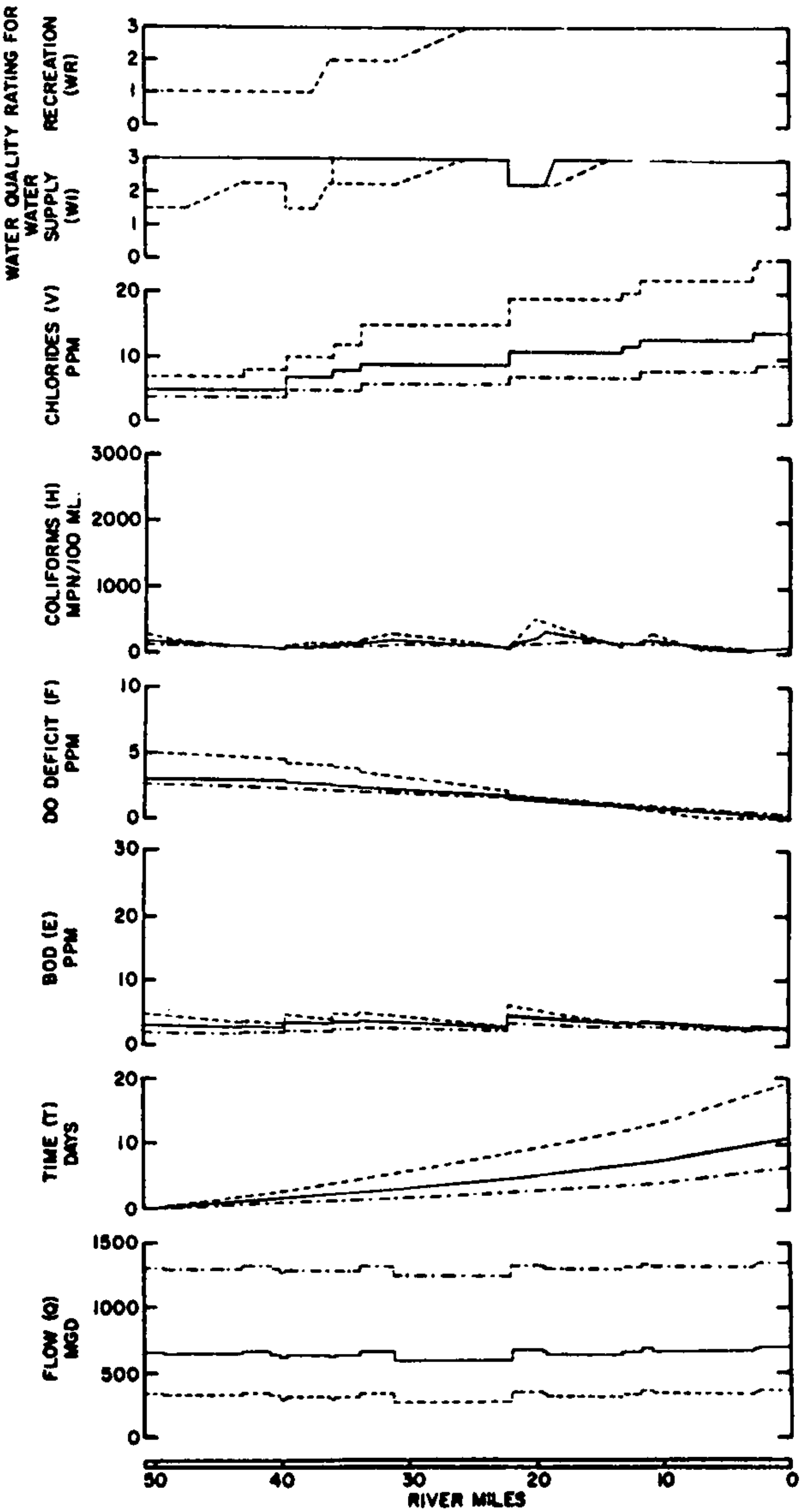

Figure 3. Merrimack River--results for all secondary treatment.

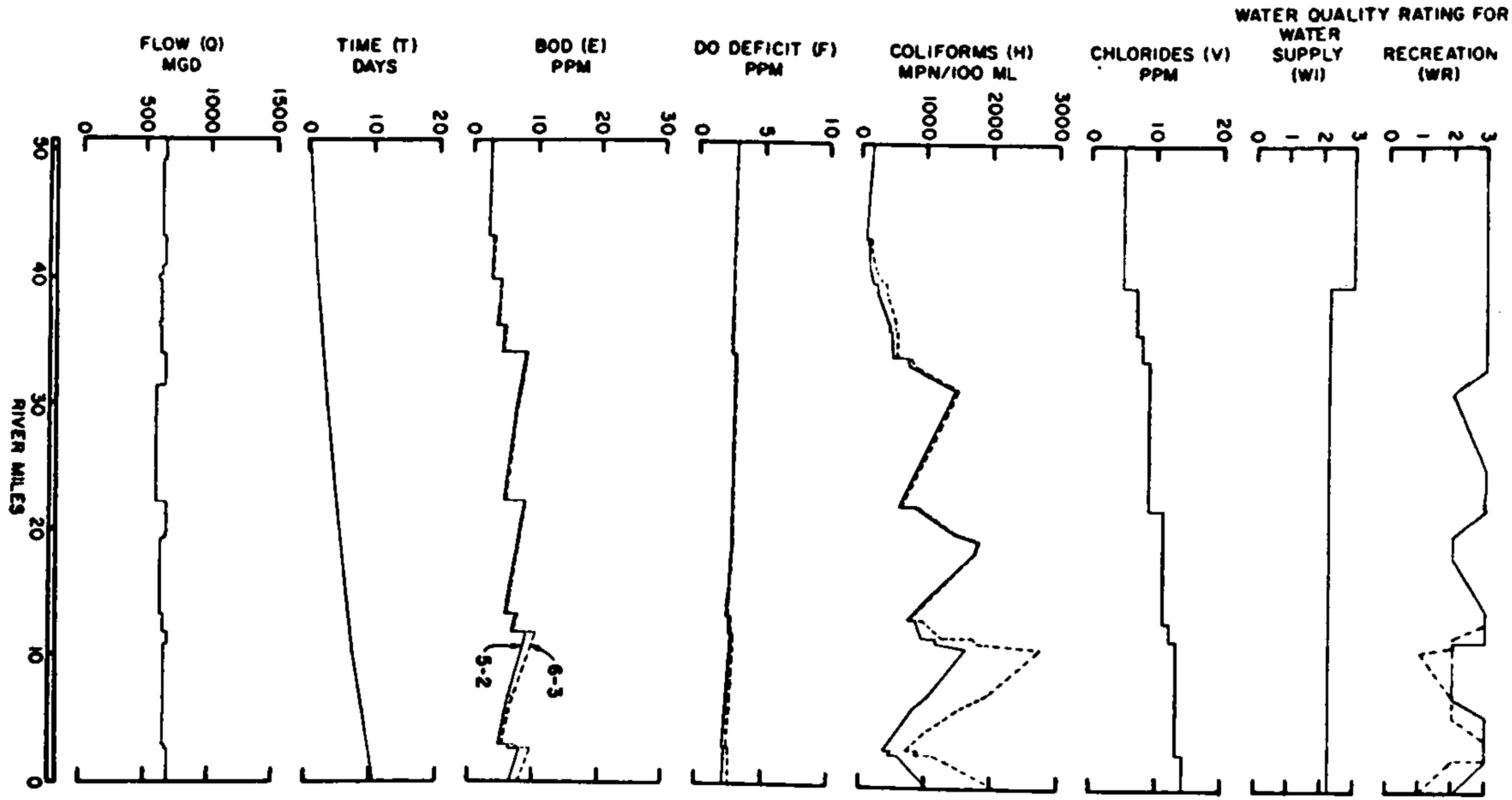

Figure 4. Merrimack River--results for optimum treatment.

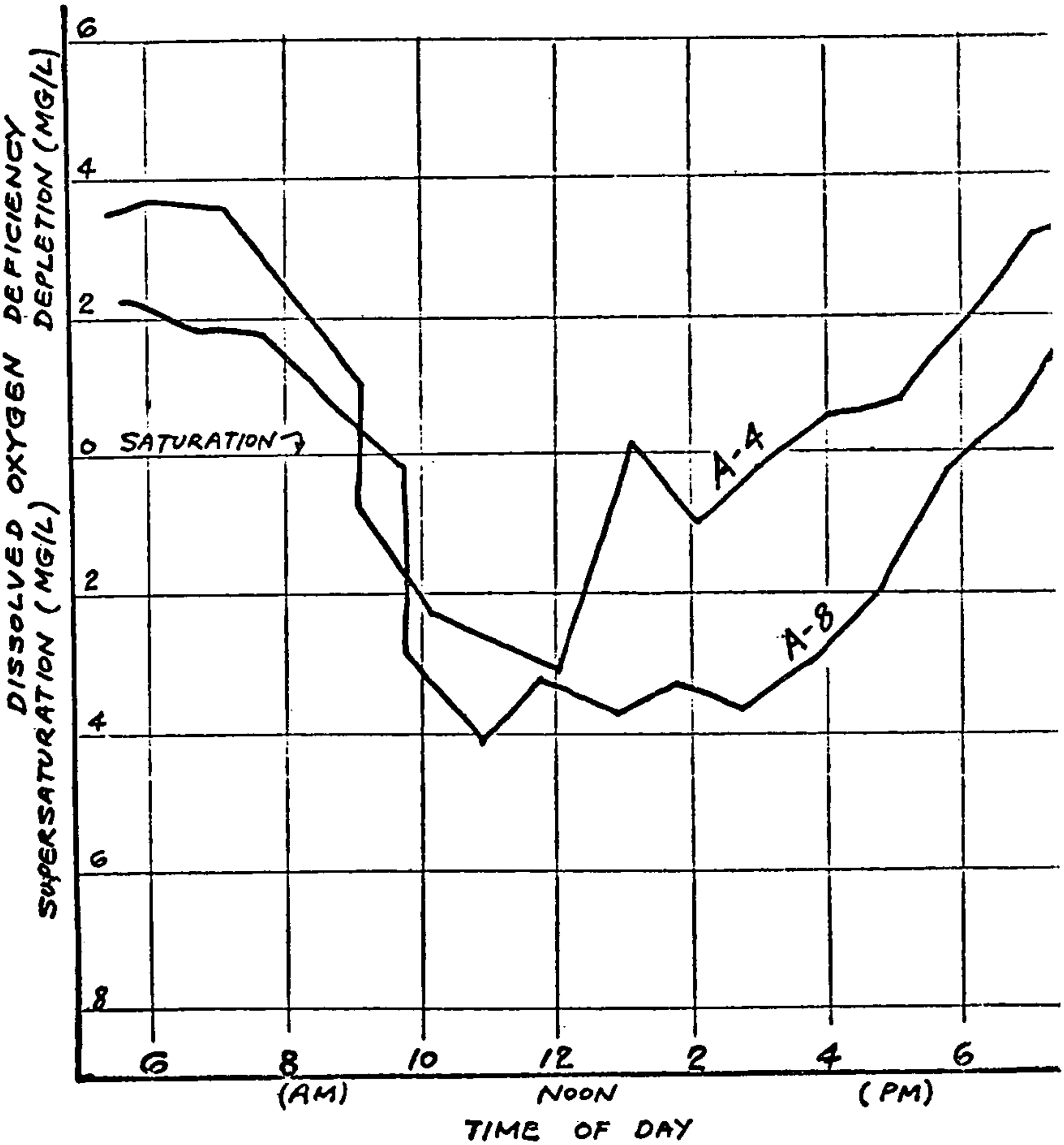

Figure 5. Canacadea Creek (Cehmung River) diurnal variations in DO at two stations.

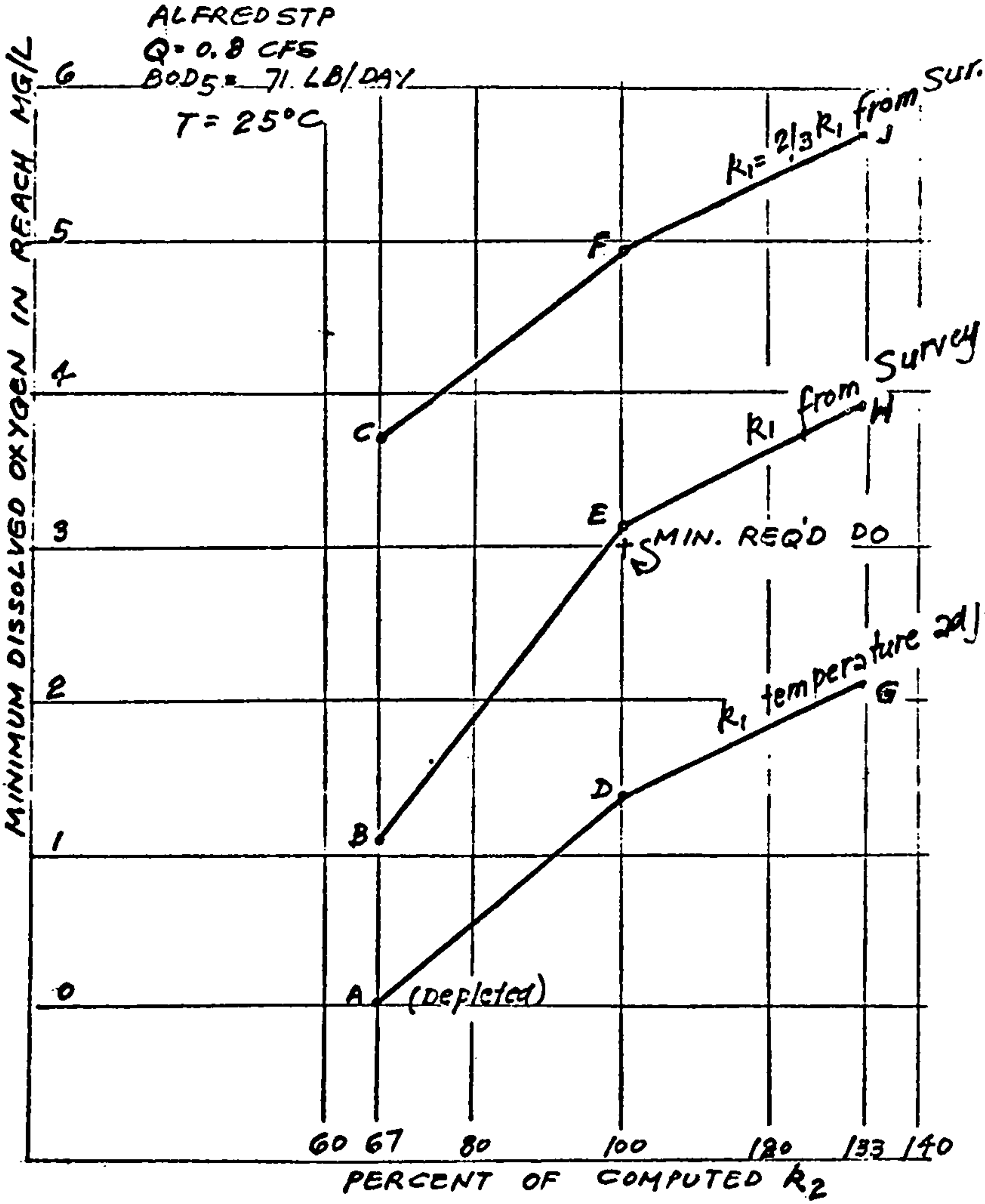

Figure 6. Sensitivity analysis for Canacadea Creek.

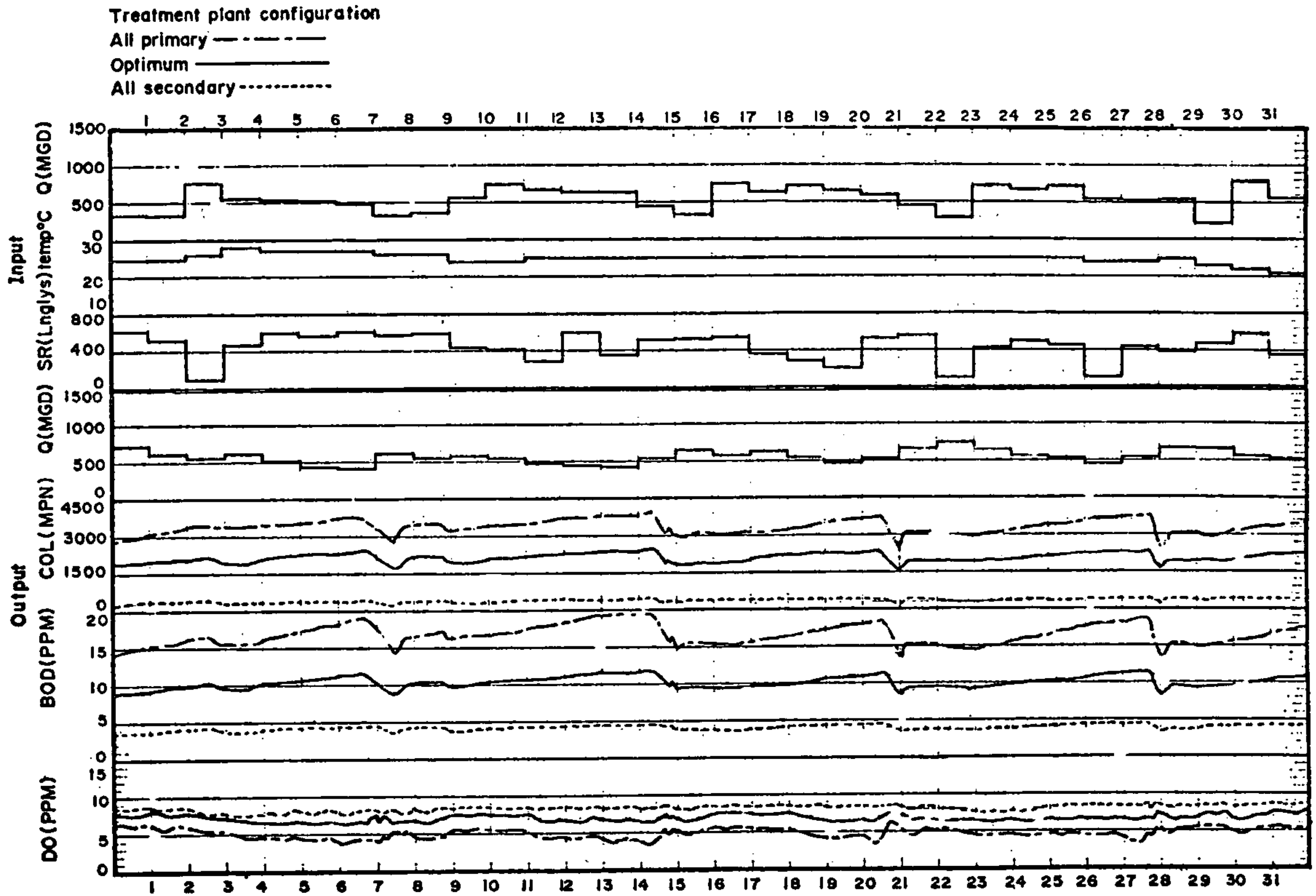

Figure 7. Example of time varying simulation for one station for one month.

MICRO-POLLUTION IN ORGANISM

by

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FOREWORD

What is the real meaning of "water pollution?" This is a very complex question which hardly can be answered by a single sentence. Maybe a simplified explanation is the following:

The polluted water can cause damage or fatal effect on the fauna and flora, including the lowest level of life. The effect may not necessarily be uniform for every living organism.

During the human history there were temporary water contamination which was able to cause great disaster to the human population, and it was well known from the middle ages on. The polluted water was able to cause communicable diseases such as, cholera, typhus, malaria, dysentery, etc. Sometimes the situation was so bad that certain people changed their drinking habit to avoid disaster. For example; in China tea was established as the drink among the wealthy, but the poor took only water to drink, and they avoided major disasters from the infected waters for thousands of years. In Europe, in the 15th and 16th centuries the name for typhus was "Morbus Hungaricus," because the bacterial contamination of the water was general in this country. Some changes occurred in the 18th and 19th centuries when the Industrial Revolution evolved. With the development of technical and scientific knowledge, they soon found out the cause of these rare diseases and curbed it to a minimum. The industrial and capitalist nations established financial laws which regulated the market and money exchange to make the industrial life more prosperous and financial life safer. To produce cheaper than the competitor was the practice and this part of the industrial development passed unchecked. For the cheaper product, the manufacturers dumped the disposal into the waterways, our lakes and our rivers. Some of this water became so badly contaminated with chemicals and other poisonous substances that many rivers and lakes became unsuitable for animal or plant life. Meanwhile the air became unhealthy.

After the first World War, when the first Communist country developed, their final target was the industrialization, as quickly as possible, and the price was not important. They also polluted the water and air in large scale.

Today many people are aware of the harmful effect of pollution, and they tend to do something about it. However, there is another environment which is a controlled environment of the living body, the organs and cells, and now this environment also is endangered. The water which must be used to replace the natural water loss of the organism is not safe. Our food and drink is contaminated with so-called safe chemicals; such as, stains, preservatives, artificial chemicals, medically claimed safe drugs. All find a way into the uncontrolled environment of the body. Yes, many of these chemicals have been used for centuries by millions of people and nobody noticed any harmful effect. This observation was superficial and not thoroughly investigated. Most of the observation was with adult organisms which were already developed, and these drugs made little or no harm at all. At the same time nobody was questioning the reaction of the young undeveloped life, which may be more sensitive to the exposure of these artificial drugs.

The purpose of this experiment is to make man aware of the sensitiveness of the unborn animals, especially mammals.

"All things that live, endure for some span: The century-old tree, the one-day beetle, grow conscious, joy and love, and pass away when they have reached their own appointed aims. Time does not move. 'Tis only we who change. A hundred years are but as one brief day."

Lucifer, in The Tragedy of Man
Imre Madach

Experimental teratology and drug testing is an extremely sensitive operation. Not so long ago, in the early twenties, mammalian experimentation was unknown, but the malformed, defective human and animal newborns were not. In this time and a decade later, the general view was that the mammalian embryo is in the safest place in the world, where no harmful effects can reach it. Thus, all malformations of the embryos in the maternal womb were blamed on genetic errors.

In the 1930's Josef Warkany of the Medical School of Cincinnati carried out animal experimentation on a large scale. His experiments proved that external factors could definitely cause malformations in research animals. This new discovery turned the animal research in 180 degrees.

Congenital malformations are structural defects present at birth. They may be gross or microscopic; on the surface of the body or within it; frequent or sporadic; hereditary or non-hereditary; single or multiple. It is necessary to make clear definitions of words like congenital malformations and teratology because many times the two terms are misused. In short, the name of this science is congenital malformations. If physiological malfunctions are present it is called congenital anomalies. Teratology is an adjective related to the science. Teratogenic implies causation or production of congenital malformations. Although the word "teratogen" is chiefly applied to environmental causes of congenital malformations such as drugs, chemicals, and viruses, it is obvious that abnormal genes and chromosomes can also be teratogenic.

Animal experimentation can be very useful for the interests of human evaluation. However, there are certain serious difficulties that do not permit the application of animal experimental results to the human level. Some of the difficulties are the following:

1) The reaction to a teratogen may vary greatly according to the route of administration. Oral administration to the mother may be harmless, whereas intravenous or intraperitoneal injection may easily reach the embryo and destroy it.

2) There exist differential susceptibilities to drugs at different ages. The effects of a drug differ greatly before, during, and after organogenesis.

3) Animals that carry more than one offspring demonstrate that a teratogen administered to the mother may produce different types of malformations in different numbers in a litter. Some of the embryos may be affected by the drug and others may not.

4) The time of administration does not always determine the morphologic changes in the embryos. The offspring can be genetically different. Although they may have been formed correctly they can still be deformed by secondary destructive forces so that malformations can arise after the organogenic period.

5) The reactions to a teratogen vary greatly from species to species. There are teratogens, including drugs, which regularly affect rats but not mice and vice versa.

6) Effective doses sometimes vary greatly in different species even when adjusted to the weight of the test animal.

These well established facts imply that animal experiment results, which can vary from one species to another, are not necessarily applicable to human beings. Even within a species a drug may have varying teratogenic effects on the embryo of different strains. This has been shown clearly by the effects of cortisone on different strains of mice.

Failure to observe offspring with congenital malformations may be due also to drug effects that are serious as to cause death of the embryo in utero before they are born. Since such embryos can be reabsorbed in some species, teratogenic effects will go undetected unless a special search is made for deformed embryos at early stages.

These are some of the facts, which explain the limited value of tests performed on animals in predicting effects of drugs on human embryos. Teratologic experiments on animals can only suggest similar effects in man but never prove them.

The experimenters in this research paper followed precisely the "Teratologist's Creed," the so-called "TTDS" which stands for: 1) appropriate Time, 2) appropriate Treatment, 3) appropriate Dose, and 4) appropriate Susceptibility (Fraser 1964). The fact that the teratologists creed was followed as closely and accurately as possible, makes the experimental results for the animal used as a parallel, more valid. The results of this experimentation cannot be applied to human beings. It is only a warning that the chemicals used may be harmful to humans. Much human experimentation and observation are necessary before this data can be related to the human being.

In this laboratory teratogenic effects have been studied since 1971. At that time the model animal was the amphibian <u>Rana pipiens</u>. Lysergic Acid Diethylamide (LSD; granted by the H E W) and caffeine were investigated. <u>Rana pipiens</u> was chosen for many reasons. For example, it has external fertilization and the day by day development can be observed without difficulty. Also, the fertilization time can be precisely pinpointed by means of induced ovulation and artificial fertilization.

In the cases of both drugs and the human lethal dose was used as a guideline and was broken down according to body weight of the frog. This certainly was a violation of the "TTDS" and the principles of teratologists, because data from one species was applied to another without an experimental approach. By this method the researcher was not able to determine whether the dose was too high or too low for the amphibians. 0.1 micrograms of LSD was injected into the dorsal lymph sac of female frogs concurrently with the induction of ovulation. Twenty-four hours later ovulation started. The control group received the same amount of pond water. The results were striking. The control group averaged about 93.1% fertilization. Two thousand eggs were involved in the fertilization process and only 0.4% developed to the tail bud stage. Many of the tadpoles had severe damage to the central nervous system, some developed as a "belly" embryo, missing the head and central nervous system.

Frogs treated with 0.1mg of caffeine averaged only 12.5% fertilization. When an additional 1.5mg of caffeine was added to the eggs of the treated females fertilization dropped to 4.4%. These experiments were not without criticism but they dramatically demonstrated a point.

In this laboratory in 1973/74, with Lambert and Restaino, investigated the effects of caffeine and aspirin, the most commonly used human drugs, on Rana pipiens. To avoid the former mistake, the lethal dosage was not directly transferred from human data but experimentally determined for the frog. The results showed that Rana pipiens was 25% more sensitive to caffeine and aspirin than rats and humans. Using 15-25% of the lethal dose of aspirin the fertilization rate dropped drastically from 70% to 6%. Another group of frogs, given 2.5% and 7.5% of the lethal dose of caffeine, reached fertilization rates of 80% and 59% respectively.

In 1975 with Restaino and Vacante set to the task of using mammalian models for their investigations. They encountered certain difficulties using laboratory rats as models. They were:

1) Pinpointing ovulation time.

2) Introducing the drug.

3) Determining the time when the fetal development must be observed.

4) Determining the lethal dose.

The vaginal smears of mated females were checked every morning for the presence of sperm. If sperm were found it was considered the zero day of development. Then the drug was administered via the stomach of the female. After the threshold dosage of each drug was determined, 25% of this dose was used for administration. Interestingly this experiment showed major malformations in 12 day old fetuses of these female rats; especially in the central nervous system.

The researchers used caffeine labeled with C^{14} and traced the drug 6 hours and 12 hours after the injection. The labeled caffeine showed the highest level of concentration in the uterus, ovary, oviduct, brain, spleen, and liver with the lowest concentration. This did not explain why the caffeine accumulated at such a high in the genital system and such a low level in the liver and brain. The question remained open.

In the next year, 1976, with Smith and Vacate, further investigated these drug effects. The researchers first changed the method of administration of the drug. The intraperitoneal injection had two weaknesses. Both drugs in humans are taken by mouth, and are never taken by intraperitoneal injection. A gavage needle was devised which guided the drug directly to the stomach. Thus, there was no chance of making contact with the urogenital system first as it could with the intraperitoneal injection. This way the drug had to go through the regular route of metabolism of food particles; intestine, hepatic portal, posterior vena-cava, heart, and different parts of the body.

In those experiments 12% of the lethal doses were used in both drugs. Most of the offspring had abnormalities in the nervous system and limb development. Labeled caffeine and labeled aspirin were used for tracing. In both cases again the ovary, oviduct and uterus were the sites of the highest concentration of the drugs. In the case of the caffeine the oviduct had 18 times higher readings than in the liver.

Histological methods were also used to demonstrate the deformities encountered. Dead implantation sites were removed from the uterus of drug injected females on the twelfth day of pregnancy. Cross sections of these sites showed evidence that these sites were reabsorbed, because the syncytiotrophoblast cells reversed themself and invaded the deciduous now attached to the embryo. The cells phagocytized the embryo until it was completely reabsorbed.

MATERIALS AND METHODS

Animals Used

The animals used were _Rattus norvegicus albicans_, the common laboratory white rat. The Sprague-Dawley (S/D) strain was selected for uniformity. The animals were purchased from the "Sunrise Farms" in New Jersey. The female rats' body weight ranged from 200 to 250 grams and the male rats' body weight ranged from 250 to 300 grams. All of the animals were in good condition and their health excellent. The rats were kept in the animal room where they received the necessary care.

Mating

To introduce the drug into the female rat as soon after mating as possible it was important that the mating time be known. Therefore, an artificial day and night sequence was established in the animal room. It is known that the mating of rats usually occurs in the early hours of the morning while it is still dark under natural conditions. In our animal room darkness was set to start at two o'clock in the morning. This was important for two reasons. First, the sperm can be found in the vaginal smears which indicates mating. Second, the drug could be administered only a few hours after mating. (In our estimations about six hours after mating). When administration took place the zygote was still in the one cell stage. The day on which sperm were found in the vaginal smears was the zero day.

Chemicals Used

Labeled caffeine and aspirin were purchased from New England Nuclear, Boston, Massachusetts.

Anesthesia

All pregnant female rats were sacrificed. First the female rat was put under deep anesthesia by ethyl ether and then killed by cardiac puncture after opening the abdomen. The anesthetized rat was placed on a small operating table and the abdomen opened along the linea alba. Then the xiphoid process was held up with a pair of forceps and the diaphragm cut to open the thoracic cavity. Finally the ascending aorta and the anterior vena cava were severed with a pair of scissors.

B. Administration of the Drugs to the Mated Female

The determination of the effects of a precisely controlled amount of drug on an animal's system is more accurate if the drug is introduced directly into the stomach. The gavage method was selected. The gavage needle was made by Clay Adams Company. It was custom made for rats; was a 16 gauge, four inch long gavage needle with a small metal ball at the end to avoid injuries when inserted into the pharynx and esophagus. The needle was attached to a three cm^3 syringe for measuring the exact amount of drug.

Anesthesia was not required for the administration of the drug into the stomach of the female, because of the quickness and painlessness of the method. Also it was necessary for the rat to be in an awakened state to be sure the drug entered the stomach and not the lungs. One researcher held the rat immobilized and the head was at a 45^o angle to the stomach. Usually, in this position the rat opened its mouth and no force was required to insert the gavage needle. The researcher could then insert the needle with a free hand. Care was taken to follow the curvature of the mouth and pharynx with the bulb of the needle before entering the esophagus. A small force was necessary to push the instrument through the isthmus of the nasopharynx.

C. Threshold-Lethal Dosage Determination

It is important to follow the teratologist's creed. The appropriate time was determined by the workers, one cell stage zygote. The appropriate treatment was established also and the drug was sent through the regular metabolic pathway; through the stomach and liver.

It was necessary to determine the appropriate dosage by establishing the lethal threshold of caffeine and aspirin. The lethal threshold is the dose at which 50% of the rats die within 24 hours, but others survive. First, a very large dose was given, 200mg in the case of caffeine and 1g in the case of aspirin. All of the rats died. The dosages were cut in half, 100mg of caffeine, 500mg of aspirin and the results were the same; all of the animals died. In the third trial the dosages were cut in half again, 50mg of caffeine and 250mg of aspirin. The animals which were given the 50mg of caffeine all survived the 24 hour period but in a very weak condition. Some of the rats given the 250mg of aspirin died in the first 24 hours but others survived. The lethal dose of caffeine was established as 60mg and the lethal dose of aspirin as 250mg.

It is just as important to determine the lowest dosage threshold which is not harmful to the animals. The dose was measured.

Results From the Caffeine Administration

Control group was established. The rats received only saline through the stomach, the same amount of liquid which will be administered in the rats.

After 12 days the pregnant control female rats were sacrificed and the uterus exposed. Each horn contained 7 implantation sites. The vascularization was excellent,the color light, not dark. The implantation site in the uterine horn measured 5mmx 10mm. Then, the embryos were operated out from the uterus and measured and examined gross anatomically. The crown to rump (CR) measurements were 5mm per embryo.

Two control rats were examined and only one partially absorbed embryonic site was found of the 28 implantation site which is only 3.57%.

It is necessary to explain the entire evaluation procedure which was followed through this experiment. The rats which were killed by cardiac puncture, were then removed of all the viscera from the abdomen, except the urogenitals. First the uterine horns are layed down to investigate the implantation sites. The uniformity of the sites, the vascularization, and the color were registered, also the number of the embryonic sites and the distances from each other. The reasons for this data collecting are the following: 1) Uniformity is checked for retardation or dead sites. 2) Vascularization is checked for the sufficient blood supply from the uterine artery. If branches supply the uterine horn well, where no implantation site is visible, there is good reason that was an early dead embryo, and the site is already reabsorbed, only the vessels indicate the former place of the embryo. 3) Number of site is noted and also the number of the corpus lutea in each ovary. 4) Color was important for determining the living shade of the site.

When the general appearance of the uterine horn and the ovary were registered, the embryo was removed from the uterine horn.

With two watch maker forceps the uterine wall was torn over the implantation site. It needed a steady hand to separate the amnion from the chorion and the placenta.

Upon tearing the uterine wall the stressed amnion emerged from the uterine wall, naturally enclosed the embryo.

Then the embryo with the amniotic sac will be worked out from the uterus with watch maker forceps. Dexterity and care are needed for this because of the thin layer of the amniotic sac. When it is out, with the aid of a microspatula this embryo will be placed in warm (38oC) physiological saline (.9%) in a petri dish and examined under the dissecting microscope for further inspection and observation.

The observation must be done quickly and accurately; even the embryo's heart was still beating about 1.5 hours after the maternal death. (Picture 1)

The embryo in the amnion was transferred under a zoom dissecting microscope to see if there were any abnormalities which could be determined with the amnion intact. Gross deformities could be seen through the amniotic membrane which proved that the observed deformity was not caused by the removal of the membrane or secondary injury during the operation.

When the membrane is removed the final gross phenotypic examination occurred. If the embryo was a subject for abnormalities, but it was not observable to the phenotype, serial cross sections were made.

Caffeine

A 13% solution of the lethal dosage was made in solution, 160mg of powdered caffeine was dissolved in $40cm^3$ of water and containing 4mg per cm^3. On each occasion $2cm^3$ of solution or 8mg caffeine was administered which was equivalent to 13% of the lethal dosage (lethal dosage 60mg). Gavaged 2 rats with 13% of caffeine, and sacrificed at the 12th day of gestation, we had the following results.

The uterus was almost empty only one reabsorbed site can be seen close to the junction of the two uterine horns, but the uterine horn in the whole length was thicker than normal. The ovary showed good size of the corpus luterum, which indicated the pregnancy.

It was interesting to know if the 13% of caffeine was evenly distributed to the 12 days of pregnancy, would it make any difference in the development of the embryo; or in other words giving 1% of the drug daily. Two rats were involved in this experiment. In both cases the diagnosis was the same.

Vascularization is good, ovaries have corpus lutea. There were no reabsorption sites, the left horn had 5 sites and the right had 9 sites. In the other rat the right horn had 8 sites, and the left 6. The implantation sites were not uniform but alive. Embryos from the right horn showed slight retardation in size, more severe retardation was found in embryos coming from the left horn.

Final experiment in the 13% group was to introduce 13% of caffeine at the 6th day of gestation. In this experiment only 1 rat was used with the following results: General condition of the uterus and the implantation sites were good and they were well vascularized. The right horn contained 6 sites; the left horn also 6 sites. The sizes of the implantation sites were uneven. Counting from the ovary the first and second sites were smaller than the others but they were alive. In the left horn also the 1st site was smaller. The other sites were unevenly placed. Checking the corpus lutea in the left ovary disclosed that there were originally 8 developing embryos.

It was clear that 13% injection of caffeine administered at 0 day of pregnancy can cause serious damage in the developing embryos, so they die before they reach the 12th day of gestation. It is also clear that the same dosage given evenly divided in 12 cause little or no visible damage. If the whole dosage were administered at the 6th day of gestation, same site were found reabsorbed, but it can not prove it was caused by the drug. To follow the appropriate time, the rat embryos are the most sensitive to the drug if it was administered at the 0 day.

The next group of pregnant rats received only 6.5% of the lethal dosage. The results were mixed, only one specimen of the 6 females used in this part of the experiment had fatal reabsorbance.

It is demonstrated that 3 slightly enlarged uterine segments can be seen. The uterine horn with one of these segments was cut out for further physiological examination.

The next female had good vascularization. The sites were evenly spaced in the right uterine horn. The 6 implantation sites were differently developed from each other. Counting from the ovary the first site was only 5x6mm. The second CR measurement was 4mm., which shows poor development, and the third site was almost normal measuring 5x9mm. The other sites were under reabsorption. (Picture 2)

A histological section of this site going through reabsorption, only the placenta and the lumen with the embryonic remnant was found. (Picture 3)

In higher magnification (X100) the embryonic remnant can be seen better in the small lumen. Surrounded by large invading syncytiotrophoblast cells and the outer layer consisting only of cytotrophoblastic cells.

In x1000 magnification is shown the large syncytiotrophoblast cells. The third female had 11 implantation sites; 5 in the right horn and 6 in the left. (Picture 4)

In this left horn the first two sites were reabsorbed.

The fourth specimen had excellent vascularization, none of the sites showed the state of reabsorption, all were alive, with their hearts palpitating. The size of the embryos were different, some were very small and retarded.

Here two embryos are being compared; one is normal and the other is retarded. (Picture 5) Even in the retarded embryo the blood in its heart and some of its blood vessels can still be observed. But it is small and monstrous in appearance. The telencephalon is underdeveloped, there is a notch in the metencephalon area just behind the isthmus. The mesencephalon is severely retarded and the mandibular arch is widely separated from the maxillary process, the front leg looks larger than in the normal embryo but the hind leg can barely be seen. In the cross section, the lens is not detached from the ectoderm and the sensory retina lies closely on the developing lens; in other words, the vitrous humor chamber is not developed at all. This specimen had 9 embryos in the right horn and 7 in the left. The fifth female in this series had 7 embryos in the left horn and 8 in the right uterine horn.

The general conclusion of the 6.5% group is that many malformalities occurred, as well as reabsorption. The 6.5% is administered to the pregnant rat on the zero day, with the being very critical, but variable. In the last series of the caffeine experiment was the 3% lethal dosage. Four female rats were used. All of them received the caffeine on the zero day. The results were still mixed. One female rat had thickened enlarged uterine horns. Some implantation sites were found as a small dark area within the horn. The vascularization is still a strong indication for former embryonic positions. The ovary had corpus lutea. The next female had evenly spaced embryonic sites on the uterine horn, but were unevenly developed in size. A few were dead and some of the living embryos were malformed. Six sites were observed on either side of the uterine horn.

The third specimen had 17 implantation sites, 9 in the right horn and 8 in the left. Ten of them appeared as normal in gross observation, but two were in the reabsorption state, and five as appears retarded, especially in the brain area as compared to a normal embryo.

The last female of this group had 7 sites on either side of the uterine horn. All sites were alive, individual embryonic showed that only 3 had visible retardation in the brain development, but no others. There remained a lot of questions as to whether these embryos which were judged as normal, by gross observation, were they structurally normal or not. Making slides of fetal specimens in serial cross sections revealed that they are far from normal. Many had circulatory malformations, the posterior vena cava wasn't developed, but the posterior cardinal veins were the principal veins, also single chambered atrium and ventricles. Paired dorsal aorta and anterior cardinal veins had malformalities. The mesonephrose and metanephrose rudimentally developed. Split external naris which open dorsally and ventrically in the rostrum, and also the under-developed eyes! (Picture 6) The septum development of the heart is malformed. (Picture 7.)

Results of Aspirin Administrations

All of the methods for administering the drug on the zero day of the pregnant S/D rats were the same for the aspirin experiment as was with caffeine. It was clear from the work of Smith and Vacante that 12% aspirin caused severe damage to the rat embryo. This experimentation started with a 6% solution of the dosage of aspirin diluted in oil. Four pregnant rats were used in this experiment. The first rat uterus had excellent vascularization. Each uterine horn had ten implantation sites, all together, 20 conceptus. Three of them were in the reabsorbing state. Seven conceptus developed and 10 were normal in gross phenotypic examination.

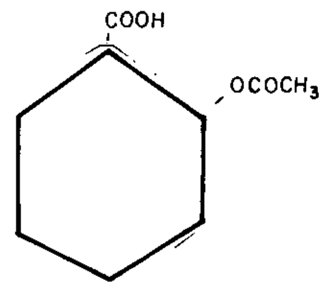
Picture 8 is a pair of embryos, the right one is a monster. The whole brain area is malformed, especially the eyes which are poorly developed. The mesencephalon and there is a deep notch present within the metencephalon. Against this abnormal embryo is a normal one to compare. The strong and healthy development of the brain area is evident by the size and shape of the embryo. Both embryos were alive, determined by the beating heart.

Tracer C^{14} Labeled Caffeine and Aspirin in the Early Pregnant Female Rat System.

An explanation of the destroying effects on the early embryo by caffeine and aspirin would only be partial if the biotransportation of these two drugs was not investigated. It was planned that radioactive labeled aspirin and caffeine would be tested.

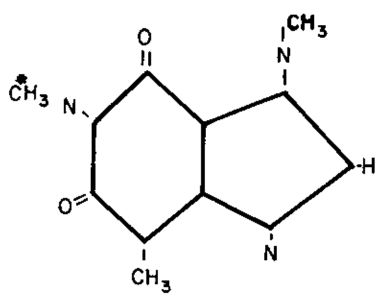
The drugs were administered by the gavage needle; four rats received caffeine, and four received aspirin. The rats were sacrificed 18, 24, and 48 hours after administering the labeled drug. The fourth rat was injected on the eighth day of pregnancy and sacrificed 6 hours later. We used these times since Smith and Vacante, 1976, used the 6, 12, and 24 hour timing; we wanted to compare our results to make them conclusive, while also receiving new pertinent information about the pathway of these two drugs.

From the sacrificed rats, six organs were removed and prepared for radioactive readings. The brain was selected since both drugs affect the brain which receives substantial vascularization. The second organ is the liver. This organ was selected for the reason that any substance absorbed into the blood stream must enter into the liver via the hepatic-portal system, also the liver is the first and major filter of the body against all harmful drugs and chemicals. The third choice was the kidney because the blood is filtered there, where toxic wastes are removed and the kidney is of mesodermal origin. The remaining three organs are the ovaries, oviducts, and uterus. The purpose was to see if the drugs were absorbed by these organs and to what extent. All organs were prepared for the radioactive reading in the same manner. For the labeled caffeine study, each rat received .04mg and .05mci of radioactive drug; for the labeled aspirin study each received .04mg and .05mci. The metabolic breakdown of aspirin or salicylic acid occurs in three steps:



1) salycilovic acid, 2) Ether or salycilate (Phinolic glucuramide) and 3) Ester of salycilate (Acylglucuramide). Part of the metabolic product is oxidized to geutisic acid, the metabolites found in urine. Salicylates are excreted by the kidney, and only a small portion leaves the body as a metabolite, staying in the body for one or two days.

Caffeine is a methylated purine which has stimulating effect on the central nervous system. Its structure is:



The caffeine is also a weak stimuli for gastric secretions.

At this time we were interested to know with the aspirin and caffeine, when administered into the stomach and had gone through the metabolism, did they reach the target organ? In what dosage? Also, what concentration was present after a specific time? The C14 labeled caffeine and aspirin were purchased from New England Nuclear (NEN).

In 1976, Szebenyi, Smith and Vacante used C14 labeled aspirin and caffeine in the body, introducing the drug into the system and sacrificing 6, 12, and 24 hours later. They used the following list of tissues: brain, liver, spleen, ovaries, oviducts, and uterus. According to their experiment the highest reading for aspirin after 6 hours was in the ovaries at 148, oviduct next at 92, uterus 38, spleen 16, liver 6, and brain 2. After 12 hours the highest reading was in the uterus at 362, and after 24 hours the highest reading was still in the uterus but in a lower concentration at 60.

The labeled caffeine after 6 hours was read and found to be the highest in the oviduct at a reading of 198, next the ovaries at 168, uterus 66, spleen 12, brain 10 and liver 7. At 12 hours after administration the oviduct had a reading of 312, ovaries 202, uterus 90, spleen 14, brain 8, and liver 2. Finally at 24 hours the ovaries again had the highest reading of 126, then the oviduct at 106, uterus 36, spleen and brain 4, and liver 2. This data suggest that the highest concentration of the labeled drugs accumulated in the genital system.

Szebenyi, Smith and Vacante used only non-pregnant females in the radio-tracing experiment. In this years' experiment, we decided to check the accumulations of the two labeled drugs in fertilized females at 18 hours, 24 hours, 48 hours, and also a pregnant rat on the eighth day of pregnancy and gavaged 6 hours before it was sacrificed as mentioned earlier.

In this year's research a different technique was used from the 1976 experiment for radioactive reading. After removing the organs we chose from the pregnant rat, they were homogenized and mixed with .9% sodium chloride to a fixed value. Tables III and IV. At St. Mary's Hospital, under the supervision of Dr. Hordynsky, the samples were centrifuged at 2200 rpm for ten minutes. One millimeter of the supernatant was removed and then was mixed with either 5 or 10 cm3 of a phosphorous cocktail solution. We read the emission for one half a min, in a machine designed to count C14 radiation in solutions. This technique appeared more accurate than last year's ashing technique because some of the C14 radiation could escape as a volatile hydrocarbon, thus influencing the reading unless very strict procedures were followed. After computing the readings to counts per minute per gram of the tissue and percentage present in comparison to the oviduct, we got the following results. In the labeled aspirin experiment, the 18 hr. rat had the highest concentration in the oviduct at 600, next the uterus at 440, ovaries 400, kidney 156.5, brain 75, and the liver the lowest at 17.2. The 24 hr. rat had the highest readings in the uterus at 1200, next the oviduct and the ovary with 1000, the brain 153.8, kidney 75 and the liver with the lowest reading at 21.6. The 48 hr. rat had the highest reading in the oviduct with 2000, ovaries 400, uterus 200, brain 81.1, liver 66.6 and kidney with 6.6. The 8 day rat had its highest reading in the oviduct with 2800, uterus 1946.7, ovaries 1733, kidney 1109, brain 191, and liver 107. (See table III.)

In the labeled caffeine experiment the following results were observed. The 18 hour rat had the reading in the oviduct at 8000, ovaries 2400, uterus 1120, kidney 360, brain 185, and liver 158. The 24 hour rat we had to leave out because we had a large % error and we felt that it made this data invalid. Se Table I and II for absolute reading of labeled aspirin and caffeine experiments. The 48 hour rat again had the highest concentration in the oviduct at 1400, ovaries 800, uterus 333, brain 188, liver 140, kidney 107. The 8 day pregnant rat, after administration of the labeled caffeine was found to have the highest concentration in the brain at 2957, uterus 2733, ovaries 2300, oviduct 2000, kidney 463, and liver with 372. (See Table IV). To summarize the results of the labeled caffeine and aspirin experiment, the readings were calculated into a percentage where the oviduct reading was equivalent with 100 percent. In the labeled caffeine experiment, Table IV, it is clear that of the organs examined the oviduct, ovaries, and uterus showed the highest readings among all the organs consistently. Special attention can be given to the 8 day old pregnant which was at 38% of her gestation time, more than 1/3, and here the uterus with the implanted embryo had the highest reading with 2733 counts per gram. At this point mention must be noted that it wasn't investigated which, the uterine wall, the placenta, of the embryo of these absorbed the drug and it wasn't investigated if these embryos are affected at this point of development if the drug is administered this late time of pregnancy.

In the labeled aspirin experiment, Table III, that out of the organs examined the oviduct, ovaries and uterus again had the highest readings and the oviduct was the highest except in the 24 hour reading where the uterus was found with a reading 20% in excess of the oviduct.

The dosages of 6% and 3% were used in this experiment. These were calculated from the lethal dosage and at this amount it is considered low. Further experimentation with labeled drugs can also give light whether the males' genital organs collect higher concentrations of salicilates and caffeine. If it does, maybe the pathways and reasons for high concentration in these organs can be seen more clearly.

> "Earth engendered the members most grotesque;
> Monsters, half-man-half-woman, footless and
> handless, void of mouth or eye....
>
> Nature checked their vile growths....
>
> Hence, doubtless, many a tribe has
> sunk suppressed, powerless its kind to breed.--
>
> Einpedocles 495-435 B.C.

DISCUSSION

In the issue of Science November 26, 1976, was an editorial "Irrational Drug Prescribing and Birth Defect." The article is an important one and it states:

"Few physicians receive formal training in the correct use of drugs, but the average practitioner writes 7,934 prescriptions each year. Many of these prescriptions are irrational in the sense that the drug has not been shown to be effective for the purpose for which it has been prescribed, many are completely inappropriate because they represent a substantial hazard to the patient without any compensating benefits."

This article is an argument against the unnecessary drug uses by the physicians. The drugs are used frequently and some times with no experimentation against side effects. Therefore this makes more important, the animal experimentations which were introduced by Hale and then in larger scale by Warkany. By 1961 it was known to the teratologist that many drugs, including salicylates are teratogens when given at the right time, in the right dose to the right animals. In recent times caffeine came into the focus of the teratogenic research, which now strangely suspects that the caffeine had teratogenic effects in the human. This experimentation deals with the two most commonly used human drugs, caffeine and aspirin, to prove they have teratogenic effects on animal models. In 1970 Bartholomew reported that the caffeine has positive mutagenic effects. The most dangerous among the many mutagenic drugs are these which can cross the placenta as free drugs. Among those are the salicylates and the caffeine. Evans states that (1975)- Probably the most critical factor involved in drug-induced teratogenesis is in the utero age of the developing fetus. In a figure they show the adult female to have teratogenic susceptibility. In this chart they believe that the first 20 days of human development, the so-called "pre-differentiation" period is usually not susceptible to teratogenesis. They also stated, Organogenesis in humans begin about the twentieth day of gestation (the first somite stage) and continues for the most part through the third month. The risk of morphologic analysis is therefore greater during the first trimester (day 20-day 90) cie. during the period of the greatest organ development. Harbijou and Becker 1972 used DPH in the rat. If the drugs were administered during early gestation (day 7-10), hydronephrosis was the prominent morphological observation. However, administration on days 10 through 14 resulted in cleft palate formation. This categorical determination that the early embryonic life, (before the first somite) is not sensitive for the teratogenic effect of a drug is not an overall truth. It can be certainly true for the drug DPH, but not so for other drugs. It must be recalled the experiment with the rats, when the drug was administered on the zero day of pregnancy, its effects were more damaging when the drugs were administered through the half time of the pregnancy.

In this paper the embryos were in the earliest stage possible, there was no connection at this time with the maternal blood supply, it was possible to be able to enter in the upper third of the oviduct of the mother. Then an important question arises, how can the administered drug influence the early one cell stage preimplantation embryo? The possible answer may be from the results obtained by the radioactive labeled drugs. Why were both the caffeine and aspirin accumulating around the ovary, oviduct, and the uterus in the highest level; why are they not neutralized by the liver for excretion? When the drug administration occurred, the zygote still was covered with the corona radiata, and the follicular cells. It is possible that the follicular cells transported the chemical into the zygote? Certainly not is the answer: the follicular cells are separated from the maternal organism just like the zygote itself. But the tubat fluid is labeled the zygote with the surrounding corona radiata and this way maybe the follicular cells can pick up some of the part of the drugs. It is not proven yet but this can be the project to the next experiment to establish the route of the drug to the preimplantation embryo.

This experiment has the conclusions only for the Rattus norvegicus albicans and not in any way to apply for the human population. Many reasons can be listed which make the animal results not suitable for human condition. First the greater degree of inbreeding in any strains of laboratory animals than in the man, for example, the different metabolism of drugs in man compared to other mammals. The possible protective effect of the larger size and larger gestational period of the human fetus.

A one-day exposure to a drug, for instance, affects about 1/21st of the embryonic period of a mouse but only about 1/26th of the comparable period in the human. On the other hand, malformations of the human fetus might possibly result from massive doses of certain drugs given during a major part of the embryonic period, which fortunately are rarely administered to pregnant women in that fashion. If the reader agrees with Irvin Emanuel (1976) then a question arises in this experiment.

The preimplantation periods are similar in the mouse, rat, rabbit, in man and many other mammals. These 5 days of development are the same, and five days in some animals as development are concerned with be equivalent with 5 days in the other animals. During this time there is no organ differentiations, the five day term and in all of the cases with the development of the blastocyst stage. (Picture 9). this shows the four day old preimplantation embryo in the rats. This picture was taken in this laboratory, can be compared with any human embryology book development stage the hour day old human blastocyst stage confusingly similar. This also means that during this four day journey before the implantation is true in all mammals and can be compared on a day to day basis.

But to compare the drug effect is certainly not in the scope of this paper.

ACKNOWLEDGEMENT

My thankful appreciation to my many students who helped to carry out this chain of experiments since 1971. Without their enthusiastic and responsible work, the results could not be reached.

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TABLE I - Data of the Absolute Reading of Labeled Caffeine Experiment.

Rat #32, 18 Hrs.	Brain	Liver	Uterus	Ovaries	Oviducts	Kidneys
Weight in grams	12,1,3	7,11,4	8,.5	10, .1	11, .1	9,2.5
Homogenized solution in cc	10	50	10	10	10	30
Reading B group	24.0	36.0	56.0	24.0	80.0	30.0
% Error	0	0	0	0	0	0
Rat #34, 24 Hrs.						
Weight in grams	10,1.7	11	8,.16	6,.92	9,.37	7,2.6
Homogenized solution incc	35	50	10	10	10	30
Reading 1-12(a)	26.0	206.0	28.0	26.0	6.0	68.0
% Error	0	20.0	0	0	0	0
Rat #33, 48 Hrs.						
Weight in grams	5,1.6	12	1,.3	2,.2	4,.2	3,1.7
Homogenized solution in cc	30	50	10	10	20	30
Reading	0	0	0	0	0	0
Rat #30, 8 days						
Weight in grams	2,1.4	1,18	5,1.2	4,.2	6,.1	3. 4.8
Homogenized solution in cc	30	50	20	10	10	30
Reading	138.0	134.0	164.0	46.0	20.0	74.0
% Error	-	-	-	-	-	-

TABLE II - Data of The absolute Reading of Labeled Aspirin Experiment.

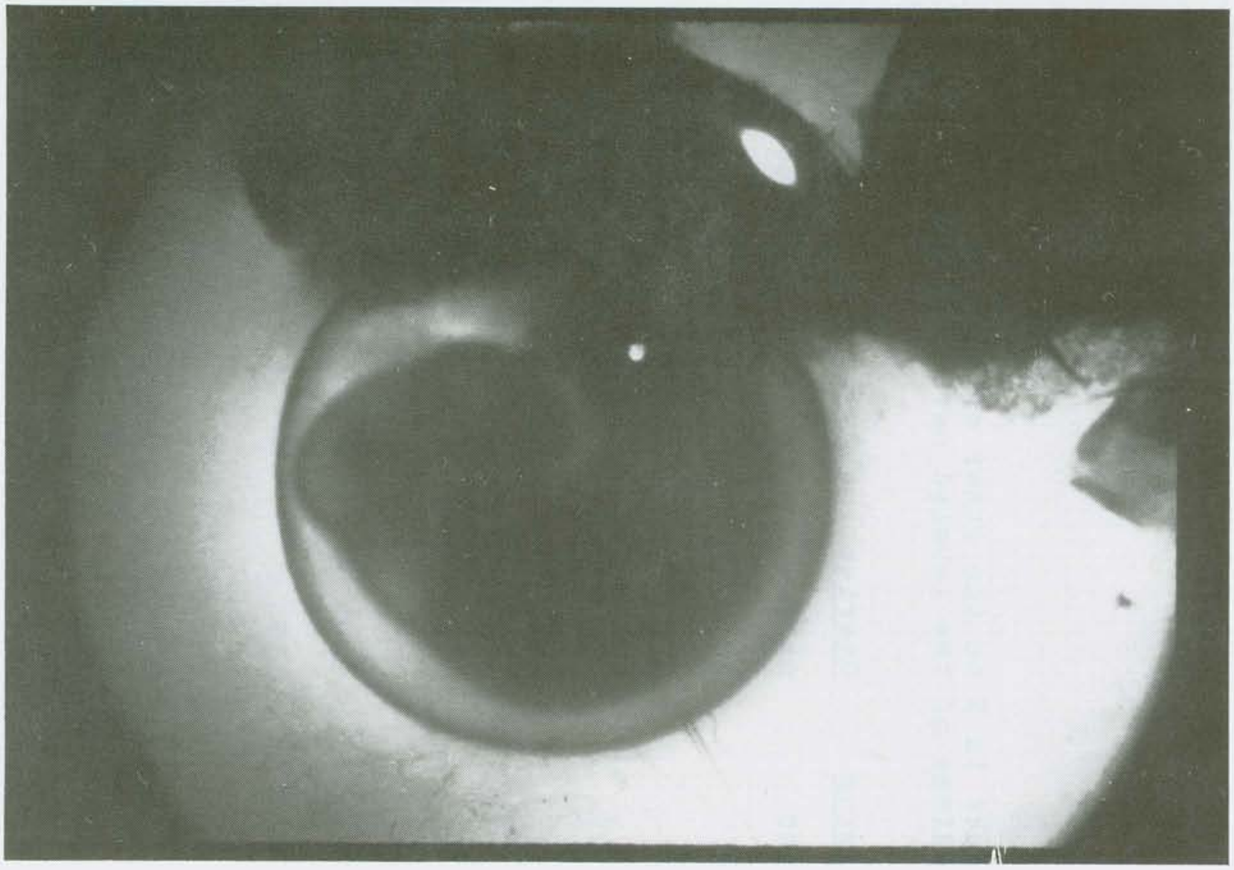
Rat #35, 18 Hrs.	Brain	Liver	Uterus	Ovaries	Oviduct	Kidneys
Weight in grams	16,1.6	14,11.6	11,.5	17,.1	18,.1	13,2.3
Homogenized solution in cc	10	50	10	10	10	30
Readings	12.0	4.0	22.0	4.0	6.0	12.0
% Error	-	-	-	-	-	-
Rat #31, 24 Hrs.						
Weight in grams	19,1.3	20,13.9	21,.2	22,.1	23,.1	24,2.4
Homogenized solution in cc	15	50	10	10	10	30
Readings	12.0	14.0	10.0	8.0	20.0	6.0
% Error	-	-	-	-	-	-
Rat #24, 48 Hrs.						
Weight in grams	25,2.2	26,10.5	27,.5	28,.2	29,.1	30,2.7
Homogenized solution in cc	10	50	10	10	10	30
% Error	-	-	-	-	-	-
Rat #29, 8 days						
Weight in grams	31,2.4	32,14	33,.75	34,.15	35,.1	36,3.3
Homogenized solution in cc	10	50	10	10	10	30
% Error	-	-	-	-	-	-

TABLE III Comparison of the oviduct in % to other organs and Computation of reading of lab, asp. experiment

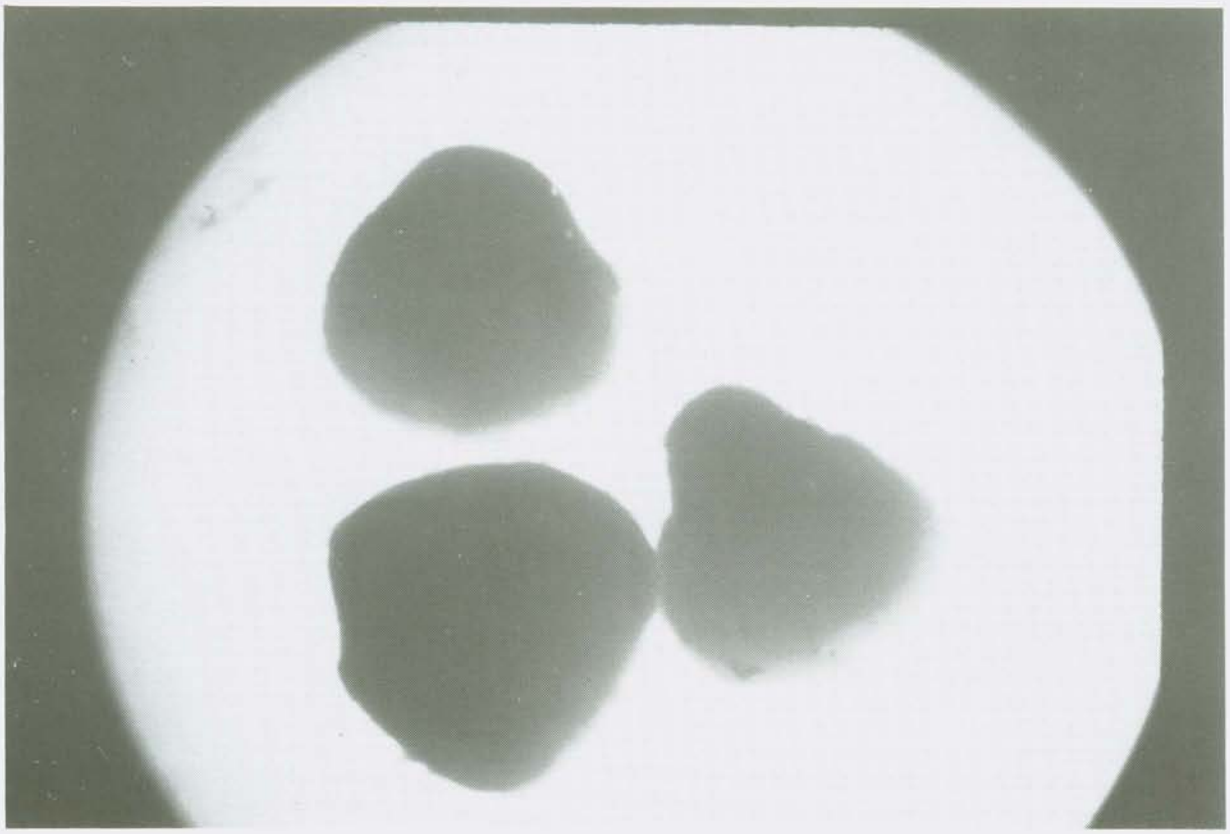
Rat #35, 18 Hrs.	Brain	Liver	Uterus	Ovaries	Oviducts	Kidney
cpm/gram	75	17.2	440	400	600	156.5
% in comparison with oviduct	12.5	2.8	73	66	-	26
Rat #31, 24 Hrs.						
cpm/gram	153.8	21.6	1200	1000	1000	75
% in comparison with oviduct	15.4	2.2	120	100	-	7.5
Rat #24, 48 Hrs.						
cpm/gram	81.8	66.6	200	400	2000	6.6
% in comparison with oviduct	4	3.3	10	20	-	.3
Rat #29, 8 days						
cpm/gram	191.6	1947.7	1733	107.1	2800	1109.1
% in comparison with oviduct	6.8	3.8	69.5	61.9	-	39.6

TABLE IV Comparison of the oviduct in % to the other organs and Computation of the readings of the labeled caffeine experiment.

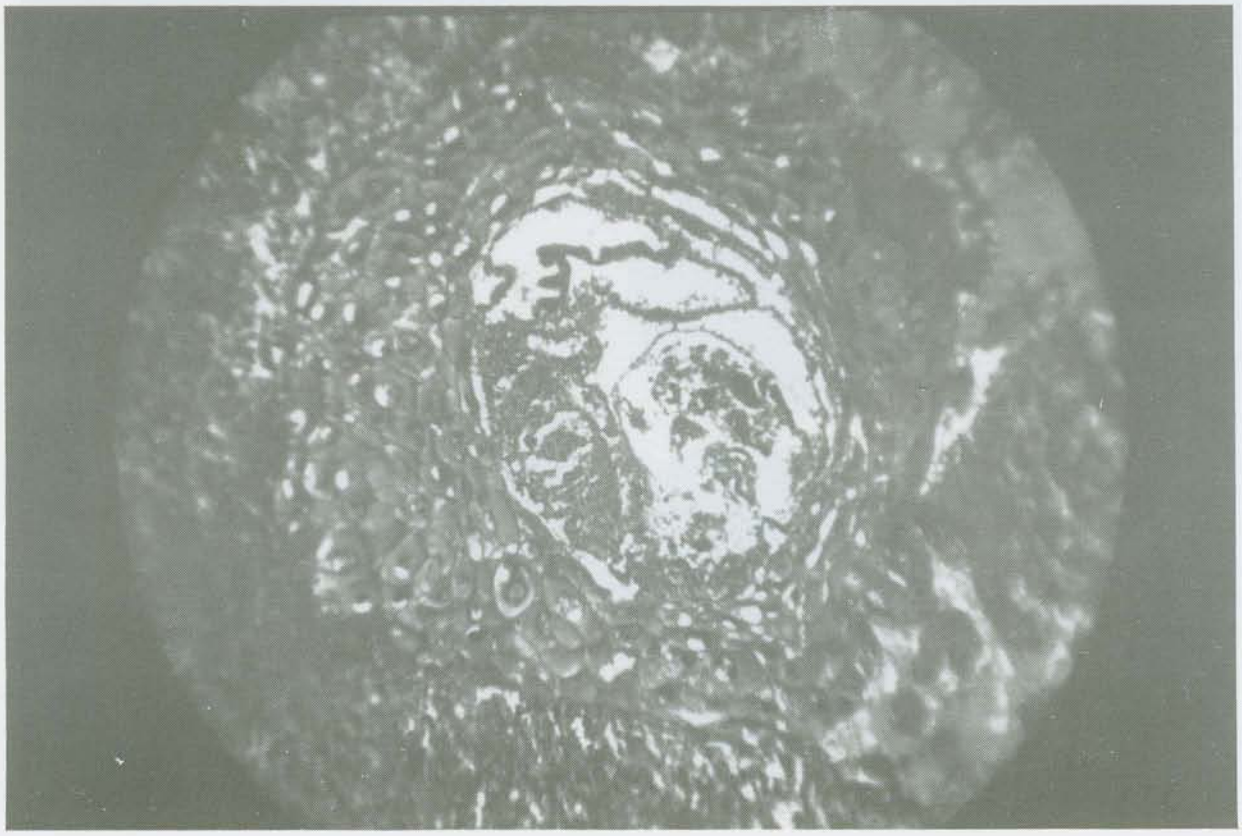
Rat #32, 18 Hrs.	Brain	Liver	Uterus	Ovaries	Oviduct	Kidney
cpm/gram	185	158	1120	2400	8000	360
% in comparison to oviducts	2.3	1.9	14	30	-	4.5
Rat #34, 24 Hrs.	-	-	-	-	-	-
Rat 33, 48 Hrs.						
cpm/gram	188	140	333	800	1400	107
% in comparison to oviducts	13	9.9	23	57	-	7.5
Rat #30, 8 days						
cpm/gram	2957	372	2733	2300	2000	463
% in comparison to oviducts	147	18	136	115	-	23.1



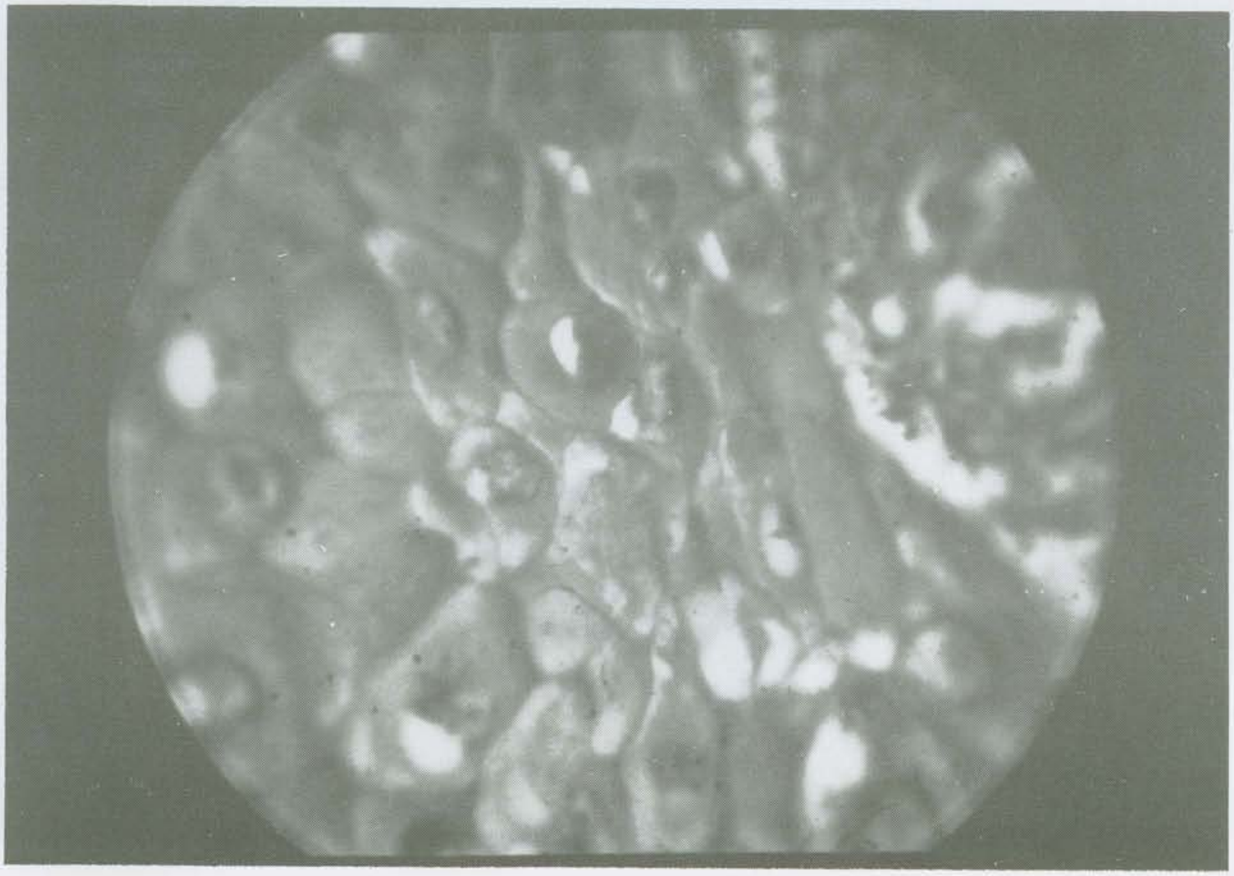
Picture 1. The embryo in the amnion.



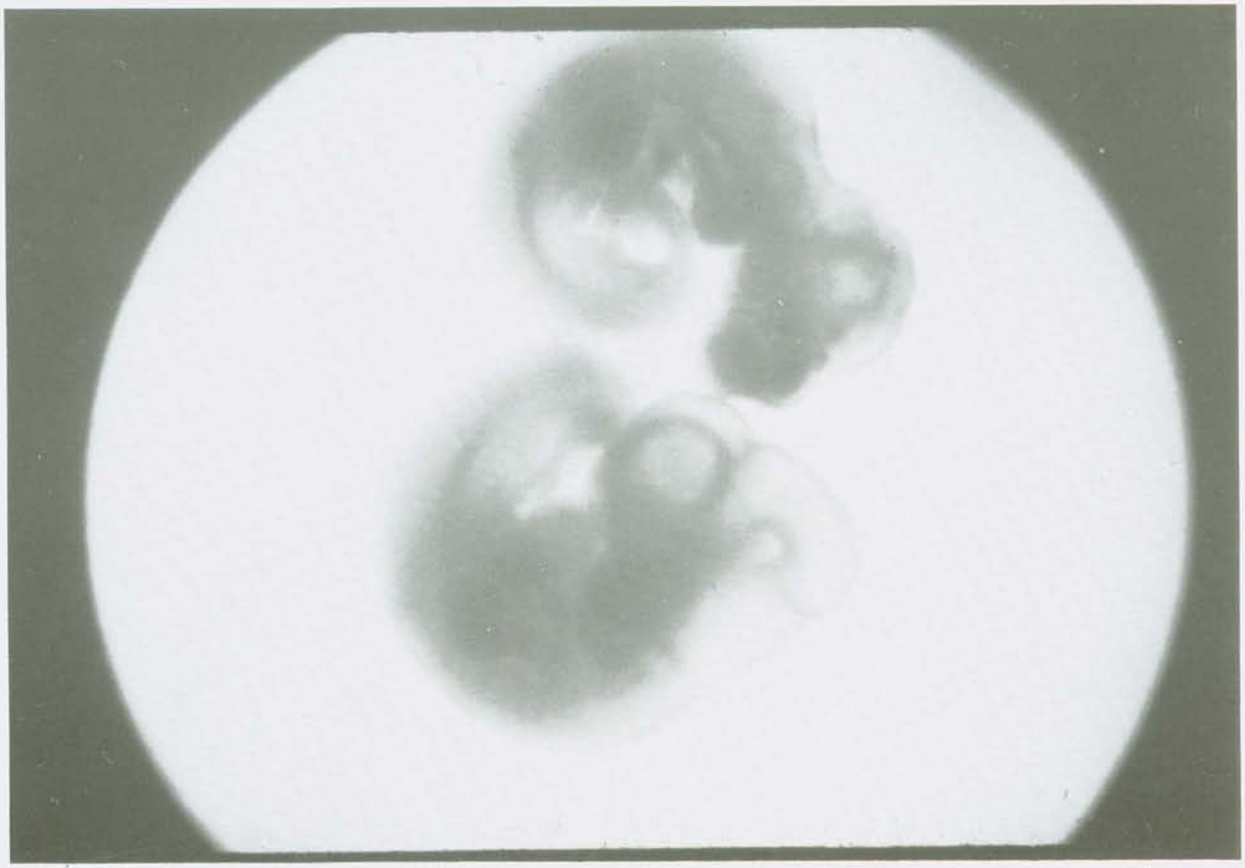
Picture 2. The embryos under reabsorption.



Picture 3. Histological section of the uterus and reabsorbing embryo.

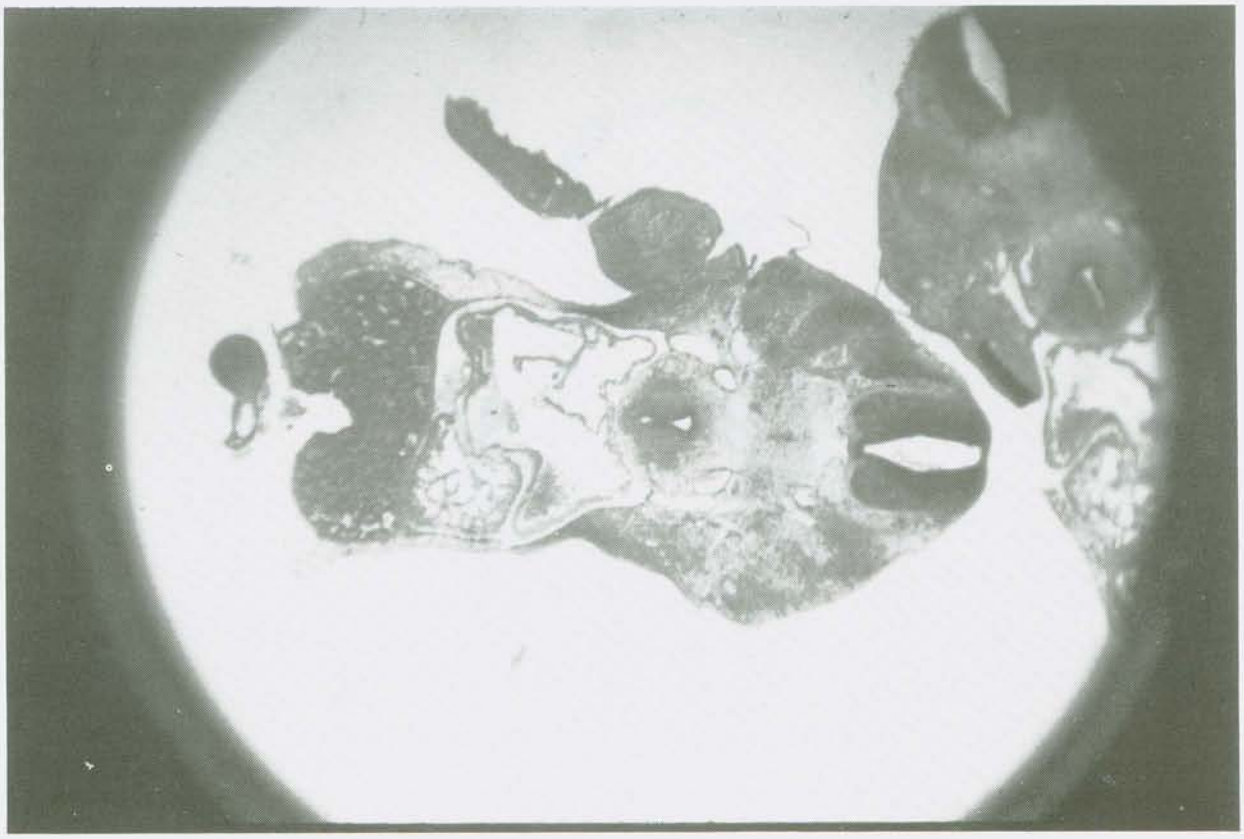


Picture 4. Same as above with showing the reversed syncytiotrophoblast cells. x 1000.



Picture 5. Two embryos are compared normal and monster.

Picture 6. Underdeveloped eyes can be observed in histological section.



Picture 7. Abnormal heart septa development.

Picture 8. Again comparing two embryos, a normal and abnormal once treated with 6% aspirin.

Picture 9. Rat preimplantation embryo in the 5th day in the lower tubal area.

EXTREME RUNOFFS IN REGIONS OF VOLCANIC ROCKS IN CENTRAL EUROPE AND IN NORTHEASTERN U.S.A.*

by

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(1) INTRODUCTION

Generally, it is accepted that--especially in smaller watersheds (up to 350 km^2) and at similar climatic conditions--the extreme surface flows (100-year maxima and minima) are depending mainly on the permeability of the soil and the geologic subsurface including their saturation, the topographic conditions (slopes) and the size of the watershed. As secondary factors for peak runoffs are the yearly rainfall with its distribution, the point rainfall intensity, the storm characteristics, the retardation effect of the vegetative cover, the lake and swamp area and finally the roughness of the surface.

The above factors are the most important elements governing the peak flows. The coefficients of the lowest flows are slightly different. They are depending also on permeability of the geologic subsurface and the size of the watershed, but to a greater extent on the evapotranspiration than on the slope characteristics (topographic conditions). The length of the drought, the frequency and the amount of rain, the retardative effect of forest and lake and finally the relative elevation of the watershed to the adjacent region are the additional factors modifying the minimum flows.

Based on these principles, they were two areas investigated in the 1960's and 1970's: East-Czechoslovakia in Central Europe and New Jersey in Northeastern U.S.A. (1) and (2). In both cases, the above listed principles were confirmed and extreme flow equations were established in accordance with the various geologic formations. Since in both areas are geologic formations of volcanic or plutonic origin, it has merit to describe the findings.

(2) HYDROGEOLOGIC DESCRIPTION OF THE VOLCANIC ROCKS IN THE CARPATHIAN BASIN (EAST-CZECHOSLOVAKIA) AND IN NEW JERSEY, U.S.A.

In East-Czechoslovakia, the Central Slovak Carpathians mostly Paleozoic Crystalline formations, Granite, Gabbro, Sandstones in the North and Mesozoic Basalt, Andesite and Tuff in the South interwoven and surrounded mainly in an arc form from West to East can be found. The general layout of volcanic rocks of the area together with the geologic pattern of the adjacent region is given in Fig. 1. The yearly average rainfall varies from 750 mm in the South to 2100 mm in the North. The peak floods are caused either by transcontinental cyclones or by local torrential rains. The point rainfall intensity reaches 125 mm per day value. The recorded storm pattern is an ellypsoid 15 km by 50 km, with the highest intensity in its focus (3). The valleys' elevation is 400-700 m and the peaks of the mountains reach in the North 2600 m and in the South 1300 m elevation. Vegetative cover (forest) is 40%, the lake and swamp area is insignificant. Evapotranspiration amounts to 40% in the South and to 35% in the North of the yearly rainfall values.

The area can be divided into three hydrogeologic regions (4). The coarse grained Granite and Gneiss, some times with Porphyry, Diabase and Trachyte have few local springs with a limited capacity up to 1 l/sec. On the other hand, the Porphyritic Basalt and Andesite region is characterized by numerous springs of little capacity up to 2 l/sec. The increased voids in this region are only near to the surface, therefore, these springs of low yield can be found on various elevation and their location is quite scattered which makes any substantial concentration of water supply extremely difficult. Water can be found mainly along contact lines of the various formations. Geologically in some areas the Basalt and Andesite are mixed with Trachyte. The third hydrogeologic region can be called the fine grained Andesite interwoven with Tuff including some agglomerates etc. (Ryholite, Trachyte, Dacite etc.) and Tuffite. The weather-beaten Granite and Gneiss areas chiefly on the southern more fractured slopes and more exposed side of the formations and in areas of accumulated piles of debris caused by weathering and erosion belong also to this hydrogeologic region where the springs are generally in the lower part of the depressions similar to the previous region: along contact lines of the formations with a capacity up to 4 l/sec.

In New Jersey, U.S.A., there are two areas where rocks of volcanic or plutonic origin can be detected (5). The bulk of the Appalachian Highland Province in the North is formed by Precambrian Gneiss, Granite and Gabbro. The Highlands are characterized by the flat-topped ridges which have an average elevation of 300 m above sea level. These are cut by narrow, steep-sided valleys 60 to 240 m below the summit level. Between the Highlands and the Coastal Plains, the Piedmont Province is comprising the central part of the State and has in Northwestern part extrusive Triassic Basalt (Watchung Basalt lava flows at some points accumulated to a total thickness of 240 m). Along the Hudson River intrusive Triassic Diabase sill (300 m thick) is dominant which reappears in the Southwestern part of the Piedmont. The ridges have a 200 m elevation and the valleys are at 50 m above sea level. Fig. 2 gives information about the igneous rocks and other geologic formations of New Jersey. The yearly average rainfall is 1125 mm. The peak runoffs are caused by local thunderstorms, cyclonic continental storms or extratropical storms (hurricanes). The point rainfall intensity reaches 250 mm/day value. The recorded storm pattern area is 30 km by 105 km. The vegetative cover (forest) is 47%; the lake and swamp area is in general 2% and reaches up to 17% in some areas. Evapotranspiration amounts to 45% of the yearly rainfall (500 mm) (6).

The volcanic formations in New Jersey have also three hydrogeologic regions but less differentiable than those in East-Czechoslovakia. The groundwater is available only to a depth of 180 m below the surface. Boring tests proved that below that level there is a very marked decrease in fractures and fissures from which water can be obtained. There is also evidence, of course, that certain fracture zones may give abundant water at great depth, but these fractures are those such as the Precambrian-Triassic border fault or others that have been mapped for years. The coarse grained Granite, Gneiss and Gabbro area can be divided into two hydrogeologic regions. The whole area is distinguished by rugged topography with numerous springs and shallow wells of various capacity from less then 1 l/sec up to 4 l/sec which can be even increased by widespread stratified deposits of glacial origin. It must be pointed out that the uneven surface weathering divides this geologic province into two hydrologic regions in the area of the Precambrian formations: one with very limited amount of voids where springs and wells have a capacity only less than 1 l/sec; the other one with substantially more interstices and fractures where springs and wells reach the capacity up to 4 l/sec. The first region, therefore, can be described as poor in voids and fractures, consequently poor in water. The Biotite Gneiss, Amphibolite, Pyroxene Granite and Skarn are the most distinctive formations. The other region is the area of the weathered igneous rocks of the same formations and it can be categorized as the best water yielding area of the Precambrian formations. The third hydrogeologic region is in the Piedmont and to this can be counted also the transition between the two regions previously mentioned and some additional Precambrian formations as it will be enumerated. This region is naturally not only the Triassic Basalt-Diabase area of the Piedmont but also the Precambrian Highland where the weathering processes are slower. This latest category includes the Precambrian Alaskite, Plagioclase Gneiss and Hornblend Granite. The surveyed springs and shallow wells indicate only up to 2 l/sec yield.

(3) EXTREME RUNOFF COMPUTATIONS

The peak runoff investigations are based on records of 23 gauging stations in East-Czechoslovakia and of 19 gauging stations in New Jersey. All the observation was collected for watersheds with an area less than 400 km^2 and the records of various length of observation were gathered from a period of 1871-1972. The lowest flow observations are evaluated from the drought periods 1921 and 1947 in Czechoslovakia (7) and 1961-1966 in New Jersey (8), (9), (10), (11). Further valuable information was obtained from the over 90,000 well-record files of domestic and industrial wells throughout the State of New Jersey from a period of 1947-1973. (Area of 20,295 km^2.)

In accordance with the findings in Central Europe and in the Northeastern United States, the correlation of the 100-year peak runoff with the geologic subsurface in igneous rock regions, the topographic conditions (slopes) and the size of the watershed can be put in the following simplified equation (12):

$$Q = C.A^{-e}$$, where

Q = 100-year peak runoff in $m^3/sec.km^2$
A = area of watershed in km^2
C = coefficient depending on the geologic subsurface with a value:
  In Central Europe from 6 to 10
  In New Jersey from 59 to 81
e = topographic (slope) exponent of the watershed area depending on the topographic character of the watershed (0.40 hills; 0.45 moderate mountains; 0.50 Alpine type mountains)

The above equation's "C" value is different in the two surveyed areas and their ratio is 1:8.2 depending on the 24 hours point rainfall intensity and storm pattern.

The formula can have also the following detailed form:

$$Q = (p_1.p_2).(i_1.i_2).A^{-e}.(c_v.c_c)$$, where

Q, A, e are given as in the simplified equation.

p_1 = permeability factor of the geologic subsurface with a value from 6 to 10

p_2 = urbanization factor from 1 to 3 in accordance with the impervious land-use area and permeability of the geologic subsurface

i_1 = twenty-four hours point rainfall intensity coefficient from 0.5 to 2.0 (0.5 for 35 mm/day; 1.0 for 125 mm/day; 2.0 for 250 mm/day)

i_2 = storm characteristic with a value from 1 to 4.1 depending on the size and pattern of the extreme storms and on the wind velocity

c_v = coefficient of the vegetative cover from 0.95 to 1.05 (from 40% to 70% forested of the watershed)

c_e = concentration coefficient from 0.90 to 1.05 (0.90 for elongated shape or at least 1:5; 0.95 for horseshoe shape and 1.05 for fan-shaped watersheds)

The roughness of the surface and its retardation effect on the flow is not treated separately because this phenomenon is bound on the geological formation. Therefore, this effect is part of the geological runoff coefficient "C" in the simplified equation and of permeability factor "p_1" in the detailed formula. Both basic equations are developed for Central Europe when the parameters have a unit value (1.0) except coefficient "C" and exponent "e". The values of coefficient "C" in volcanic formations of the both areas are given in Fig. 3.

The lowest runoff formula has a similar form

$$Q = C.A^{-e} \quad \text{, where}$$

Q = lowest runoff (50-year runoff ?) value in 1/sec.km^2

A = area of watershed in km^2

C = coefficient depending on the geological subsurface with a value from 0 to 2 (Fig. 4):

In Central Europe	from 0-1.1 to 2
In New Jersey	from 0-1.7 to 0.9

e = 0.065--the exponent indicates an almost even distribution of the lowest runoff regardless of the size of watershed and the available data and values were not sufficient evidence to evaluate the influence of slopes and topographic configuration of the drainage basins in further details.

On the other hand, the constant value of the exponent "e" and the different values of the coefficient "C" in the two surveyed areas indicate that the lowest runoff is more depending on the evapotranspiration effect (% of yearly rainfall) than on the slope characteristics since the minima occur at the end of the drought period when the stored groundwater is less bound on the topographic characteristics of the watershed than on the evapotranspiration effect.

(4) CONCLUSION

The developed equation for peak runoff in smaller watershed with an area less than 300 km^2 can be considered for computations of 100-year peak runoffs. The formula of lowest runoff can be used for areas less than 50-100 km^2 and only for a 50-year lowest flow value because of insufficient length of observation further details and refinements of the formula could not be achieved.

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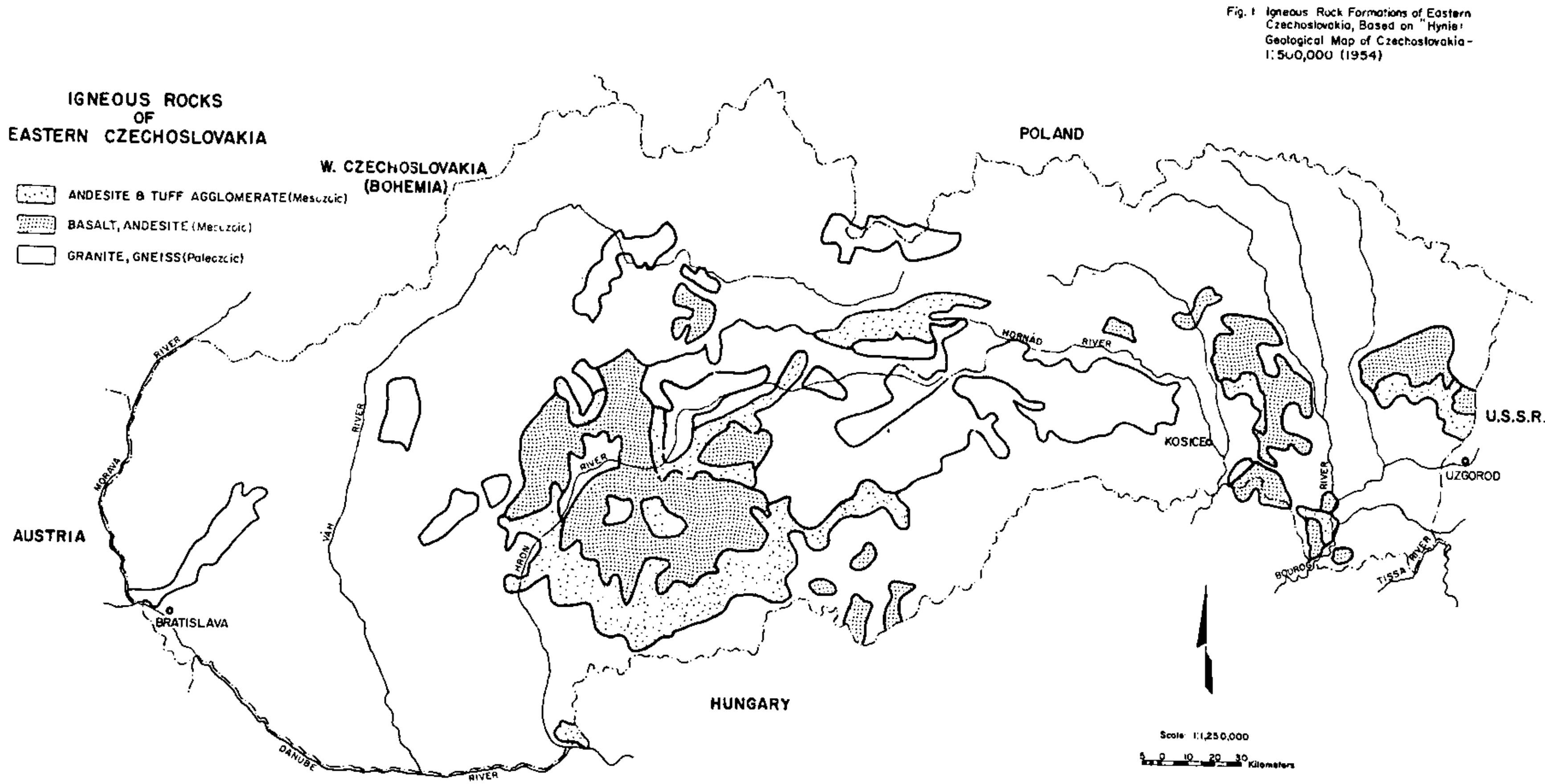

Figure 1. Igneous Rock Formations of Eastern Czechoslovakia, Based on "Hynie: Geological Map of Czechoslovakia"--1:500,000 (1954)

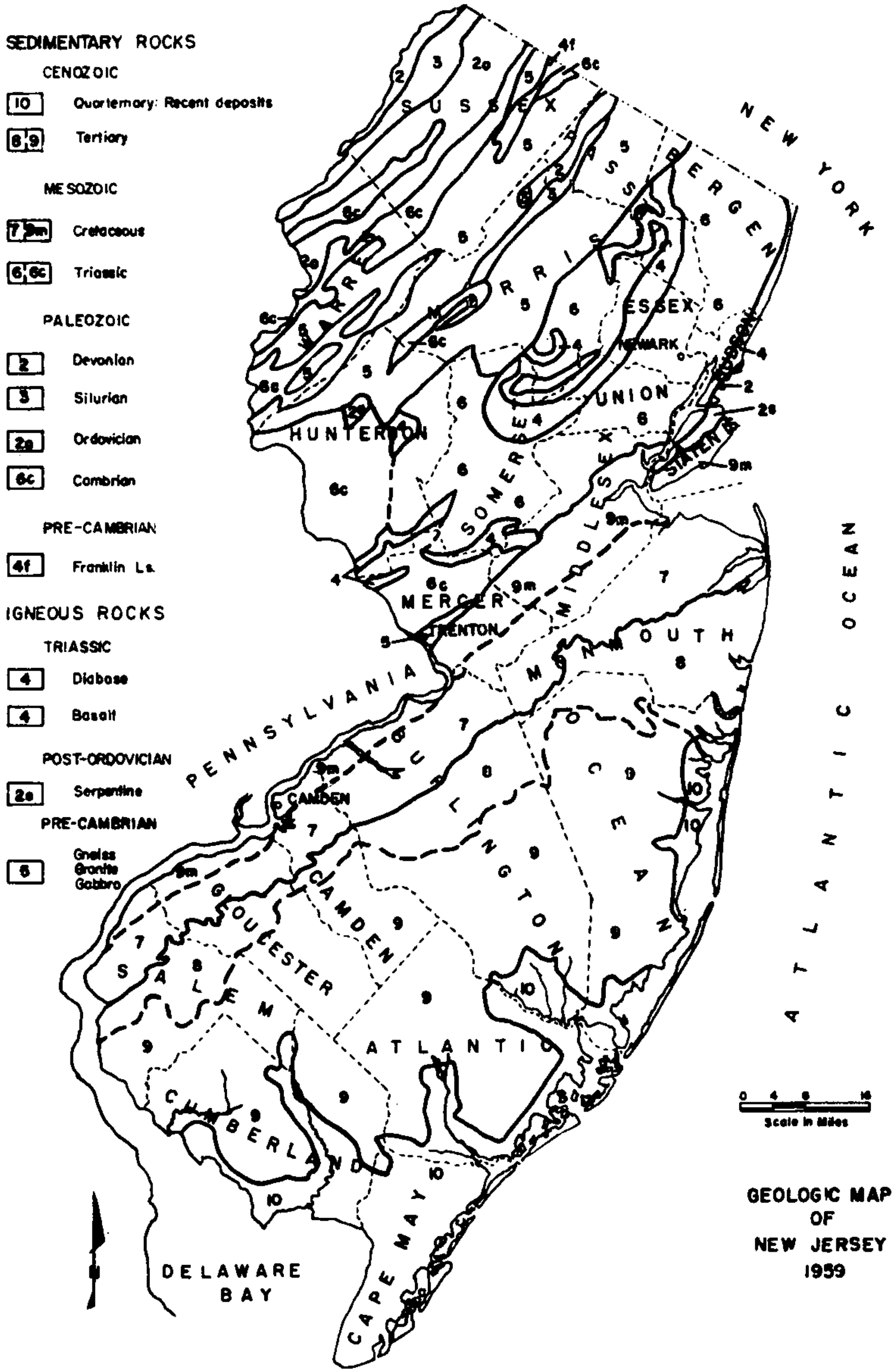

Figure 2. Igneous Rocks of New Jersey (1959)

Hydrologic Regions: (formations)	Peak Runoff Coefficient in $m^3/sec.km^2$ in Central Europe:	in Northeastern U.S.:
(1) Granite, Gneiss	10	81
(2) Basalt-Andesite (Central Europe) Basalt-Diabase (Northeastern U.S.)	8	70
(3) Weathered Igneous Rock (Tuff with agglomerates)	6	59

Figure 3. Peak Runoff Coefficient in Volcanic Rocks

Hydrogeologic Regions: (formations)	Lowest Runoff Coefficient in $1/sec.km^2$ in Central Europe:	in Northeastern U.S.
(1) Granite, Gneiss	less than 0.7* (0 to 1.1)	less than 0.4 (0 to 1.7)
(2) Basalt-Andesite (Central Europe) Basalt-Diabase) (Northeastern U.S.)	1 (0.5 to 1.5)	0.6 (0.17 to 0.8)
(3) Weathered Igneous Rock (Tuff with agglomerates)	2	0.9

*Alpine type areas (frozen most of the year) are excluded.

Figure 4. Lowest Runoff Coefficient in Volcanic Rocks

HACKENSACK RIVER

DETERMINATION OF TERTIARY SEWAGE TREATMENT

REQUIREMENTS FOR WASTE WATER DISCHARGE

by

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INTRODUCTION

The addition of phytoplankton stimulating nutrients into any body of water, via domestic waste water effluents, has the potential of significantly reducing dissolved oxygen levels in the water. This, in turn, brings about a reduction in the number and diversity of desirable life forms and creates an environment which favors the proliferation of biological and chemical pathogens.

The value of removing specific algae promoting nutrients from sewage has increasingly become recognized, especially as we experience an increased volume of waste water flow into rivers, lakes and estuaries, and as a favorable ecological balance in these areas declines. However, enthusiasm for achieving "total effluent purity" must be tempered by an understanding of which nutrients and other effluent components in fact damage the environment and to what degree natural and economic resources are affected. This is implied in the Federal Water Pollution Control Act of 1972 which admonishes that any proposed method of sewage treatment be environmentally sound and cost effective. Direct and indirect costs are a major consideration because the construction and operation of a waste treatment facility may result in changes in air quality, land use planning and energy utilization.

This report deals with the necessity for constructing a tertiary sewage treatment plant on an area of the Hackensack River near Secaucus, New Jersey, by analyzing the effect of two chemical nutrients, nitrogen and phosphorous, which have been shown in other bodies of water to be responsible for eutrophication and which can be removed from domestic waste water by tertiary treatment. It is important to note that individual eco-systems respond in different ways to these elements. For example, a nutrient such as phosphorous which causes excess algal growth in one of the Great Lakes has little effect in areas of Long Island Sound, where it is nitrogen that is responsible for eutrophication.

It is evident then that chemicals that are potentially stimulatory to algal growth must be investigated on an area basis. Differences in response of each area to specific chemical agents can be attributed to environmental modification by industrial waste, landfills, sewage outfalls, microbial populations and the fauna and vegetation of adjacent terrestrial, marsh and aquatic areas.

The economic benefits of determining and removing eutrophicating agents from sewage treatment effluent are evident. Recreational utilization of receiving waters are safeguarded, and adequate water quality is maintained to accomodate commercially valuable marine fish that utilize marshes as nursery grounds.

The economic advantage associated with determining that tertiary treatment is not necessary is more directly apparent. The millions of construction and maintenance dollars necessary to support such a facility can be saved while at the same time retaining recreational and asthetic benefits.

MATERIALS, METHODS & DISCUSSION

Water samples used in the eutrophication analysis were collected in chemically clean containers and refrigerated prior to being processed. All samples were collected from the Hackensack River in Northern New Jersey near the base of the Erie Lackawanna Railroad Bridge and this study and its evaluation is indicative of conditions in this limited area.

A portion of the water sample was filtered thru a 0.45 micron millipore filter. To this were added the chemicals, individually or in combination, that were under investigation as potential limiting factors. The enriched and unenriched water samples were then inoculated with phytoplankton indigenous to the area from which the sample water was obtained.

Experimental and control cultures was then incubated until phytoplankton growth levels were sufficient to permit a meaningful evaluation of the results. A significant stimulation of phytoplankton growth above control levels caused by chemical enrichment of the water indicates that the chemical used is a limiting factor. A failure to stimulate growth significantly beyond the level of the control indicates that the chemical being tested is not limiting and therefore, that its addition to the river water, as a component of a sewage treatment discharge, will not stimulate excessive phytoplankton reproduction.

Tests for limiting factors were conducted throughout the year, rather than just in the warmer months, because in shallow waters growth may never be seriously limited by reduced solar radiation (Riley, 1969).

Ammonium, nitrate and phosphate were analyzed as suppliers of nitrogen and phosphorous because they have been identified as being responsible for eutrophication in other bodies of water (Ryther & Dunstan, 1971) and because of their known significance in estuarine algal physiology (Lo Pinto, 1972).

A broad spectrum of meadowlands phytoplankton was utilized in each analysis. In this way, the interrelationships among the diverse populations are not artificially eliminated. Provasoli (1963) has demonstrated that many algae produce antibiotic substances which are capable of inhibiting the reproduction of other algal species. An experimental system designed to determine the presence of a limiting factor that selects against these interactions by utilizing uni algal cultures may not accurately reflect environmental conditions. Because interactions do occur in natural ecosystems, a system of analysis for limiting factors in which phytoplankton populations are tested in mixed culture insures a more accurate reflection of in situ biological responses.

Another refinement of our analysis is designed to avoid possible misinterpretation of nitrogen data. Ammonium nitrogen has been shown to be toxic to some phytoplankton even at very low levels but stimulatory to other species at very high concentrations (McLaughlin, 1957). Lo Pinto and McLaughlin (1974) have shown that high concentrations stimulate the very abundant estuarine chrysomonad, Micromonas.

In order to assure a correct interpretation of our nitrogen analysis, ammonium nitrogen was added in a broad range of concentrations so that any ammonium toxicity would be apparent. As an additional safeguard, nitrogen was supplied as nitrate. Thus any significant stimulation of primary productivity by nitrogen would be readily recognized.

RESULTS AND DISCUSSION

The water quality analysis conducted from March thru December 1976 in the area of the Hackensack River previously mentioned, is presented in the enclosed tables and figures.

Table I presents the effect on primary production of several concentrations of phosphate and nitrogen compounds. The figures reflect the potential of these compounds to stimulate algal growth throughout most of the year. The effect on primary production is recorded as a percentage of production in the control, i.e. unenriched waters (primary production equivalent to that in the control is indicated as 100% of the control).

Figure I and table I show that throughout most of the year exogenously supplied phosphate concentrations of 0.1, 0.5 and 1.0 mg% do not stimulate phytoplankton growth beyond that shown in the control. Samples collected in late June, early July and August do show an increasing stimulation of phytoplankton growth in response to the lower levels of phosphate supplied (fig. 2 - 4).

Figure 5 and table I reveal a relatively uniform response throughout the sampling period to nitrate as a nitrogen source. No significant stimulation or inhibition was apparent.

A review of figure 6 and table I reveals that low levels of ammonium show a mild stimulatory trend in samples V, VI, and VII (see figs. 2 - 4).

Figure 7 and Table II, which consolidate the data on seasonal trends of stimulation by phosphorous and nitrogen sources illustrate more clearly the trend towards increased productivity between June, July and August in phosphate and ammonium enriched cultures.

It should be emphasized, however, that neither the nitrogen or phosphate sources supplied individually to the organisms in the water samples analyzed during the summer months when water temperatures are relatively high (table III) or at any time throughout the sampling period causes an excessive increase in primary production. In all cases, production in nutrient enriched samples remains well below a two fold (200%) increase over the control. This represents but a fraction of the 1100 to 3600% stimulation that has been reported in other areas. In addition, it is important to note that no synergistic stimulation results from combining ammonium and phosphate (table I) at any time of the year.

The minor trend toward increased primary production that is seen in summer samples when ammonium and phosphate are supplied in vitro (fig. 1), probably reflects an increased depletion of these nutrients in the Hackensack River at the site studied, by phytoplankton and adjacent marsh vegetation. It may also indicate reduced inorganic regeneration rates, or both these factors may be contributory. During the remainder of the sampling period physiologically available phosphorous and nitrogen are apparently received by or regenerated in the river at a rate which exceeds demand by autotrophs.

It is evident from our analysis that the decrease in eutrophication potential that would be achieved by even total nitrogen and phosphorous removal from any industrial or municipal waste water treatment facility, intended to discharge in the Hackensack River in the area studied would provide no ecological advantage.

Indeed, the economic, energy and natural resource expenditures that would be required to construct and maintain such a plant would represent a disservice to the Hackensack River estuary.

In view of the results and conclusions expressed herein, it is evident that the 1984 EPA goal of "zero pollutant discharge" may well be worthy of reconsideration, at least for parts of the Hackensack River estuary. Furthermore, it is also important to mention, in view of the increasingly popular utilization of mathematical models to predict the effects of pollutants, that data of the type generated for this report need be included in the calculations that balance the benefits and risks of constructing waste water treatment facilities. If this is not done it is conceivable that in some circumstances natural and economic resources could unjustifiably be expended in order to gain environmental goals which do not reflect the needs of the particular ecosystem being considered.

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TABLE III

Date	30 March	29 April	24 May	10 June	30 June	22 July	4 Aug.	25 Aug.	16 Sept.	14 Oct.	12 Nov.	10 Dec.
Water Temperature (C)	14	16	20.5	25	28	27	27	29	24.5	18	-	7

TABLE II

Average Of Primary Production For Generally Non-Inhibitory Concentrations

Sample	30 March	29 April	24 May	10 June	30 June	22 July	4 Aug.	25 Aug.	16 Sept.	14 Oct.	12 Nov.	10 Dec.
	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
$NaH_2PO_4 \cdot 7H_2O$												
average for 0.1, 0.5, 1. mg%	92	108	98	90	127	152	158	93	95	98	78	112
$NaNO_3$												
average for 0.5, 1, 5, 10 mg%	114	121	93	105	121	100	89	117	126	106	98	102
NH_4Cl												
average for 0.5, 1. mg%	89	112	85	68	147	173	129	100	100	105	75	100

TABLE I

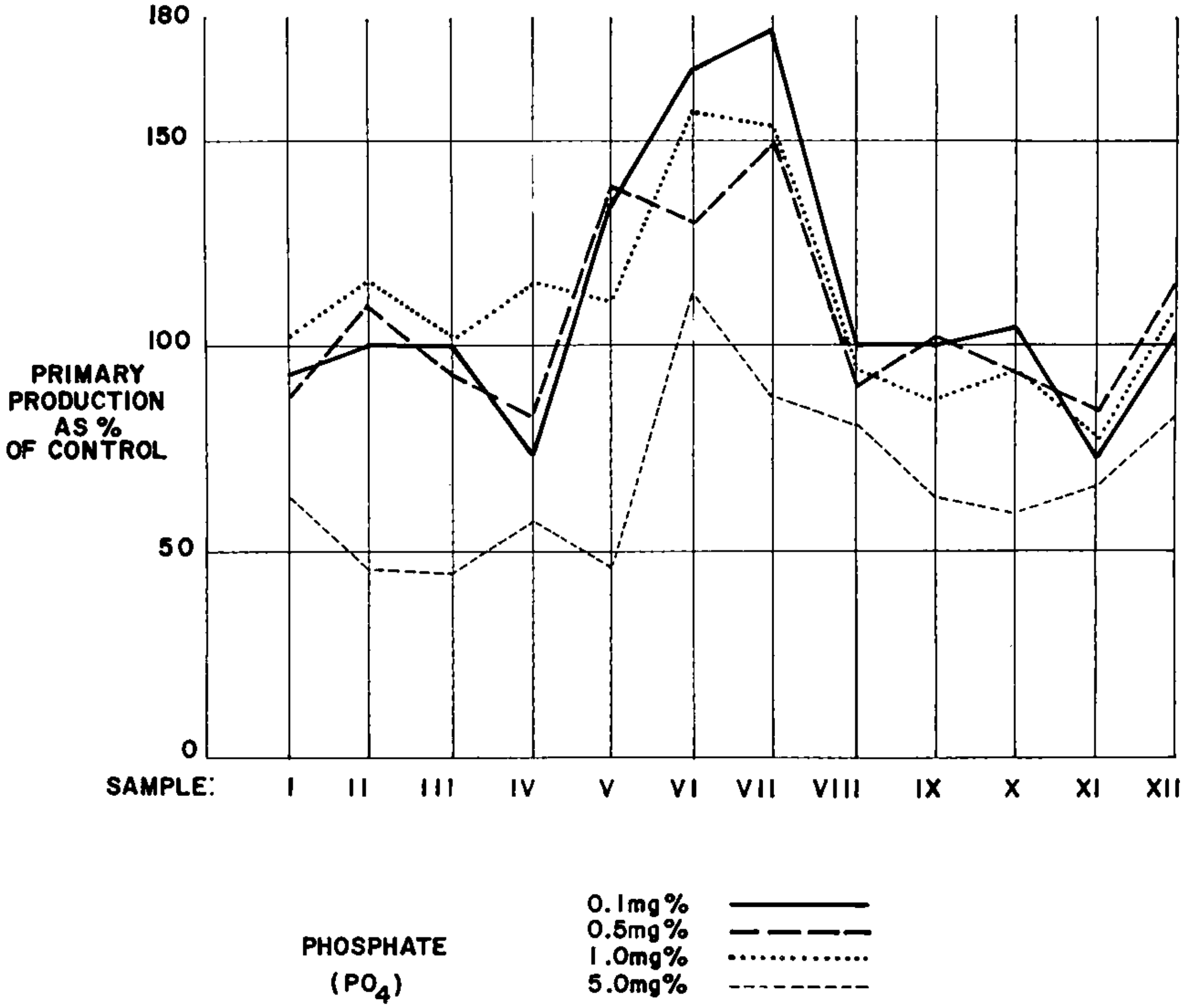
Primary Production Expressed As % Of Control

(Experimental/control x 100)

Sample	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
1976	30 March	29 April	24 May	10 June	30 June	22 July	4 Aug.	25 Aug.	16 Sept.	14 Oct.	12 Nov.	10 Dec.
$Na_2HPO_4 \cdot 7H_2O$												
.1mg%	92	100	100	71	131	167	175	100	100	105	75	106
.5	85	108	94	86	144	133	150	89	100	94	83	113
1.	100	115	100	114	106	156	150	89	86	94	75	113
5.	62	46	43	57	44	111	83	78	60	55	66	81
$NaNO_3$												
.5mg%	123	123	100	107	125	100	83	122	113	94	100	113
1.	100	131	88	107	119	100	83	111	133	116	92	100
5.	108	123	88	114	113	89	83	111	126	110	100	94
10.	123	108	94	93	125	111	108	122	133	105	100	100

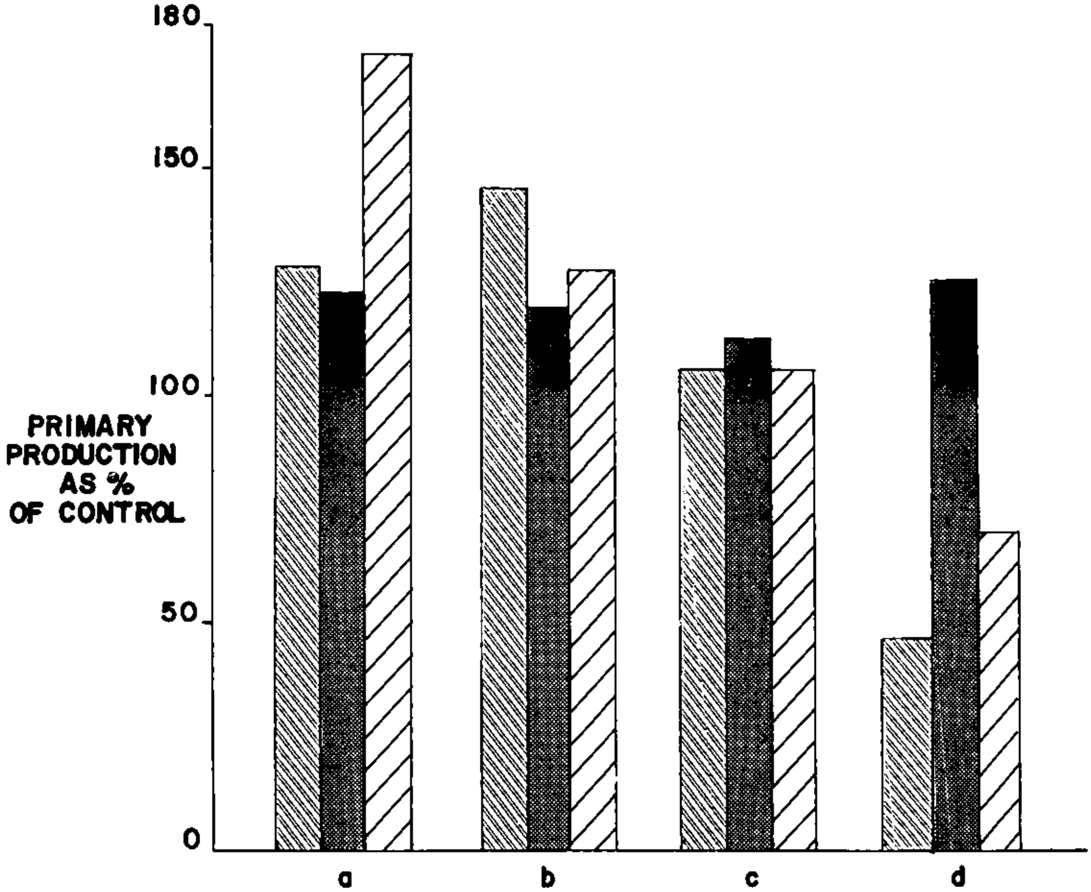
TABLE I - cont'd

Sample	I	II	III	IV	V	VI	VII	VIII	IX	X	XI	XII
NH_4Cl												
.5%	92	123	100	64	169	178	133	111	106	110	83	106
1.	85	100	69	71	125	167	125	89	93	100	67	94
5.	54	77	81	57	106	122	108	67	60	61	50	63
10.	38	62	81	50	69	111	92	56	30	44	50	56
NH_4Cl(1 mg%) + Na_2HPO_4(1 mg%)		92	81	100	113	88	92	100	86	100	92	88



PRIMARY PRODUCTION AT ALL PO_4 CONCENTRATIONS

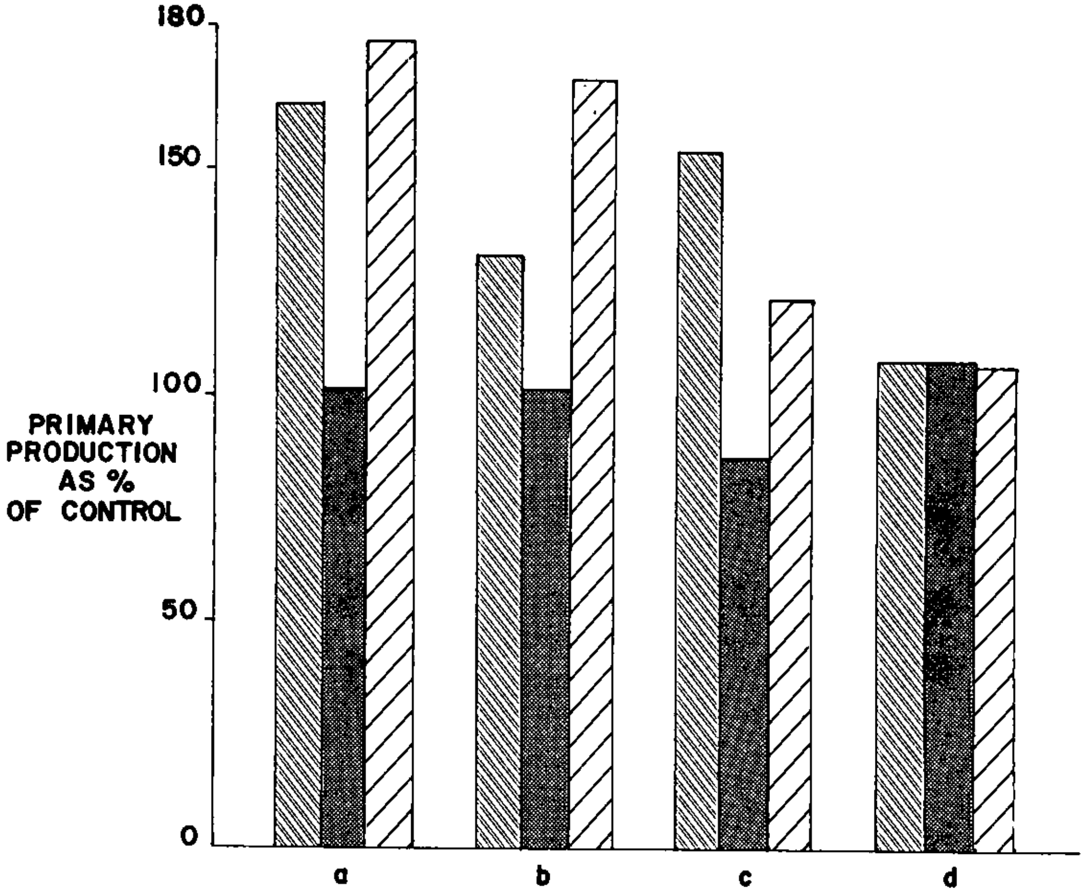
Fig. 1



CONCENTRATION
SAMPLE V
Fig. 2

Conc. Code	CONCENTRATIONS (mg%) PO_4	NO_3	NH_4
a	0.1	0.5	0.5
b	0.5	1.0	1.0
c	1.0	5.0	5.0
d	5.0	10.0	10.0

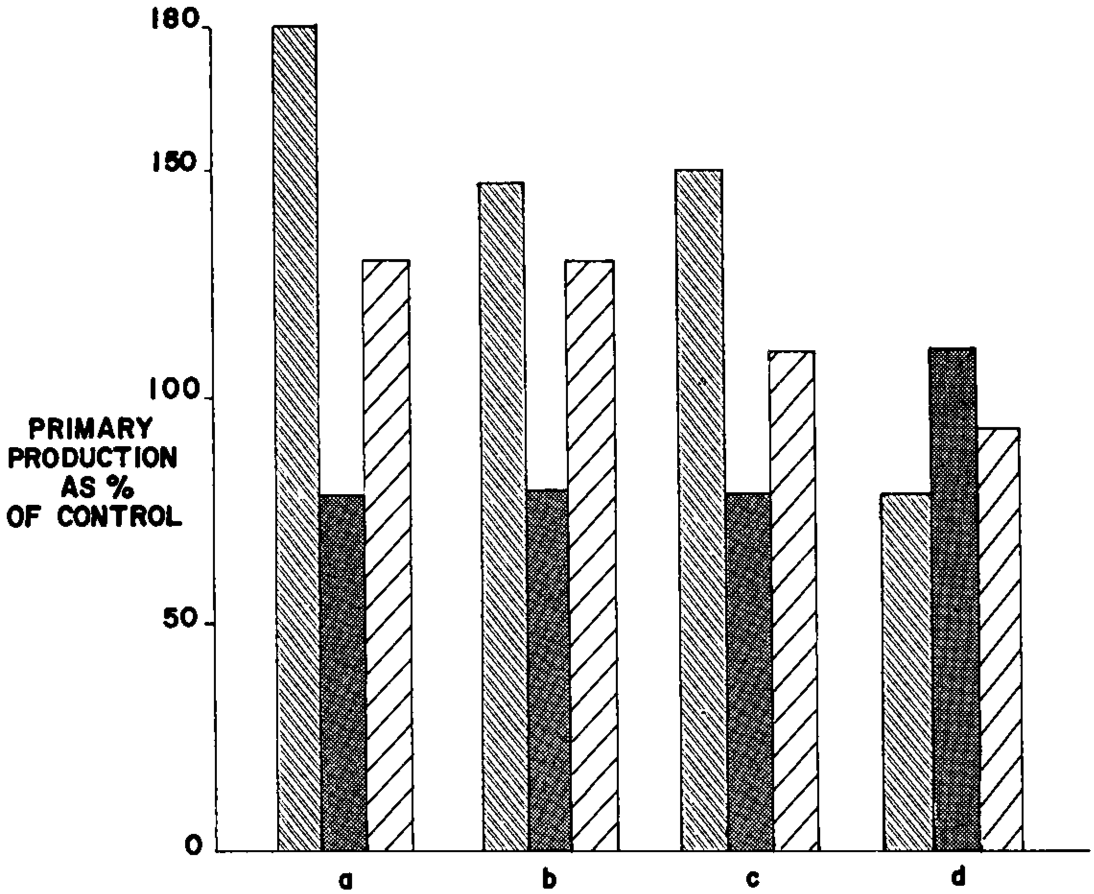
EXPLANATION OF FIG. 2



CONCENTRATION
SAMPLE VI
Fig. 3

Conc. Code	CONCENTRATIONS (mg%) PO_4	NO_3	NH_4
a	0.1	0.5	0.5
b	0.5	1.0	1.0
c	1.0	5.0	5.0
d	5.0	10.0	10.0

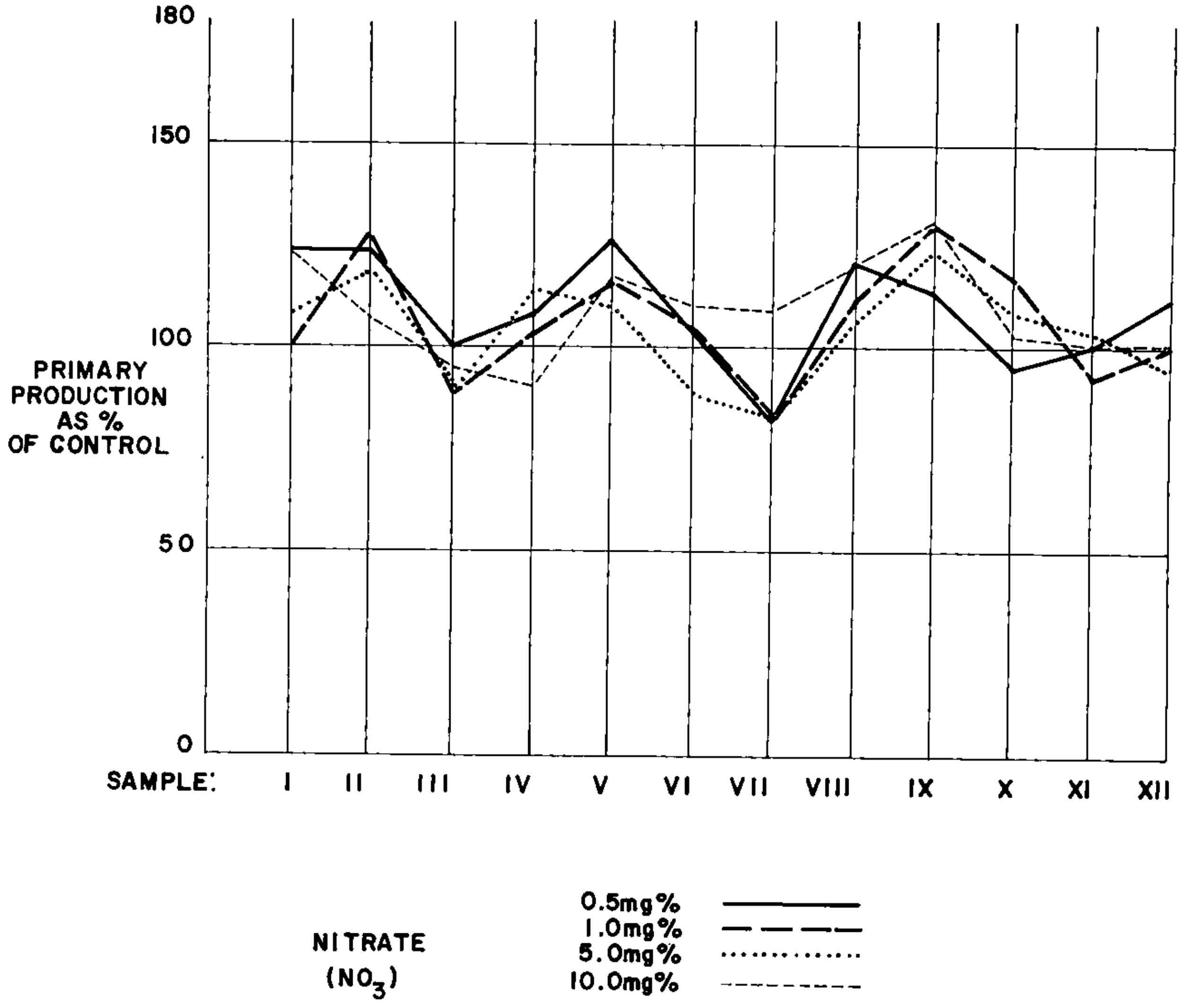
EXPLANATION OF FIG. 3



CONCENTRATION
SAMPLE VII
Fig. 4

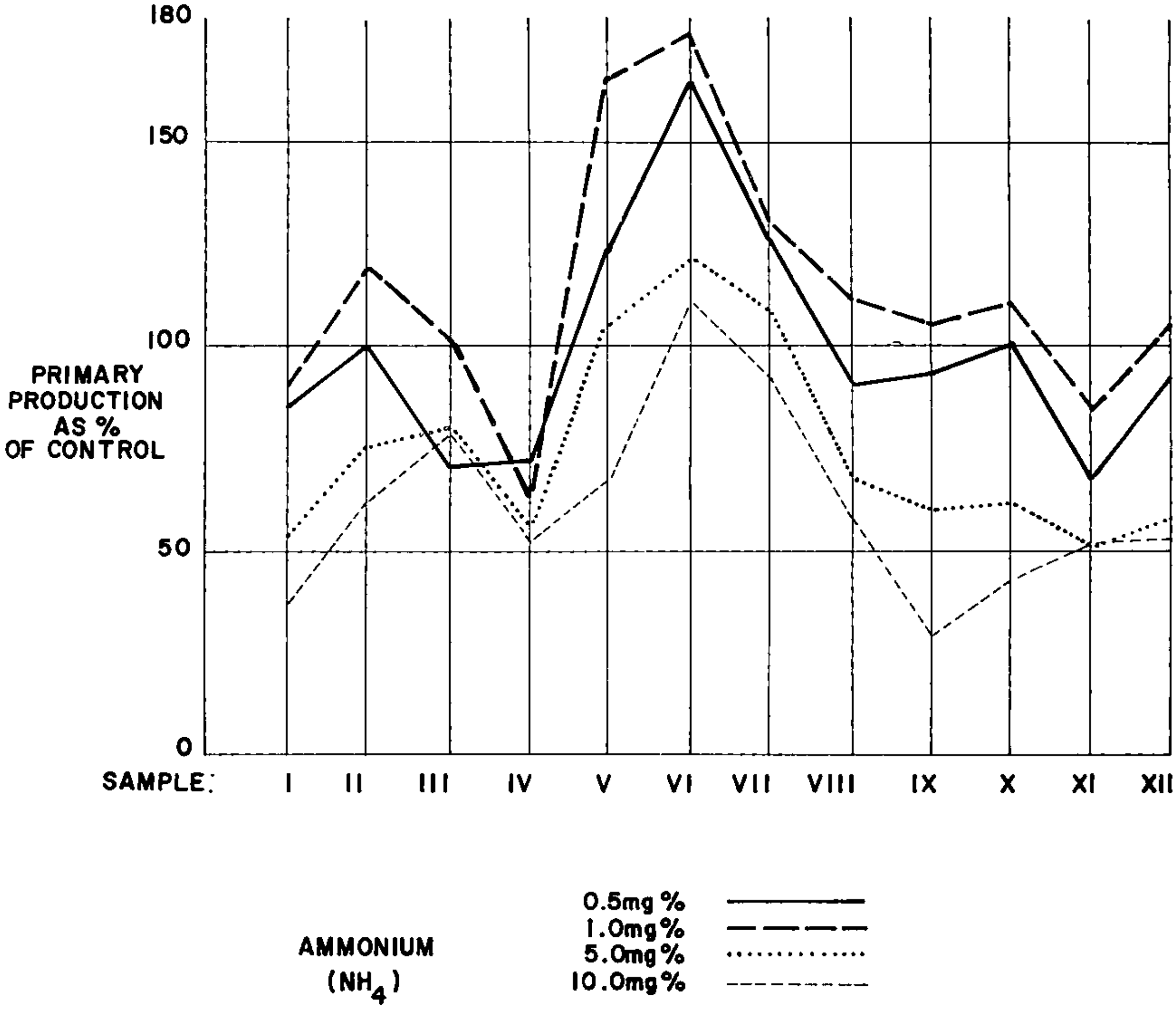
Conc. Code	CONCENTRATIONS (mg %) PO_4	NO_3	NH_4
a	0.1	0.5	0.5
b	0.5	1.0	1.0
c	1.0	5.0	5.0
d	5.0	10.0	10.0

EXPLANATION OF FIG. 4



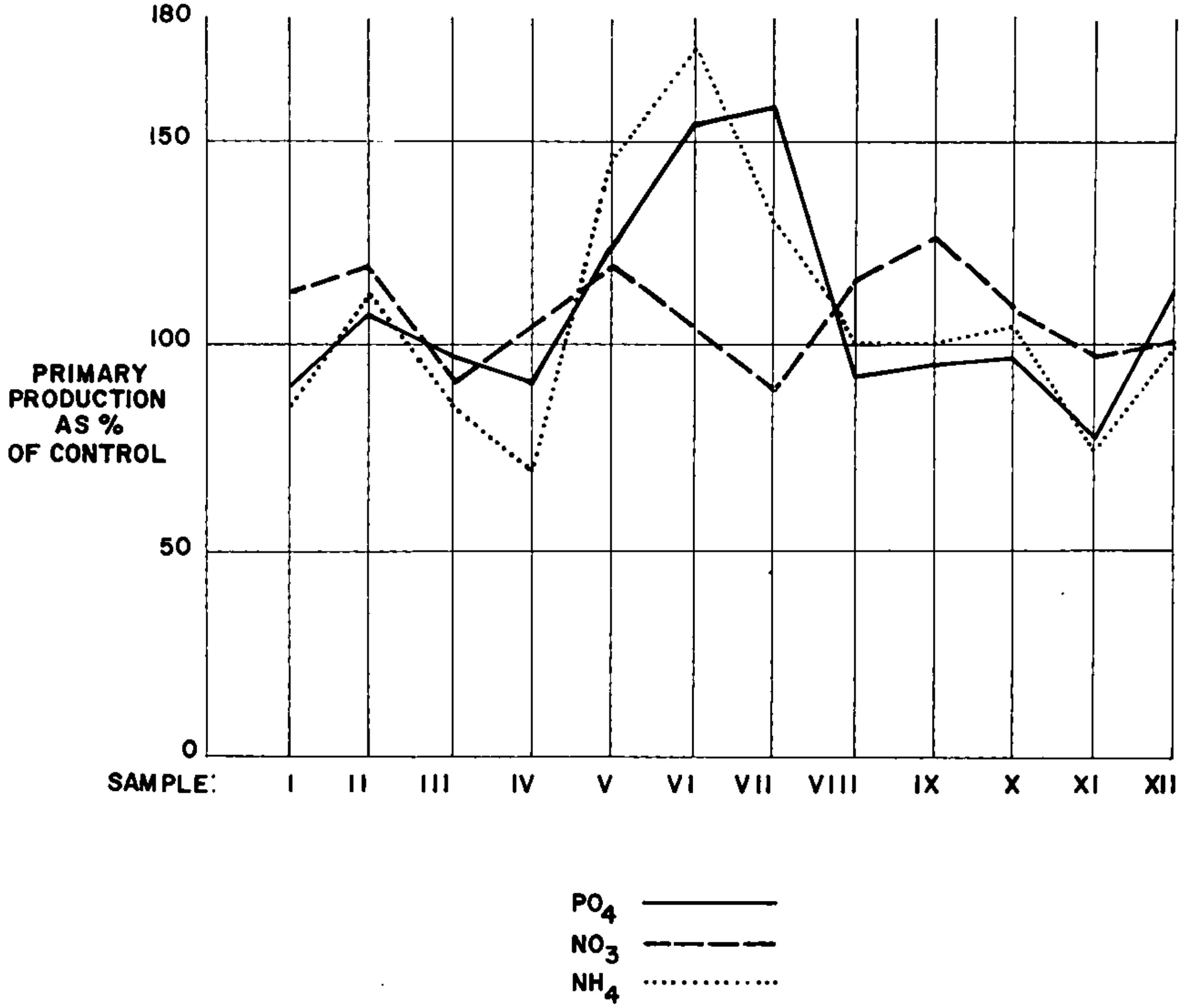
PRIMARY PRODUCTION AT ALL NO_3 CONCENTRATIONS

Fig. 5



PRIMARY PRODUCTION AT ALL NH_4 CONCENTRATIONS

Fig. 6



AVERAGE OF PRIMARY PRODUCTION AT GENERALLY NON INHIBITORY CONCENTRATIONS OF PO_4, NO_3, AND NH_4

Fig. 7

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