# PREDICTION OF THE CHEMICAL QUALITY OF STREAMFLOW BY AN INTERACTIVE COMPUTER MODEL

by

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## INTRODUCTION

A prototypical computer simulation model which predicts dissolved chemical concentrations in streamflow runoff has been developed to aid watershed management specialists and land use planners estimate the impacts of alternative management practices on water quality. The model allows users at remote locations to readily obtain predictions of stream chemical quality with modest computer equipment and commonly available data. The model, called CHEM, is structured in an interactive format to facilitate operation by persons not familiar with computer operations. The model, written in ANSI Standard FORTRAN, requires approximately 5,000 words of core and is currently operative on a DEC-10 computer at the University of Arizona. The prototypical version of CHEM has been developed to represent dissolved chemical constituents in water yield from snowmelt in southwestern ponderosa pine forest ecosystems in central Arizona; however, the conceptual framework is considered applicable to other types of runoff and ecosystems.

## CONCEPTUAL SIMULATION MODEL

Instantaneous dissolved chemical concentrations in surface runoff from a watershed may be represented by functions of several variables. A time related variable changing most appreciably for a given event is discharge. Parameters other than discharge may be variable in a longer temporal sense, but are considered constant for a single runoff event, such as stream pH. Herein, concentrations of dissolved chemicals are considered to be represented by functions of discharge and stream pH for individual runoff events.

In general, discharge, q, is a function of time. With this in mind, a runoff event with a total runoff Q, flowing for a time T, is given as:

$$Q = \int_0^T q(t)dt \tag{1}$$

The volume of water, $dQ_1$, leaving a watershed in time element dt at time $t_1$ after initiation of surface runoff is given as:

$$dQ_1 = q(t_1)dt \tag{2}$$

This expression, multiplied by the instantaneous concentration of a chemical, $f(q(t_1), pH)$, at a time interval dt, gives the weight of dissolved chemical discharged $dW_s$, in that interval. This is expressed as:

$$\begin{aligned}(dW_s)_1 &= f(q_1,pH)dQ_1 \\ &= f(q(t_1),pH)\ q(t_1)dt\end{aligned} \tag{3}$$

The integration of this relationship over the duration of the surface runoff event gives the total weight of dissolved chemicals carried by water as:

$$W_s = \int_0^T f(q,pH)\, q(t)dt \tag{4}$$

In general, a surface event hydrograph is composed of both a rising and a receding component. If the crossover from one to the other component occurs at time $T_1$ after initiation of surface runoff, the total weight of a dissolved chemical yield, $W_s$, from the watershed for the duration of the event is given as:

$$W_s = \int_0^{T_1} f_1(q_1,pH)\, q_1(t)dt + \int_{T_1}^{T} f_2(q_2,pH)\, q_2(t)dt \tag{5}$$

where:

$f_1(q,pH)$ = concentration of dissolved chemical for rising stage;

$q_1(t)$ = discharge function for rising stage;

$f_2(q,pH)$ = concentration of dissolved chemical for receding stage; and

$q_2(t)$ = discharge function for receding stage.

Here, the rising and receding chemical concentration functions are different for a given discharge.

In general, one would numerically integrate equation (5) to yield total weight of a chemical discharged from a watershed in a surface runoff event of Q area inches, over T hours. The above relationships are typical for water release during the summer. However, as CHEM has been structured to represent chemical quality of streamflow from snowmelt, relationships for winter release are required.

Winter release is approximated by a constant value discharge function throughout the day. A daily release of Q cubic feet would yield a constant flow, $q_c$, of:

$$q_c = \frac{Q}{86400} \text{ cfs} \tag{6}$$

Using this constant flow in a dissolved chemical concentration function gives total daily chemical yield as:

$$W_s = f(q_c,pH)Q \tag{7}$$

Several predictive equations for instantaneous chemical concentrations in streamflow from snowmelt have been developed from data sets on ponderosa pine forests in central Arizona (Gregory, 1976). These equations are:

| | | |
|---|---|---|
| Calcium | $4.8 \leq w \leq 8.0$; | (8) |
| Magnesium | $1.0 \leq w \leq 3.0$; | (9) |
| Sodium | $w = 2.0 - 8.88\ q$; | (10) |
| Chloride | $w = -.81 + .41\ pH$; | (11) |
| Sulfate | $w = -10.93 + 2.95\ pH$; | (12) |
| Carbonate | $w = 0$; | (13) |
| Bicarbonate | $w = -46.6 + 11.32\ pH$; | (14) |
| Fluoride | $w = .01 + .76\ q$; | (15) |
| Nitrate | $w = .02 + 1.08\ q$; | (16) |
| Phosphate | $w = .17 - .8\ q$; | (17) |

| | | |
|---|---|---|
| Total Soluble Salts | $w = 15.32 + 9.81\ pH;$ | (18) |
| Conductivity | $w = -.14 + .28\ pH;$ | (19) |

where: $w$ = concentration in parts per million (ppm);

$q$ = discharge in cubic feet per second (cfs); and

$pH$ = that of the stream.

These equations resulted from analysis of source data from watersheds ranging from 15 to 40 acres in size. The watersheds are underlain by sandstone and alluvial material. Soils derived from this material are principally fine sandy loams which are relatively shallow (60-150 cm.).

As can be seen from the predictive equations (Equations 8-19), some chemical concentrations are functions of discharge, while others are functions of stream pH. From the data sets selected, two of the constituents, calcium and magnesium, were not found to have a significant correlation with either streamflow or stream pH; as such, they are represented by the range in values they were found to lie within.

These equations have been incorporated into CHEM. Concentrations of the various chemical constituents of streamflow are presented as ranges rather than point measurements as given by the predictive equations. The range for each chemical constituent is associated with the scatter in the data used to generate the predictive equation; the more the scatter, the wider the range.

Relationships similar to the above can be assembled from existing source data from other locations, with resultant equations readily incorporated into the framework of CHEM (Figure 1). The ability to introduce other chemical response functions into the prototypical model has been one of the main design criteria in the development of this simulator. This feature should be useful in predicting the chemical quality of streamflow in locations other than Arizona. For example, source data from Colorado and Minnesota are currently being analyzed for development of appropriate functions for these locations.

While the current version of CHEM predicts the dissolved chemical constituents of snowmelt runoff, the framework has been developed to allow predictions to be made for summer thunderstorm events. This structure is detailed in a paper that describes a model which predicts the concentration and yield of suspended sediment for either summer or winter events (Rasmussen and Ffolliott, 1979). CHEM is similar to the winter prediction portion of this latter model. The summer component of CHEM is to be incorporated into the model when appropriate chemical concentration response functions are available.

## APPLICATION OF MODEL

Perhaps the best way to illustrate the application of CHEM in predicting concentrations of dissolved chemicals in surface runoff is through an example. For illustration, a hypothetical 20 acre watershed of southwestern ponderosa pine forest was examined to estimate chemical concentration in streamflow from snowmelt.

Operation of the model begins by presenting a list of dissolved chemical constituents (Figure 2). The user selects which of these are of interest. In the example, we wished to examine all of them. Watershed area, 20 acres, was input next. Streamflow pH is then requested. A default value of 6.9 is offered and was selected in the example. This default value represents the "best" or most frequent response to a statement or question. Acceptance of a default value allows a simulation exercise to continue without explicit knowledge of the input requested. It should be noted, however, that the user has the option of overriding any default value offered, if desired. The daily streamflow was input at 0.1 area-inches. Following this, a table displaying the predicted ranges in the various chemical constituents dissolved in the stream is output.

After the table, a question is asked whether EPA water quality standards are requested. If the user wishes to examine the predicted chemical concentrations against standards for several types of usage, he may do so. In the example, this comparison was desired and so indicated (Figure 2). The table which shows EPA water standards gives the level of acceptability for three forms of use: aquatic life, irrigation, and public water supply. The standard values may be easily changed to reflect changes in the standard, or another standard may be introduced if considered appropriate.

The end of the example is signified to the computer by the input of -1 to the request for the daily streamflow (Figure 2). Another operation of the model could have been made if it were desired to observe the predicted consequences of a vegetative modification which resulted in a change in snowmelt rate for the same index day over the watershed.

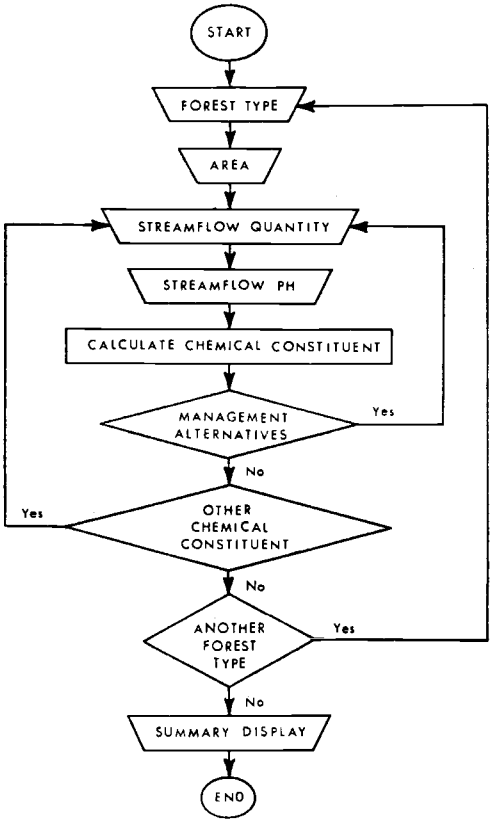


Figure 1 - Flow of activities in executing CHEM to predict dissolved chemical constituents in streamflow.

## INTERACTIONS WITH OTHER MODELS

While this simulator has been designed to operate alone, it has also been structured to be linked with other simulators, if desired. CHEM is part of a family of computer models being developed to help watershed management specialists and land use planners estimate impacts of alternative land management practices (Larson et al., 1979). This family of simulation models includes three general modules: FLORA for estimating responses of forest overstory, herbaceous understory, and organic material; FAUNA for evaluating animal habitats, carrying capacities, and population dynamics; and WATER for assessing streamflow yield, sedimentation, and chemical quality. CHEM is a component of the WATER module, with interfaces to many of the other models.

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CHEM:

DISSOLVED CHEMICAL CONSTITUENTS ARE:

    1 - CALCIUM (CA)              8 - FLUORIDE (F)
    2 - MAGNESIUM (MG)            9 - NITRATE (NO3)
    3 - SODIUM (NA)              10 - PHOSPHATE (PO4)
    4 - CHLORIDE (CL)            11 - TOTAL SOLUBLE SALTS
    5 - SULFATE (SO4)            12 - HYDROGEN ION (PH)
    6 - CARBONATE (CO3)          13 - CONDUCTIVITY
    7 - BICARBONATE (HCO3)       14 - ALL

ENTER THE NUMBER(S) OF THE CONSTITUENT(S) YOU WISH TO EVALUATE
        SEPARATED BY COMMAS.  14

WHAT IS THE WATERSHED AREA IN ACRES ? 20

WHAT IS THE STREAMFLOW PH (CR GIVES: 6.9) ?

WHAT IS THE DAILY STREAMFLOW IN INCHES (ENTER "-1" TO STOP) ? .1

STREAMFLOW OF   0.10 INCHES ON   20.00 ACRES WITH A PH OF  6.90 PRODUCES:

    CONSTITUENT              CONCENTRATION (PPM)     DAILY VOLUME (POUNDS)
    -----------              -------------------     ---------------------

    CALCIUM                     4 -    8             2.17 -        3.62
    MAGNESIUM                   1 -    3             0.45 -        1.36
    SODIUM                      0 -    1             0.43 -        0.71
    CHLORIDE                    1 -    2             0.69 -        1.14
    SULFATE                     7 -   11             3.20 -        5.34
    CARBONATE                   0 -    0             0.00 -        0.00
    BICARBONATE                23 -   39            10.70 -       17.83
    FLUORIDE                    0 -    0             0.03 -        0.04
    NITRATE                     0 -    0             0.04 -        0.06
    PHOSPHATE                   0 -    0             0.03 -        0.06
    TOTAL SOLUBLE SALTS        39 -   65            17.79 -       29.66

AVERAGE DISCHARGE =   0.08 CFS.
     HYDROGEN ION = 6.8 - 7.4
     CONDUCTIVITY =  31.48 UMHOS.

EPA WATER QUALITY CRITERIA (YES/NO, CR GIVES: YES)  ? YES

                                   LEVELS OF ACCEPTABILITY
CONSTITUENT          AQUATIC LIFE        IRRIGATION        PUBLIC WATER SUPPLY
-----------          ------------        ----------        -------------------

CALCIUM              NOT LISTED          NOT LISTED          NOT LISTED
MAGNESIUM            NOT LISTED          NOT LISTED          NOT LISTED
SODIUM               NOT LISTED        NOT PRESCRIBED*     NOT PRESCRIBED
CHLORIDE             NOT LISTED        NOT PRESCRIBED*       250 MG/L
SULFATE              NOT LISTED        NOT PRESCRIBED*       250 MG/L
BICARBONATE          NOT LISTED        NOT PRESCRIBED*     NOT LISTED
FLUORIDE             NOT LISTED          2.0 MG/L          .06-1.9 MG/L**
NITRATE              NOT LISTED          NO MAXIMUM          10 MG/L
PHOSPHATE            NOT LISTED          NO MAXIMUM        NOT PRESCRIBED

  * - CANNOT BE PRESCRIBED WITHOUT CONSIDERATION OF
        OTHER SOIL AND WATER CONSTITUENTS.
 ** - FROM PUBLIC HEALTH SERVICE DRINKING WATER STANDARDS (1962)
        LEVEL DEPENDENT UPON ANNUAL AVERAGE OF MAXIMUM
        DAILY AIR TEMPERATURE.


WHAT IS THE DAILY STREAMFLOW IN INCHES (ENTER "-1" TO STOP) ? -1
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Figure 2 - Sample operation of the predictive model CHEM.

## REFERENCES CITED

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