The International Symposium on

Water Quality Modeling

Proceedings of the International Symposium

April 2-5, 1995
Hyatt Hotel Orlando
Orlando, Florida

Sponsored by

ASAE – The Society for engineering in agricultural, food, and biological systems

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Edited by
Conrad Heatwole

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Preface

The impact of chemicals associated with agriculture on water quality has been a major concern to scientists and engineers for several decades. Simulation models have been developed to incorporate the knowledge developed from field and laboratory studies of chemical fate and transport in the environment into a complete systems approach. The goals of this work are to provide tools to improve the understanding of the complex interactions involved in the system, to better identify areas of inadequate understanding of the system, and to aid in making policy and management decisions concerning the use of chemicals in the agricultural environment.

The American Society of Agricultural Engineers Hydrologic Systems Committee (SW-215), along with other technical committees in the SW-21 Hydrology Group have sponsored technical sessions on water quality modeling at International ASAE Meetings for a number of years. In December of 1991 the Hydrologic Systems Committee (SW-215) of ASAE proposed this speciality conference to bring together researchers working on water quality modeling. The committee decided that the scope of the conference should be broad enough to include basic research on process models and parameter estimation as well as the interests of end users of water quality models. Since one important method of communicating a model's capabilities is through hands-on demonstrations, one-on-one sessions were planned to allow direct interaction between model developers and interested potential users.

Cooperating societies and members of the symposium planning committee are listed on the following page. The active participation of these people and organizations contributed to the success of this symposium.

The Symposium Planning Committee would like to express its sincere appreciation to the authors for their contributions. Special thanks go to the four keynote speakers, Stanley R. Johnson, John M. Laflen, William J. Fontenot, and C. T. Haan.

We hope that these proceedings will provide valuable, up-to-date information on water quality modeling that can lead to continued progress in this important area.

Carl E. Anderson, PE
Conference Chair
Associate Professor of Agricultural and Biosystems Engineering
Iowa State University
Ames, Iowa

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2950 Niles Road
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Phone: 616-429-0300

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S. E. Nokes
Member ASAE

F. M. Landa

J. D. Hanson[1]

ABSTRACT

The Root Zone Water Quality Model (RZWQM) is a computer model developed to simulate water, chemical, and biological processes in the root zone of agricultural management systems. RZWQM is in the beta-testing phase of development. This paper reports on a calibration and validation study performed in Ohio for the crop growth portion of RZWQM. One year of data was used in calibrating RZWQM, and two other years of data from the same site were used to check the predictions of the model once it was calibrated. The crop growth predictions were compared to observed values of leaf, stem, and seed biomass collected throughout the growing season at the Ohio Management System Evaluation Area in Piketon, Ohio. The RZWQM predicted seed or yield well for all three years, with predictions falling within one standard deviation of the observed values. Leaf and stem biomass predictions generally fell within one standard deviation of the observed values, but for all years there were dates within the growing season that the predictions were outside of the observed range.
KEYWORDS: water quality model, crop growth model, validation

OVERVIEW OF THE ROOT ZONE WATER QUALITY MODEL

Historical Perspective

The RZWQM is being developed by the Great Plains System Research Unit of USDA-ARS in Fort Collins, Colorado. ARS undertook this project in 1985 in response to requests by scientists and action agencies for a simulation model which would predict the effects of agricultural management systems on the physical, chemical, and biological processes in the root zone. RZWQM is also capable of predicting management effects on crop production. As of August, 1994, RZWQM 2.1 is in the testing phase and is being provided to a limited number of cooperators who have agreed to serve as beta-testers for the model.

[1]S. E. NOKES, Research Scientist and F. M. LANDA, Research Associate, Department of Agricultural Engineering, The Ohio State University, Columbus, Ohio. J. D. HANSON, Systems Ecologist, GPSR USDA-ARS, Ft. Collins, Colorado.

The Management Systems Evaluation Areas (MSEAs) are cooperating with the Great Plains System Research Unit to beta-test the RZWQM. In October, 1992, five post-doctoral scientists were charged with evaluating the sub-processes within RZWQM. Each state administering a MSEA project (Ohio, Nebraska, Missouri, Minnesota, and Iowa) agreed to perform an evaluation of RZWQM, using the MSEA data for calibration and validation purposes. The MSEAs have collected extensive data on agricultural systems, with the objective of evaluating agricultural practices for their impact on water quality, productivity, and profitability. These data provided input information to initialize RZWQM and to evaluate crop production and agri-chemical fate predictions. Ohio was charged with evaluating the crop growth sub-model of RZWQM. This paper reports the results of the calibration process on one year of field corn data, and compares the predictions of the calibrated RZWQM on two independent data sets consisting of two other years of Ohio MSEA field corn data.

General Features of RZWQM

The principal objective of RZWQM is to simulate water, chemical, and biological processes in the root zone (DeCoursey et al., 1992). The primary use of RZWQM is as a tool for assessing the environmental impact of alternative agricultural management strategies on a field-by-field basis. RZWQM is intended primarily for comparative purposes as opposed to rigorous quantitative predictions.

RZWQM, Version 2.1, simulates the movement of water, nutrients, and pesticides over and through the root zone. It is primarily a one-dimensional model, designed to simulate conditions at a representative point in a field. Therefore agricultural practices which are two-dimensional in nature, such as ridge-tillage, banded chemical application, or subsurface drainage are not considered. Measures of the micro and macro-porosity differentiate between rates of flow through the soil matrix. Chemical, nutrient, and pesticide processes are simulated in great detail. The crop growth model simulates plant size and yield as affected by temperature, water and nutrient stress. Management processes include the effect of tillage and other management practices on infiltration rates and micro-topographical features, and impose controls on other processes. In its current state RZWQM can only simulate one year at a time.

A large number of interrelated hydrologic processes are simulated, including: Green & Ampt infiltration; chemical transport during infiltration; transfer of chemicals to runoff during rainfall; water and chemical flow through macropore channels and their absorption by the soil matrix; evapotranspiration, root water uptake, and soil water redistribution; and chemical transport during redistribution.

The soil inorganic chemical environment is simulated to support the prediction of nutrient processes, chemical transport, and pesticide fate and transport. The inorganic processes include bicarbonate buffering; dissolution and precipitation of calcium carbonate, gypsum, and aluminum hydroxide; ion exchange involving bases and aluminum; and solution chemistry of ion pair complexes. The chemical state of the soil is characterized by the soil pH, solution concentrations of the major ions, and adsorbed cations on the exchange complex. The model is capable of predicting soil solution chemistry across a wide range of soil pH.

The nutrient submodel defines carbon and nitrogen transformations within the soil profile. Given initial levels of soil humus, crop residues, other organics, and nitrate and ammonium concentrations, the model simulates mineralization, nitrification, immobilization, denitrification, and volatilization of appropriate nitrogen. A multi-pool approach is used for organic carbon cycling. Process rate equations are based on chemical kinetic theory, and controlled by microbial population size and environmental parameters such as soil temperature, pH, water content, and salinity. Levels of soluble nutrients are used in estimating crop growth, nutrient extraction in surface runoff, and movement through and below the root zone.

Pesticide processes include the transformations and degradation of pesticides on vegetative surfaces, crop residue surfaces, the soil surface, and in a given layer of soil. The model simulates the amount of pesticide reaching the soil surface and the amounts adsorbed and transported through each soil layer. In addition to a "lumped" dissipation, volatilization, photolysis, hydrolysis, biodegradation, oxidation, and complexation dissipation pathways are provided if data are available to drive them. Equilibrium and kinetic adsorption/desorption isotherms are used to obtain a balance between adsorbed and solution pesticide phases.

The management sub-model consists of a description of management activities influencing the state of the root zone. Included are typical tillage practices for most common crop rotations and the impact of these tillage practices on surface roughness, soil bulk density, and micro and macro-porosity. The timing of typical management practices such as fertilizer and pesticide applications, irrigation, planting, primary tillage cultivation, and harvest operations are functions of soil water conditions. Algorithms to describe soil bulk density reconsolidation as functions of time, rainfall, and tillage have been adopted and modified from the WEPP project (Laflen et al., 1991).

PLANT MODEL STRUCTURE

The RZWQM plant growth sub-model is a generic plant model, which can be parameterized to simulate a specific crop. The basic equations will be described here mainly to give the reader a sense of the plant model's strengths and limitations. It is not the authors' intent to fully describe the plant model. Additional information can be found in Hanson and Hodges (1992).

Environmental Fitness

Environmental fitness (EVP) is used in the plant model as a measure of the suitability of the environment for providing for the needs of the plant. EVP is determined as the product of the current temperature fitness (ETP) and the minimum of the current water (EWP) and nitrogen fitness (ENP). All factors are scaled between 0 and 1, with 1 representing ideal conditions.

$$EVP = ETP * \min(ENP, EWP) \quad \textbf{(1)}$$

Temperature fitness is an empirical function of air temperature and the maximum, optimum, and minimum temperatures at which activity occurs for the crop being simulated and a shape parameter for the curve.

Nitrogen is passively taken into the plant in proportion to the plant's transpiration rate and in quantities necessary to satisfy the present N demand. The amount of N that enters the plant is determined by the concentration of N in the soil water that enters the plant. If passive N uptake is limited, then active uptake occurs in a manner similar to the Michaelis-Menton substrate model. Since water uptake affects the passive uptake of nitrogen, the water uptake equations will affect the nitrogen stress (ENP) predictions. The ENP is based on the distance the present leaf nitrogen percentage is away for the lower bound of percentage nitrogen in the leaf, as follows:

$$ENP = \begin{cases} 1 - e^{EFFN \times SPCTN}, & if\ SPCTN > 0 \\ 0 & , otherwise \end{cases} \quad (2)$$

where EFFN is the nitrogen-use coefficient, and SPCTN is the difference between the current percentage leaf nitrogen and the lower bound of percentage shoot nitrogen in the leaf.

The water fitness factor EWP is defined as ratio of actual water uptake, $\{T_r(P_r,z)\}$ to transpiration demand $\{T_a\}$:

$$EWP = \frac{\int_0^{z_0} T_r(P_r,z)\,dz}{T_a} \quad (3)$$

where P_r is the effective water potential in the root at the soil surface in cm and z_0 is total root zone depth in cm.

Water uptake $T_r(P_r,z)$ in cm/day/soil layer is computed using the equation derived by Nimah and Hanks (1973a, 1973b):

$$T_r(P_r,z) = \sum_{t=1}^{24} \frac{[P_r + (P_{res} z) - h(z,t) - s(z,t)]\, RDF(z) K(\theta)}{dx\, dz} \quad (4)$$

where t is the hour of the day, P_{res} is a root resistance term which accounts for the gravity and friction loss terms in the root water potential in cm, h(z,t) is the soil water pressure head in cm, s(z,t) is the osmotic potential in cm, dx is the distance between roots at depth z in cm, RDF(z) is the proportion of the total root activity in the depth increment dz, and $K(\theta)$ is soil hydraulic conductivity in cm/hr. Transpiration demand is calculated by the Penman-Montieth equation modified to account for a sparse crop (Shuttleworth and Wallace, 1985).

Growth Stage Development

Growth stage in RZWQM 2.1 is a theoretical index of plant development and ranges from 0 (seeds) to 1 (totally mature plant). Growth stage (GS) is defined as the development rate for the dominant class, j, modified by the current environmental fitness.

$$GS = \sum_{i=1}^{t} DEVRAT_j * FACT_j(EVP_i) \quad (5)$$

where $DEVRAT_j$ is the inverse of the minimum time required to pass through the current average phenological stage under optimal environmental conditions and $f(EVP_i)$ is an empirical function of the environmental fitness at time i which allows for acceleration or deceleration of crop growth rate depending on the stage at which stress occurs.

Phenological Development

A modified Leslie probability matrix is used to track the phenological development of the crop. At the end of the time step, which is equal to the age-class length, the plant either remains in the present class, progresses to the next age class, or dies. Environmental fitness controls the plant development rate by reducing the probability of progressing to the next stage as follows:

$$p'(j+1,j) = p\,(j+1,j) \times EVP \tag{6}$$

where $p'(j+1,j)$ is the probability of progressing to the next class under the current environmental stress, and $p(j+1,j)$ is the probability of progressing to the next class under no environmental stress.

Photosynthesis

The net carbon assimilation rate is predicted from the solar radiation incident at the top of the canopy as follows:

$$PNCA = \frac{ALPHA \times RAD \times PMAX}{ALPHA \times RAD + PMAX} \tag{7}$$

where PNCA if the net carbon assimilation rate, RAD is the solar radiation incident at the top of the canopy, ALPHA is a light-use efficiency coefficient, and PMAX is the theoretical maximum net assimilation rate. The solar radiation was symmetrically distributed around 1200 hours by estimating the average maximum light flux density for the day within the canopy from RAD.

Respiration

Whole-plant respiration rate is calculated in the RZWQM as a function of plant weight and current day photosynthetic rate based on McCree (1970).

$$WPRESP = BETA \times PNCA + GAMMA \times BIOPLT \tag{8}$$

where WPRESP is the whole-plant respiration, BETA is the proportion of the photosynthate respired for general plant maintenance, GAMMA is the temperature dependent respiration parameter determined from an empirical equation involving the respiration quotient of the plant, and BIOPLT is the plant biomass.

Carbon Allocation

The difference between PNCA and WPRESP represents the allocable carbon for the plant. The carbon is distributed among the plant components based on a hierarchy of demands. Propagules receive carbon first if the plants are in a reproductive growth stage. The remaining carbon is divided between the above and below ground organs. When the plant is in active growth, leaves receive up to 99.5% of the above-ground allocable carbon. As the plant transitions to the reproductive phases less of the carbon is allocated to the leaves (96% and 36% in growth stages 4 and 5 respectively).

Tissue Mortality

Up to 50% of the above-ground plant biomass can die during any given time step. Factors affecting the mortality rate include water stress, freezing temperatures, and tissue age. The actual contribution of each of these factors is determined by input parameters.