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Application of the Root Zone Water Quality Model (RZWQM) to pesticide fate and transport: an overview†

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Abstract: Pesticide transport models are tools used to develop improved pesticide management strategies, study pesticide processes under different conditions (management, soils, climates, etc) and illuminate aspects of a system in need of more field or laboratory study. This paper briefly overviews RZWQM history and distinguishing features, overviews key RZWQM components and reviews RZWQM validation studies. RZWQM is a physically based agricultural systems model that includes sub-models to simulate: infiltration, runoff, water distribution and chemical movement in the soil; macropore flow and chemical movement through macropores; evapotranspiration (ET); heat transport; plant growth; organic matter/nitrogen cycling; pesticide processes; chemical transfer to runoff; and the effect of agricultural management practices on these processes. Research to date shows that if key input parameters are calibrated, RZWQM can adequately simulate the processes involved with pesticide transport (ET, soil-water content, percolation and runoff, plant growth and pesticide fate). A review of the validation studies revealed that (1) accurate parameterization of restricting soil layers (low permeability horizons) may improve simulated soil-water content; (2) simulating pesticide sorption kinetics may improve simulated soil pesticide concentration with time (persistence) and depth and (3) calibrating the pesticide half-life is generally necessary for accurate pesticide persistence simulations. This overview/review provides insight into the processes involved with the RZWQM pesticide component and helps identify model weaknesses, model strengths and successful modeling strategies.
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1 INTRODUCTION

Pesticide transport models offer a cost-effective method of investigating different pesticide management strategies and studying important pesticide processes (eg degradation, sorption) under different conditions (eg management, soils, climate). Furthermore, models can help illuminate which aspects of a system are most in need of further laboratory or field study.[1] The Root Zone Water Quality Model (RZWQM) is a comprehensive agricultural systems model intended as a research tool to investigate the effects of agricultural management on crop production and environmental quality.[2] The pesticide fate component of the model has recently been modified,[3] tested[4–6] and used to investigate pesticide transport issues.[7] To use the pesticide component effectively, however, some understanding of the other components of the model is necessary because the RZWQM is comprehensive in scope and also complex. Submodels within RZWQM include: infiltration, runoff, water redistribution after infiltration, and chemical movement in the soil; macropore flow and chemical movement through macropores; evapotranspiration (ET); heat transport; plant growth; organic matter/nitrogen cycling; soil chemistry processes; pesticide dissipation and degradation processes; chemical transfer to runoff and transport through the soil matrix; and the effect of agricultural management practices on these processes.

More than 40 peer-reviewed publications have utilized RZWQM, and insight into RZWQM may be gained by reviewing model parameterization

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strategies and model performance under different conditions. This will help identify model strengths, model weaknesses and successful modeling strategies. Hanson *et al*[8] reviewed the processes simulated by RZWQM and Ma *et al*[9] reviewed RZWQM applications within whole agricultural systems. A review of the use of RZWQM related to pesticide modeling is undertaken here. Our objectives are to provide an overview of RZWQM history and distinguishing features, provide an overview of key RZWQM components, and review RZWQM validation studies pertinent to simulated pesticide processes.

2 RZWQM HISTORY AND DISTINGUISHING FEATURES

In the mid-1980s, USDA–Agricultural Research Service (ARS) scientists reviewed the state of water-quality modeling in cooperation with other federal agencies and private industry. It was concluded that a comprehensive model of the root zone processes that affect water quality was needed, and that the model must respond to a wide range of agricultural management practices and surface processes. Thus, the specific goal of modeling the interactions among hydrology, agricultural management, crop growth and chemical fate was established. The model was named the Root Zone Water Quality Model (RZWQM) and a team of ARS scientists was selected and assigned responsibility for development. This team was to evaluate and learn from other models available in the USA at the time, such as NTRM,[10] CREAMS,[11] GLEAMS,[12] Opus[13] and PRZM.[14] The team was also to incorporate additional features needed for simulating advanced soil chemistry and nutrient transformations, improved pesticide dynamics, a comprehensive plant-growth model, and important water and chemical management scenarios.

The first version of the model was completed in 1992.[15] Since then, the model has undergone extensive verification, evaluation and refinement, in cooperation with several external users. In particular, cooperative efforts with MSEA (Management Systems Evaluation Areas) water-quality projects in the five Midwestern States have been extremely useful.[16] A Microsoft Windows user interface has recently been developed to make it easier to use. This model has been adequately tested and improved for release to general users. The current version of the model is named RZWQM98.

RZWQM is an integrated physical, biological and chemical process model that simulates plant growth, and movement and interactions of water, nutrients and pesticides over and through the root zone at a representative area of an agricultural cropping system. It is a one-dimensional (vertical into the soil profile) model designed to simulate conditions on a unit-area basis. The model can simulate a fluctuating water table and the flow of water and chemicals to tile drains. It allows simulation of a wide spectrum of management practices and scenarios including: evaluation of conservation tillage, residue cover and conventional tillage; methods and timing of fertilizer and pesticide applications; manures and alternative chemical formulations; irrigation and drainage technology; methods and timing of water applications; and different crop rotations. Tillage and residue management affect soil physical and hydraulic properties, micro-topography and surface roughness, energy and water balance, and chemical transfer from soil to surface runoff. Tillage-induced changes to soil hydraulic properties are simulated to change back slowly to their original conditions as rainfall reconsolidates the tilled layers.

The model contains special features such as the rapid gravitational transport of surface-applied chemicals through macropores, and the preferential transport of chemicals within the soil matrix via mobile-immobile zones. The transfer of surface-applied chemicals (pesticides in particular) to runoff water is also an important component.

The model's generic crop-growth component plays a major role in affecting the state of the simulation system. Shading from the plant canopy reduces soil evaporation, while transpiration links root water and nutrient extraction from soil layers to atmospheric demand. Seasonal sloughing of leaf material and dead roots, coupled with harvest residue, provide a source of carbon and nitrogen for the soil nutrient transformations. Estimates of crop production and yield allow for a relative economic evaluation of the simulation results.

The chemical system within the soil matrix features a complete interaction between nutrient transformations and equilibrium soil chemistry. These two processes characterize the pH and chemical state (salinity) of the soil. Pesticide process dependencies on soil pH are simulated. A multi-pool accounting system for carbon and nitrogen forms the core of the nutrient transformation system. Micro-organism populations respond to food sources, environmental conditions and chemical constraints. Chemical equilibrium concentrations of the major ions in the soil solution and on the exchange complex are modified by soil moisture changes, temperature fluctuations, tillage and application of residues and manures.

To evaluate adequately the effect of certain long-term management practices on water quality and production, RZWQM can be run for up to 100 years using automated execution of certain management operations relative to crop growth stage, such as fertilizer application based on recommended practices, irrigation scheduling, and harvesting. Long-term simulations are important for comparing alternative crop rotations and associated nitrogen and water management practices, since many impacts are only observed after the system has stabilized over many years.

For long-term simulations, over-winter processes of snow accumulation and snow melt are modeled.[17]

More detailed snow and freezing–thawing routines are being tested for future inclusion.

3 KEY MODEL COMPONENTS

3.1 RZWQM simulated processes

Table 1 summarizes the major model components and input requirements. Details on governing equations are provided elsewhere.[8,18]

3.1.1 Hydrology and macropore flow

Rainfall infiltrates into the soil as described by the Green–Ampt equation until the soil's maximum infiltration capacity is exceeded; excess rainfall (or irrigation) is routed into macropores (if present). The maximum macropore flow rate and lateral water movement into the surrounding soil are computed using Poiseuille's law and the lateral Green–Ampt equation, respectively.[39] Macropore flow in excess of its maximum flow rate (if macropores are present) or excess infiltration (if macropores are not present) is routed to runoff. Most of the parameters concerning infiltration, water redistribution, macropore flow and ET listed in Table 1 are common, but the lateral sorptivity reduction factor accounts for impeded lateral water movement into the soil surrounding macropores due to an organic coating or compaction.[19] The effective soil radius will be discussed below (Section 3.1.2). Soil water is redistributed between rainfall using a numeric solution to Richards' equation.[40]

3.1.2 Pesticide processes

Wauchope *et al*[3] describe the pesticide component in detail, and other papers in this series[4–7] deal with various aspects of this component. Briefly, RZWQM has a detailed pesticide component that uses partition coefficients to simulate pesticide sorption to soil and half-lives to simulate degradation (Table 1). RZWQM may simultaneously simulate pesticide sorption on instantaneous equilibrium sites, slower 'kinetic' sites and irreversibly bound sites. Sorption may use a linear or Freundlich isotherm. Kinetic sorption is first-order, onto a defined fraction of total sorption sites. Irreversible sorption assumes a fraction of the pesticide is slowly sequestered in the soil and becomes unavailable for transport, simulating 'aging'. Pesticide sorption and degradation in soil are summarized in Fig 1 and details are provided by Malone *et al*[6]. Other simulated processes include: pesticide degradation and washoff from foliage and mulch; ionic and non-ionic species sorption; adjustment of soil half-life for soil-water content, temperature, and depth; plant uptake; and metabolite formation and transport.

Despite this complexity, the RZWQM pesticide model can be run with a fairly rudimentary amount of pesticide input data. For most of the important pesticides in commercial use the active ingredient (AI) need only be identified and its application timing and mode of application (foliar, soil surface, broadcast, soil incorporated, etc) specified. RZWQM will then supply default values for essential parameters (eg foliar washoff fraction, soil organic carbon sorption constant, aerobic soil half-life, soil-water content and temperature adjustment factors). If a particular parameter is not supplied in the database the model will observe that the value is 'missing' and will not apply the process for which the parameter is required. For example, non-ionic pesticides will not have an acid/base dissociation constant and so the calculations of simultaneous sorption of ionic and non-ionic equilibrium species are not made.[3] The user may edit any default value or add values when defaults are not provided. Wauchope *et al*[3] give details of the RZWQM simulated pesticide processes.

Parameterizing the macropore component may be important to simulate pesticide transport accurately. In addition to the input described in Section 3.1.1 above, the effective soil radius is important when simulating pesticide transport through macropores.[20] The effective soil radius is the lateral radius of soil surrounding macropore walls that interacts with water moving through macropores. Basically, the effective soil radius indicates the volume of soil surrounding macropores available for pesticide sorption.

3.1.3 Chemical transport

Chemical transfer to runoff and macropore flow is simulated using the non-uniform mixing model (Table 1). The degree of mixing between rainwater and soil solution is assumed to be complete at the soil surface ($z = 0$) and decreases exponentially with depth as a function of the non-uniform mixing factor. This parameter may be calibrated, but a value of 4.4 works under many conditions.[18]

The soil matrix is divided into mobile (mesopore) and immobile (micropore) regions and is treated separately from macropore flow. During rainfall or irrigation (infiltration), water and chemicals only move through mobile regions in the saturated zone by 'partial piston displacement', which introduces a degree of preferential transport of chemicals in the soil matrix. During each infiltration step, partial piston displacement is followed by partial chemical mixing in each 1-cm soil increment, which simulates dispersion.[18] Chemical is transferred between mobile and immobile regions during each infiltration time step by diffusion. The only two controlling parameters specific to these processes are the fraction microporosity and the chemical diffusion rate in water.

3.1.4 Agricultural management processes

Allowable RZWQM management options include crop rotations (corn, soybean, simplistic 'quickplant' and 'quickturf' for other plants), tillage, and irrigation, fertilizer, pesticide and manure applications. Crop planting and harvesting are scheduled by the user and crop residues are returned to the soil surface if desired. Surface residue is important in RZWQM because of its effects on soil water, soil carbon and surface soil

Table 1. Summary of RZWQM components and input parameters needed

Processes	Modeling method	Required Input	Comments
Infiltration and water redistribution between rainfall or irrigation	Green–Ampt equation during infiltration Richards' equation during redistribution	Soil crust K_{sat} Soil texture Horizon deliniation Bulk density Soil water retention curves or, 1/3 or 1/10 bar SWC (if available) Initial SWC	The other parameters describing the Brooks–Corey soil-water relationships can be input, but RZWQM will compute these. Runoff is equal to difference between rainfall and infiltration/macropore flow.
Macropore flow	Poiseuille's law and lateral Green–Ampt	Lateral sorptivity reduction factor (reduces lateral water movement simulated from Green–Ampt) macroporosity Effective soil radius Fraction dead-end macropores Average radius of cylindrical pores Width of cracks Length of cracks Depth of cracks	For bromide movement in macropores, Ahuja *et al*[19] assumed water to mix with 0.5 mm of the macropore wall, but this parameter (effective soil radius) can be adjusted. Malone *et al*[6,20] found that an effective soil radius of 0.6 cm worked well for pesticides.
Evapotranspiration	Modified Penman–Montieth[21,22]	Albedo of dry soil Albedo of wet soil Albedo at crop maturity Albedo of fresh residue Pan coefficient (only with pan evaporation) Dry mass of surface residue	Actual ET is bound by water availability as estimated from Richard's equation. The modified Penman–Montieth accounts for a partial canopy and surface residue.
Tile drainage	Hooghoudt's steady state equation[23,24]	Drain depth Drain spacing Radius of drains Water table leakage rate Lateral K_{sat}	The sensitive parameters are effective porosity, initial water content, and lateral K_{sat}.[25]
Heat transport	Partial mixing and displacement during infiltration Heat convective-dispersive equation during redistribution	Soil textural class Dry volumetric soil heat capacity Initial soil temperature	Thermal properties of the soil and water are estimated from the schemes of De Vries.[26] Heat transport during infiltration (partial mixing and displacement) is treated similarly to chemical transport during infiltration, described in Section 3.1.3.

Plant growth	A generic plant growth model for corn and soybean[27]	Maximum nitrogen uptake rate Photosynthate to respire Specific leaf density Plant density Propagule age effect Seed age effect Maximum rooting depth Minimum leaf stomatal resistance Nitrogen sufficiency index Luxurious nitrogen uptake factor	Default parameters are given for corn and soybean but site-specific value should be given or the values should be calibrated. If plant production is not needed, simplistic approaches ('quick plant' and 'quick turf') are available to simulate crop (eg fescue, carrot) effect on ET, water uptake, and nitrogen uptake.
Organic matter/nitrogen cycling	OMN[28]	Fast residue pool Slow residue pool Fast humus pool Transition humus pool Stable humus pool Aerobic heterotrophs pool Anaerobic heterotrophs pool Autotrophs pool Initial urea-nitrogen Initial NO_3-nitrogen Initial NH_4-nitrogen	An initialization wizard is available to aid the user in estimating this input. Generally, good estimates of site-specific total organic carbon and nitrogen will suffice.
Pesticide processes	Wauchope *et al*[3]	Freundlich sorption coefficient (= K_{oc} when $n = 1$), Freundlich exponent ($1/n$) Parameters governing kinetic and irreversibly bound pesticide sorption Acid/base dissociation constants Parameters governing pesticide washoff from foliage and mulch Pesticide half-life (foliar, residue, soil surface, soil subsurface) Half-life adjustment coefficient for soil depth Half-life adjustment coefficients for soil temperature and soil water content Metabolite (daughter) formation fraction	Default input parameters are incorporated into RZWQM from Wauchope *et al*[29] and other sources. Ionic, non-ionic, kinetic (slow sorption/desorption), non-linear (Freundlich), and irreversibly bound sorption may be simulated. Dissipation is simulated as a function of half-life and can be adjusted for soil temperature, moisture, and depth. Foliar and residue washoff, metabolite formation and fate, and root uptake can be modeled. Details concerning the RZWQM pesticide input parameters are provided in Wauchope *et al*.[3]

(*continued overleaf*)

Table 1. Continued

Processes	Modeling method	Required Input	Comments
Chemical transport	Non-uniform mixing model for chemical transfer to runoff[30–32] Partial displacement for matrix transport.[18]	Non-uniform mixing factor (∼ 4.4) which is a mixing parameter dependant on soil type, surface roughness and cover conditions Fraction microporosity Diffusion rate	The degree of mixing between rainwater and surface soil solution is assumed to be complete at the soil surface ($z = 0$) and decreases with depth to 2 cm. Partial displacement during infiltration induces chemical dispersion and preferential flow of chemicals. Chemical is transferred between 'mobile' and 'immobile' regions during infiltration by diffusion.
Agricultural management	Bulk density after tillage[33] Bulk density re-consolidation after tillage[34–35] Soil hydraulic properties after tillage and re-consolidation[36] Surface residue decomposition[37]	Management timing (eg fertilizer application date, tillage date) Management or application type and quantity (eg quantity of fertilizer surface broadcast; chisel plow) Initial surface residue properties (C:N ratio, dry mass of residue, age of residue)	Allowable RZWQM management options are: Crop rotations (corn, soybean, and 'quick plant' and 'quick turf'), three harvest timing options, and five harvest types; 29 different tillage implements, five tillage timing options, tillage depth, and tillage intensity; Sprinkle, flood, furrow, and drip irrigation, with three irrigation timing options; Six fertilizer application options with seven timing options; Eight pesticide application options with five timing options; 15 manure types, four manure application options, and five manure timing options. Note that application is assumed 100% except pesticide application efficiency is dependant upon application type.[38]

Note RZWQM simulates soil chemistry (salinity) processes, however, this component is not described in detail because it has not been tested and described by model users in the peer-reviewed literature.

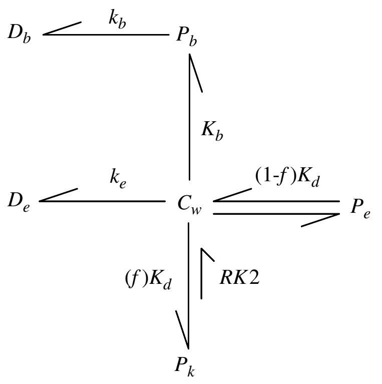

Figure 1. RZWQM sorption, desorption, and degradation. Where P_b = pesticide on bound sites (µg g^{-1}), P_e = pesticide on equilibrium sites (µg g^{-1}), P_k = pesticide on kinetic sites (µg g^{-1}), C_w = pesticide in water (µg ml^{-1}), K_d = equilibrium sorption coefficient (ml g^{-1}), K_b = bound pesticide formation coefficient (ml g^{-1} d^{-1}), $RK2$ = desorption rate constant from kinetic sorption sites (day^{-1}), f = fraction of sorption sites that are kinetic (dimentionless), k_b = degradation coefficient on irreversibly bound sites (day^{-1}), k_e = degradation coefficient of sorbed pesticide in equilibrium with water (day^{-1}), D_e = unspecified daughter product from the water phase, D_b = unspecified degradate from the irreversibly bound sites.

nitrogen.[8] Surface residue decomposition is a function of the residue nitrogen, residue moisture, and daily air temperature.[37] At this time RZWQM allows 29 different tillage implements (eg chisel-till), five tillage timing options (eg pre-plant, specific date) and input of tillage depth and intensity. Tillage modifies soil bulk density and residue pools.[33] Soil reconsolidation with time after tillage is simulated as a function of rainfall energy and quantity.[34,35] Tillage effects on soil hydraulic properties are also simulated.[36] Fertilizer and manure may remain on surface or be incorporated (other options are also available). RZWQM allows seven fertilizer application timings (eg specific date; based on leaf nitrogen content). Eight pesticide application options are available (eg surface broadcast) with five timing options (eg pre-emergence). Irrigation may be applied by sprinkler, flood, furrow or drip methods. Timing of irrigation can be fixed-interval, specific dates, or connected to soil water depletion. Water, fertilizer and manure application efficiency is assumed 100% but pesticide application efficiency is based upon application method.[38] Crops may be harvested on a specific day or at a specific growth stage. Harvest options include multiple or single harvests of seed, above-ground biomass, or root.

3.2 Model calibration/parameterization

Insight into RZWQM components can be gained by investigating parameterization strategies used in previous model studies. Input parameters for RZWQM may be measured, estimated from easily determined soil properties (eg soil texture), estimated from literature or experience, found by calibration, or estimated from RZWQM default data. The minimum data requirements to run RZWQM are provided in Table 2, whereas Table 1 gives more specific input requirements for each model component. As with most chemical transport models, some parameters are difficult to measure or estimate (eg detailed soil hydraulic properties, organic matter pools and plant growth parameters), and are usually calibrated by comparing simulated output to measured data (eg runoff quantity, crop yield). Calibration is usually required for: water balance, organic matter/micro-organism pools and carbon/nitrogen cycling, plant growth and chemical fate. Many RZWQM users calibrate the model using measured data from one time period and validate it using data from other time periods.[41–43] Other strategies include: calibrate using one agricultural management condition then validate

Table 2. Minimum data requirements to run RZWQM

Data file	Minimum data requirement
Breakpoint rainfall	Two pairs of rainfall amounts and times (eg 0 cm rainfall at 100 min; 1 cm rainfall at 200 min)
Daily meteorology	Minimum air temperature
	Maximum air temperature
	Wind run
	Solar radiation
	Relative humidity
Site description	Soil horizon delineation by depth
	Soil horizon physical properties: bulk density, particle size fractions for each horizon (optional soil properties, if available, include: 330 or 100 cm suction water content and saturated hydraulic conductivity for each horizon)
	Estimate of dry mass and age of residue on the surface
	General pesticide data such as common name, half-life, partition coefficient, dissipation pathway (this information can be found in the ARS pesticide database)
	Specifying a crop from supplied database with regional parameters
Initial state	Initial soil moisture contents
	Management details (eg tillage type and timing, chemical application and timing)
	Initial soil temperatures
	Initial soil pH, CEC values
	Initial nutrient model inputs (soil residue, humus, microbial populations, mineral NO_3-N, NH_4-N, may use incorporated RZWQM98 wizard to determine)

(test model) under other conditions;[44] calibrate hydrology component of model and soil parameters using hydrology data and validate pesticide component of model using measured and simulated pesticide concentrations from the same plots and same time periods as calibration data;[6] calibrate using one set of undisturbed soil blocks and validate using different soil blocks but same soil type and management.[20] Common to all model calibration is the requirement that model testing is accomplished using different data from those used for calibration.

A summary of the calibrated and site-specific (measured) input parameters, and the soils and field conditions of selected RZWQM validations, is presented in Table 3. This information outlines potential parameterization strategies and provides insight into RZWQM. It should be noted that the selected assessments do not always make a clear distinction between calibrated, estimated and measured input. For example, Hanson *et al*[41] reported that measured hydraulic parameters were available (eg K_{sat}), but they calibrated these parameters to better predict hydraulic output. Also, Jaynes and Miller[45] estimated herbicide half-lives from the literature to simulate dissipation, but they also report simulated dissipation using calibrated half-lives because of poor modeling results using estimated values. Therefore, input parameter classifications in Table 3 are not always clear-cut. Parameters not listed in Table 3 are literature determined, RZWQM defaults, or difficult to determine. In general, a parameter is listed in one of the two categories (calibrated or site-specific) if it clearly fits.

3.2.1 *Soil parameters*

The soil texture, water content at field capacity (10 or 33 kPa) or water retention curves, bulk density and organic matter or organic carbon have generally been obtained from site-specific measurements.[6,43,44,49,50,55,56,59] Other studies have calibrated water retention curves or field capacity[20,45] and/or K_{sat}.[20,42,54] When initial soil water content (SWC) was unknown it was calibrated.[25,47] The model is sensitive to effective porosity and lateral K_{sat}[25] which have been calibrated when drains were simulated.[25,47,48,53,54] Malone *et al*[6] and Ma *et al*[57] calibrated the hydraulic conductivity of surface crust.

3.2.2 *Macropore parameters*

Macroporosity of the soil has sometimes been measured.[20,45,54] However, Malone *et al*[20] had to input effective macroporosity, defined as 50% of percolate producing macropores, for accurate simulations. Under different management scenarios (eg long-term no-till, short-term no-till, recently tilled) it is difficult to estimate macropore radius. Therefore, Malone *et al*[6] calibrated average macropore radius and produced good simulations by keeping the number of macropores constant and reducing the average macropore radius between long-term no-till, short-term no-till and recently tilled soil.

3.2.3 *Soil organic matter pools*

Soil carbon cycling is simulated in RZWQM. However, short-term pesticide simulations are not sensitive to this because total soil C changes slowly. For long-term simulations RZWQM has a wizard to assist the user with inputting the carbon cycling parameters. Calibration is also necessary for these parameters.[41,42,50,55] Parameters related to carbon/nitrogen cycling have been calibrated by comparing simulated and measured crop yield,[44] nitrate in drainage solution[53] and soil organic matter content.[45]

3.2.4 *Plant growth*

Most studies that considered plant growth important to the simulations report that the plant growth parameters were calibrated.[43,44,58] Five input parameters are generally adjusted for plant growth,[41] but studies indicate that the model is most sensitive to conversion factor from biomass to leaf area index, and much of the crop growth calibration has been done on that parameter.[41,42] These parameters are generally calibrated by comparing simulated and measured crop yield and/or aboveground biomass.[41]

3.2.5 *Pesticide and chemical parameters*

Calibrated chemical parameters include pesticide half-life and partition coefficient.[47,54] Malone *et al*[6] also calibrated the pesticide half-life, and the bound and kinetic parameters. In addition, when runoff or macropore flow was simulated, the non-uniform mixing factor, the pesticide washoff parameters (from crop mulch and/or foliage), and/or the effective soil radius (the soil surrounding macropores that is effective in sorbing chemicals moving through macropores) have sometimes been calibrated.[20,42] More complex pesticide processes may be simulated (eg ionic sorption, metabolite formation, root uptake), but these processes have not been thoroughly examined to date.

4 RZWQM VALIDATION STUDIES

Confidence is gained when a model provides accurate simulations. Validations test one or more model component(s) and are a necessary part of model development.[60] We define validation as comparing model results to observed field or lab data different from the data used for calibration. Validation studies demonstrate effective model parameterization strategies and identify model components that need improvement or modification. In this section we briefly discuss hydrology and plant growth/yield results because a model must correctly predict the hydrology of a system to predict pesticide transport accurately. For example, a model may over-predict the quantity of runoff yet correctly predict runoff chemical concentration, thus surface chemical transport is over-predicted.

For brevity, nitrate results are excluded, although these have often been important aspects of the studies.

Hydrologic parameters (eg K_{sat}) may also directly affect herbicide concentration. For example, Malone *et al*[20] observed that an increased K_{sat} resulted in both less water movement through macropores and lower herbicide concentration moving through macropores (Table 3), possibly resulting in substantially under-predicted sub-surface herbicide transport. In addition, RZWQM simulates pesticide degradation as a function of soil moisture and soil temperature.[3,6] A more detailed RZWQM hydrologic review has been presented elsewhere.[2]

Table 3 summarizes 22 selected RZWQM validation studies out of more than 40 reported RZWQM studies. Reasons for omitting articles include: (1) the evaluation was from a modified version of the model not widely distributed; (2) the article did not evaluate the model against measured data, or (3) the article was primarily a comparison of sub-models within RZWQM that included data, but was not a comprehensive evaluation of RZWQM. Most evaluations commented on the model performance compared to the validation data using subjective terms such as 'reasonable' or 'adequate', and these terms were included in Table 3. All comments and conclusions in Table 3 (rightmost column) concern validation data and not calibration data unless otherwise noted. Model acceptability generally requires subjective judgement from the model assessor.[61] However, objective model performance descriptions are included for nearly all pesticide assessments in Table 3 or in the discussion below (eg predictions were within a factor of two of observations). Two common quantitative measures of model performance in Table 3 are percentage difference from observed and the coefficient of determination (R^2) between observations and predictions.

4.1 Hydrology and plant growth

Table 3 reveals that most hydrologic and plant-growth assessments were adequate for the purposes of the study. However, guidance for improved simulations can be gained from these studies. Drainage, percolate and/or runoff predictions may be improved by simulating macropores.[25,48,54] Moreover, modifying RZWQM to simulate cracking soils, dynamic effective macroporosity and/or the dynamic lateral sorptivity factor may improve runoff simulations.[6,42] Incorrect parameterization of soil restricting layers may contribute to poor soil-water content (SWC) simulations.[49,59] In addition, Ghidey *et al.*[42] modeled a clay pan soil and found that simulated SWC beneath an argillic horizon was too dry, possibly due to incorrect parameterization. Incorrect evapotranspiration simulation may also contribute to poor SWC simulations.[55,58]

For crop production, RZWQM should be used to project maximum yields under given soil and weather conditions because weeds, insects and disease are not considered. Also, yield evaluations should ideally be done over many years, because, if an abnormal year is used to calibrate or evaluate the crop-growth component of RZWQM, the evaluation may not accurately reflect RZWQM performance.

4.2 Pesticide fate and transport

Studies have found that RZWQM can reasonably simulate herbicide transport in percolation and runoff for individual events and can reasonably simulate averages over a season or year (Table 3). RZWQM simulated individual runoff and/or percolate events within a factor of 10 or within the range of field/laboratory measurements.[6,20,42] Yearly or seasonal percolate and/or runoff simulations were within a factor of two or three of field measurements.[6,42,54] These assessments[6,20,42,54] included macropores in the simulations. When simulating macropores, water moves through a small portion of the total porosity and a smaller portion of the soil is available to sorb pesticide.

Ahuja *et al*[46] and Azevedo *et al*[47] found that individual soil concentration predictions (depth and time) were generally within an order of magnitude of those observed, and Ma *et al*[57] found RZWQM gave reasonable predictions of concentration by depth ($R^2 = 0.73$). Jaynes and Miller,[45] in contrast, observed that RZWQM did not adequately predict soil pesticide distribution because observed peak concentrations were at the soil surface (0–7.5 cm) but the predicted peak concentrations were at 15 cm (using the equilibrium-only model). Azevedo *et al*[47] also observed that the simulated pesticide concentrations in deeper soil (below 20 cm) were generally higher than the observed (using the equilibrium-only pesticide model within RZWQM).

Activating the equilibrium-kinetic model, in which a portion of the sorbed pesticides are strongly held and released more slowly than pesticides in equilibrium with soil and water, may improve simulated pesticide concentration with depth. Ahuja *et al*[46] accurately simulated pesticide concentration with depth using the equilibrium-kinetic model, and Ma *et al*[57] noticed, using the equilibrium-only pesticide model, that pesticide peaks were predicted deeper in soil than observed, possibly due to kinetic sorption/desorption.

Calibration was necessary to simulate pesticide persistence accurately; using a default half-life resulted in less accurate predictions.[6,45,46,57] Using the two-site equilibrium-kinetic model where the sorbed pesticide on kinetic sites is not subject to degradation improved persistence simulations[6,46] but this requires determination of additional pesticide input parameters, and half-life calibration is still required. Earlier versions of RZWQM included the option of two-stage dissipation but this is no longer available in RZWQM because it amounted to double-accounting for independent processes added in later versions (eg kinetic sorption where RZWQM does not simulate pesticide degradation); therefore, it will not be discussed here.

The equilibrium-kinetic approach may improve simulated persistence and simulated pesticide concentration by depth. However, it is more complex,

Table 3. RZWQM parameterization and validation summary

Source and {RZWQM version}	Calibrated input parameters	Site-specific input parameters	Soils, crops, and management	RZWQM simulated output	Conclusions and comments
Ahuja *et al*[46] {2.5}	Herbicide half-life	Soil texture; bulk density; 10 kPa SWC; K_{sat}	Loamy sand; 12 × 30 m bare field; conventional-till	SWC at various depths;	Reasonable except the 0–3 cm was over-predicted.
				Soil bromide at various depths;	Reasonable.
				Soil metribuzin and cyanazine concentrations with depth;	Reasonable for metribuzin ($R^2 = 0.83$) and cyanazine ($R^2 = 0.97$) using the two-site equilibrium-kinetic model. Nearly every prediction was within an order of magnitude of observed. Somewhat over-predicted both herbicides, especially at lower concentrations.
				Cyanazine and metribuzin persistence in soil;	Predictions matched field concentration using the two-site equilibrium-kinetic model.
Azevedo *et al*[47] {not provided}	Lateral K_{sat}; effective porosity;[a] initial SWC; pesticide half-life; partition coefficient	Soil texture; bulk density; soil carbon	Kenyon, Readlyn, and Floyd soils; no-till and conventionally-tilled continuous corn	Atrazine concentration with depth;	Predicted concentrations were within an order of magnitude of observed concentrations but the simulated concentrations were generally higher than observed, especially late in the growing season. This may indicate that the persistence was over-predicted. The model correctly predicted depth of atrazine penetration but generally over-predicted concentrations deeper than 20 cm. It was reported that the predictions may have been improved by simulating: macropores, variation of K_{oc} and half-life with depth, interception by surface residue (faster dissipation on residue).
Bakhsh *et al*[48] {3.25}	Effective porosity;[a] lateral K_{sat}; plant growth parameters	None discussed	Kenyon and Readlyn loam; chisel plow corn–soybean rotation	Sub-surface drain flow;	Average difference between simulated and observed flows were +2% for corn and −10% for soybean. Overall flows were over-predicted by 5%. In general, the model over-predicted flow in wet years and under-predicted flow in dry years. Simulating macropores may have improved results.
Cameira *et al*[49] {2.5}	Plant growth parameters	Soil texture; bulk density; 10 kPa SWC; 33 kPa SWC; 1500 kPa SWC; organic matter; C/N ratio	Fluvissol; rototilled, flood irrigated maize hybrid	Soil-water distribution by depth and in the entire profile;	Seasonal average profile simulated volumetric water within 5% of observed. The restricting layer K_{sat}, however, may have been over-predicted, which possibly led to an under-prediction of daily profile soil moisture as indicated by regression analysis of simulated versus observed profile soil moisture (slope <1). Soil water was generally under-predicted in the surface 30 cm of soil above the restricting layer, especially when soil moisture was high.
				Grain yield;	Simulated within 5% of observed.

Farahani *et al*[50] {not provided, but probably 3.2}	organic matter pools; plant growth parameters	Soil texture; bulk density; 33 kPa SWC; 1500 kPa SWC; organic matter; dry surface residue	Numerous loam, clay loam, and loamy sand soils; dryland (no-irrigation), no-till corn and irrigated corn that was disked, chisel plowed, and row cultivated	Seasonal soil-water depletion (excluding toeslope), crop water use, or average volumetric SWC;	Within ±18%.
				Seasonal seepage below the root zone;	Within ±3%.
				Crop nitrogen uptake;	Within ±28%.
				Dry grain yield;	Within ±23%.
				Dry biomass;	Within ±21%.
Farahani *et al*[51] {3.2}	None discussed	Soil texture; bulk density; organic matter	Soil not indicated; furrow irrigated corn	ET;	Reasonable predictions (540 mm modeled vs 517 mm observed; $R^2 = 0.78$). RZWQM tended to under-predict ET at LAI less than 0.5 and over-predict ET at higher LAI.
Ghidey *et al*[42] {3.2}	K_{sat}; organic matter pools; plant growth parameters; non-uniform mixing factor[b]	Soil texture; bulk density; porosity; 33 kPa SWC; saturation SWC	Clay pan soil; Aeric Vertic Epiaqualfs, Vertic Albaqualfs, and Vertic Epiaqualfs; corn/soybean rotation; minimum-till, no-till, and conventional-till	SWC (0.15, 0.3, 0.45, 0.6, 0.75, 0.9 m);	The model generally under-predicted volumetric soil water. Predicted values compared well with measured soil water except at 30 and 45 cm, where the model greatly under-predicted soil water.
				Runoff;	Total runoff was adequately predicted, but it was generally over-predicted on a yearly basis and under-predicted large events. RZWQM predicted runoff during small events when none occurred, possibly due to increased soil cracking not simulated by model.
				Corn and soybean yield;	Generally the simulations were good but over-predicted. Soybean yield was under-predicted during a low-yield year (1994).
				Atrazine and alachlor runoff;	Reasonable when predicted and measured runoff agreed. Predicted and observed were within a factor of 3 for 5 of 6 events.
				Surface soil herbicide concentration (0–5 cm);	Under-estimated early after application, over-predicted much of remaining time, possibly indicating that persistence in soil was over-predicted.
				Daily pan lysimeter atrazine loss for 71 days;	Within the range found in the field when macropores were simulated but the field variability was very high.
Hanson *et al*[41] {3.2}	Organic matter pools; plant growth parameters	None discussed	Soil from six states; corn and soybean; various tillage and mgt. practices (13 comparisons)	Corn yield;	Reasonable in most cases (within ±25% for 11 of 13 comparisons).
				Total corn biomass;	Reasonable in most cases (within ±25% for 11 of 12 comparisons).
				Corn nitrogen uptake;	Reasonable in most cases (within ±25% for 10 of 12 comparisons).
				Soybean yield;	Within ±25% for 2 of 4 comparisons.

(*continued overleaf*)

Table 3. Continued

Source and {RZWQM version}	Calibrated input parameters	Site-specific input parameters	Soils, crops, and management	RZWQM simulated output	Conclusions and comments
Jaynes and Miller[45] {3.2}	Soil-water retention parameters; organic matter pools; crop growth parameters	Soil texture; bulk density; macroporosity; soil carbon	Clarion loam; fine-loamy, mixed, mesic Typic Hapludoll; corn/soybean rotation; disk till	ET;	The model under-predicted ET during the growing season by about 5 to 25% and seemed to under-predict mostly during dry conditions and during September.
				SWC (40, 60, 100 cm);	Generally within field variability, but the simulated water content was much more dynamic than the actual water content.
				Yearly deep seepage;	Reasonable when runoff within the sub-basin was accounted for.
				Soybean yield;	Reasonable (within ±1 standard deviation of measured).
				Corn yield;	Under-predicted by about 2 standard deviations of measured.
				Metribuzin and atrazine in-entire soil profile;	Needed to use a much shorter half-life than published. A two-parameter dissipation model worked better for atrazine but not for metribuzin.
				Metribuzin and atrazine concentration with depth;	Not adequately modeled. Observed peaks at 0–7.5 cm; modeled peaks were at 15 cm.
					It is noted that yield evaluations over many years may be necessary because of things not simulated by the model (eg weeds, disease, insects). If these effects are significant during a calibration or evaluation year and not the other year, simulated yield may not be accurate.
Johnsen *et al*[52] {not provided}	None discussed	None discussed	Primarily Tomatly sandy loam; corn, soybean, potato, wheat;	Subsurface drain flow using water table elevations;	Reasonable but tended to over-predict water table depth (ie, simulated water table deeper than observed). Simulations may be improved if more accurate ET were simulated.
Kumar *et al*[53] {3.25}	Effective porosity;[a] lateral K_{sat}; organic matter pools; plant growth parameters	Soil texture; surface horizon bulk density;	Kenyon loam; fine-loamy, mixed, mesic, Typic Hapludoll; chisel plow; continuous corn with swine manure added	Sub-surface drain flow;	Daily sub-surface drain flows were in close agreement with predicted values (within −3.9% for combined calibration and evaluation years).

Kumar *et al*[54] {3.25}	Effective porosity;[a] lateral K_{sat}; surface layer K_{sat}; lateral sorptivity reduction factor;[c] macropore fraction going to drains; dead end macropore fraction; atrazine half-life; atrazine K_{oc}	Soil texture; surface horizon bulk density; macroporosity	Kenyon, Readlyn, and Floyd soils; continuous corn; modified no-till or moldboard plow	Sub-surface drain flow;	Predictions were good given the spatial variability (within −11.6% of measured for two evaluation years).
				Atrazine in drainage water;	Reasonable (within ±12% for two evaluation years). Macropore simulation was necessary to adequately predict annual atrazine losses.
Landa *et al*[55] {3.2}	Organic matter pools; plant growth parameters	Soil texture; bulk density; 33 kPa SWC; soil carbon	Huntington silt loam; fluventic hapludoll; continuous corn and corn/soybean rotation; chisel plowing and disking	SWC at 15 cm;	Simulation was excellent for soybean. Over-predicted late in season for corn, possibly due to under-estimated ET.
				Corn and soybean yield;	Reasonable (−11 to 16.3% compared to observed).
				Leaf, stem, and seed biomass;	Reasonable for all years. Generally falling within one standard deviation of the observed values.
Ma *et al*[56] {not provided, but more recent than 3.2}	Brooks–Corey parameters	Soil texture; bulk density; 33 kPa SWC; K_{sat}; organic matter	Captina silt loam; fine-silty, mixed mesic, Typic Fragiudult; tall fescue; broiler litter applications	SWC at 10 and 30 cm;	Adequate.
				Soil-water pressure;	Adequate.
				Soil temperature;	Adequate.
Ma *et al*[44] {not provided, but more recent than 3.2}	Organic matter pools; plant growth parameters	Soil texture; bulk density; 33 kPa SWC; organic matter	Vona sandy loam; fine-loamy, mixed, mesic, Ustollic Haplargid; irrigated corn; beef manure	Water storage for entire profile;	Reasonable ($R^2 = 0.98$).
Ma *et al*[57] {not provided}	Soil crust K_{sat}; atrazine half-life	Soil texture; bulk density; soil carbon	Cecil sandy loam; conventionally tilled corn	Water distribution in soil profile;	Reasonable given the large variance of the measured data.
				Water runoff;	Reasonable ($R^2 = 0.87$).
				Atrazine runoff;	Reasonable ($R^2 = 0.92$, slope significantly different from 1 because of over-prediction).
				Atrazine persistence;	Reasonable ($R^2 = 0.97$).
				Atrazine distribution in soil profile;	Generally reasonable ($R^2 = 0.73$, slope significantly different from 1). Note that these results were obtained using the two-stage dissipation model, the soil crust K_{sat} was calibrated using the largest runoff event for each simulation year, and the regression slopes between observed and predicted atrazine runoff and atrazine distribution in profile were significantly different from one (over-predicted for both).

(*continued overleaf*)

Table 3. Continued

Source and {RZWQM version}	Calibrated input parameters	Site-specific input parameters	Soils, crops, and management	RZWQM simulated output	Conclusions and comments
Malone *et al*[6] {RZWQM98 beta version 2000.929}	Average macropore radius; soil crust K_{sat}; metribuzin half-life; kinetic pesticide parameters; bound pesticide parameters	Bulk density; K_{sat}; water retention curves; soil carbon; partition coefficient; applied metribuzin	Lowell silt loam; fine, mixed mesic Typic Hapludalf; short-term no-till (1 year) and recently rototilled	Metribuzin persistence;	Reasonable using kinetic and bound pesticide sorption ($R^2 > 0.89$). Persistence was over-predicted using equilibrium-only sorption even though the half-life was calibrated.
				Metribuzin in runoff for 70-day field experiment;	Reasonable (simulated results within a factor of three of observed). Using equilibrium-only sorption resulted in over-predicted metribuzin in runoff, but if different data were used for calibrating the half-life, the results may have been different.
				Metribuzin in percolate for 70-day field experiment;	Reasonable. Simulated chemical transport in percolate was within a factor of two of observed.
				Daily metribuzin transport in runoff and percolate;	Most simulations were within a factor of 10 of observed. The equilibrium-bound RZWQM modeling approach under-predicted transport greater than 30 days after application.
Malone *et al*[20] {RZWQM98 beta version 1.0.99.1202}	Field capacity of surface horizon; K_{sat}; lateral sorptivity reduction factor;[c] non-uniform mixing factor;[b] chemical washoff parameters; effective soil radius[d]	Bulk density; macroporosity; effective macroporosity;[e] average macropore radius; soil carbon; partition coefficient	Glenford silt loam; fine-silty, mixed, mesic Aquic Hapludalf; no-till blocks brought into laboratory	Bromide, atrazine, alachlor transport through macropores at three antecedent soil-water contents;	All nine simulations were within a factor of three of observed and were considered reasonable. The observed herbicide concentration in percolate, however, decreased with cumulative percolate volume during a rainfall event while simulated concentrations increased.
Martin and Watts[58] {not provided, but probably 3.2}	Depth of horizons; organic matter pools; plant growth parameters	Soil texture; bulk density; SW retention; K_{sat}; soil carbon	Hord silt loam; fine-silty, mixed, mesic, Cumulic Haplustolls; corn; plots were double disked, three irrigation levels and five fertilizer rates were applied; bulk density	SWC (0.15, 0.3, 0.6, 0.9, 1.2 m);	Reasonable given field variability. RZWQM tended to under-predict early and late in the season, possibly because of over-predicted transpiration at low leaf area index.
				Corn yield;	Over-predicted even though calibrated for 1 year.
				Leaf area index;	Reasonable. Under-predicted early and over-predicted late in season for 1 evaluation year.
				Above-ground biomass;	Reasonable.

Nokes *et al*[43] {2.1}	Albedo; plant growth parameters	Soil texture; bulk density; field capacity; organic matter	Huntington silt loam; fine-silty, mixed, mesic Fluventic Hapludoll; high chemical input continuous corn; chisel plowing then disking	SWC (0–15 and 45–60 cm);	Reasonable.
				Crop growth (leaf, stem, seed biomass);	Reasonable.
				Corn yield;	Reasonable. Under-predicted by 10.8% for 1993 and 8% for 1991.
Singh *et al*[25] {2.5}	Effective porosity;[a] lateral K_{sat}; initial SWC	Soil texture; surface horizon bulk density	Kenyon, Readlyn, and Floyd soils; fine loamy, mixed, mesic Typic or Aquic Hapludoll; continuous corn; chisel plow, moldboard plow, no-till, and ridge-till	Sub-surface drain flow;	Satisfactory for different soil and weather conditions but peak flow was often under-predicted. Coefficients of determination (R^2) comparing predicted and measured daily drain flow ranged from 0.51 to 0.78, with slopes ranging from 0.57 to 1.2. The slopes were generally less than one because the peak flows were under-estimated and higher values dominated the estimated slope. Including macropores in the simulations may improve predicted peak flow.
Wu *et al*[59] {not provided, but probably 3.2}	None discussed	Soil texture; bulk density; water retention curves; K_{sat}; soil carbon	Zimmerman fine sand; mixed, frigid, Argic Udipsamments; corn/soybean rotation; ridge-till	SWC (15, 35, 100 cm);	Reasonable at the upper depths. Over-estimated at the lower depths. The 15-cm and 35-cm measured soil water were much more dynamic than predicted and generally under-predicted at high soil-water content, but the 100-cm predicted soil water was more dynamic than measured. The discrepancies between predicted and measured SWC may be partly due to an inadequately parameterized restricting layer.
				Soil water in entire profile;	Over-predicted throughout the season, but it was particularly noticeable at the end of the season. Measured end of season water was about 12 cm for both corn and soybean; predicted was 16 cm for soybean year, 18 cm for corn year.
				Soil alachlor, metribuzin, and atrazine concentration (surface 15 cm);	Temporal changes were modeled reasonably well, but the pesticides were somewhat more persistent than simulated. Simulated concentration had higher peaks and lower tails than observed.

[a] Effective porosity is porosity minus field capacity.

[b] A parameter that depends on soil type, surface roughness, and cover conditions. It affects the degree of runoff mixing with soil depth.[30]

[c] Reduces lateral water movement due to compaction of organic coating on macropore walls.

[d] The soil surrounding macropores effective in sorbing chemicals.

[e] The macropores most effective in producing percolate (50% of percolate-producing macropores).

Note that entries in column 6 ‘Conclusions and comments’ correspond to those in column 5 ‘RZWQM simulated output’.

requires calibration of more parameters, and may have little effect on simulated transport in percolate and runoff compared with the equilibrium-only model.[6] Malone *et al*[6] noticed that the equilibrium-bound approach under-predicted pesticide transport greater than 30 days after application, but this had little effect on total transport because the first few events after application contributed the most to total transport.

5 SUMMARY AND CONCLUSIONS

RZWQM is a chemical transport model intended at this time for use in research on the effects of agricultural management on crop production and environmental quality. The model can be parameterized using: available site-specific input data (the rest of the input can be calculated by the model), default parameters, data from the literature or databases incorporated in the model. Some parameters (eg plant growth, organic matter/nitrogen cycling, pesticide half-life) generally require calibration for accurate simulations. Most assessments have found the model, after extensive calibration, to perform reasonably.

A few patterns were noticed in the validation studies: a restricting layer (low K_{sat}) may be difficult to correctly parameterize and lead to less accurate soil water content predictions; simulating pesticide sorption kinetics may improve RZWQM simulated soil pesticide concentration with time (persistence) and depth; and the half-life may need to be calibrated to simulate pesticide persistence adequately, rather than using a literature-determined half-life.

The performance of a single component of RZWQM (eg pesticide component) varied among different assessments (different modelers, management conditions, soils, climate conditions). For example, most assessments found RZWQM to simulate soil-water content adequately, but a restricting layer in the soil profile was sometimes blamed for less accurate simulations.[49,59] Therefore, if a restricting layer is present, it may be wise to investigate models other than RZWQM or to use detailed soil information to parameterize and/or calibrate the soil parameters (eg water retention curves for site-specific determination of soil parameters; percolate volume from pans or drains for soil parameter calibration). Comparing these different assessments and summarizing them (Table 3) may help potential RZWQM users to identify potential model weaknesses and strengths, and successful modeling strategies.

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