THE WATER, ENERGY, AND BIOGEOCHEMICAL MODEL (WEBMOD): A TOPMODEL APPLICATION DEVELOPED WITHIN THE MODULAR MODELING SYSTEM

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ABSTRACT

WEBMOD simulates hydrologic fluxes and solute concentrations using process modules coupled within the United States Geological Survey (USGS) Modular Modeling System (MMS). For example, the hydrologic fluxes are simulated using routines developed for the USGS Precipitation Runoff Modeling System, the National Weather Service Hydro-17 snow model, and TOPMODEL, a topography-based hydrological model. PHREEQC, a low-temperature aqueous geochemical model, was incorporated to simulate chemical reactions as waters evaporate, mix, or react with the soils. Modifications to several modules were made to simulate the heterogeneity in vertical infiltration rates, irrigation practices, lateral and vertical preferential flows through the unsaturated zone, tile-drains, and gains and losses to regional aquifer systems. This paper describes the WEBMOD algorithms that simulate these reservoirs and fluxes.

INTRODUCTION

In 1992, the U.S. Geological Survey (USGS) initiated the Water, Energy, and Biogeochemical Budget (WEBB) program. The program's focus is on five nearly pristine forested headwater areas; each unique in its climate, geology, soils, and vegetation: (1) the sub alpine slopes of the continental divide draining to Loch Vale, Colorado; (2) the sandy glacial outwash feeding Trout Lake, Wisconsin; (3) the forests and pastures draining to Sleepers River, Vermont; (4) the hillslopes of Panola Mountain in the Piedmont of southeastern Georgia, and (5) the weathered granodiorite in the rainforest of Luquillo Mountain, Puerto Rico. Selected process modules from the USGS Precipitation Runoff Model System (PRMS) model (Leavesley et. al., 1983) were combined with the National Weather Service's Hydro-17 snow module (Anderson, 1973) and the variable source area model, TOPMODEL (Wolock, 1993). The model, XTOP_PRMS, was built in the U.S. Geological Survey's Modular Modeling System (Leavesley et. al., 1998) using the aforementioned components that have shown to be robust and parsimonious.

Additional complexity was introduced to XTOP_PRMS to improve model fit with observations that were not possible with earlier simpler model components. For example, the sharp relief of Loch Vale and associated disparity of temperature and energy loadings required that individual models be constructed for hillslopes of similar elevation and aspect. The fate of water falling on the sandy soils around Trout Lake depends as much on variations in regional ground-water levels as it does on local topography and surface-water drainage patterns. Therefore the ability to incorporate ground-water fluxes estimated from numerical or conceptual ground-water models was added to XTOP_PRMS. Finally, heterogeneous soils and preferential flow paths documented at Sleepers River, Panola Mountain, and Luquillo Experimental Forest also were added to XTOP_PRMS.

The USGS National Water-Quality Assessment (NAWQA) Program began collecting data in 1991 to identify the sources, transport, and fate of agricultural contaminants across a range of scales (Gilliom et. al., 1995). In 2001, five NAWQA agricultural watersheds with diverse hydroclimatic regions and subject to a variety of agricultural management practices were selected for more detailed study: Mustang River, California (53 km^2); Granger Drain, Washington (160 km^2); Maple Creek, Nebraska (950 km^2); Sugar Creek, Indiana (246 km^2); and Morgan Creek, Maryland (32 km^2) (Capel et. al., 2004). XTOP_PRMS was further modified to address these unique complexities. For example, XTOP_PRMS was modified to simulate irrigation from surface water or wells of these watersheds, and field dewatering by tile drains, conditions evident in these watersheds. Stream water quality is simulated using relative contributions of new (overland flow) versus old (ground-water discharge) water predicted by XTOP_PRMS; the simplest model assumes concentrations of the new and old water to be distinct and unvarying with time. This constant concentration approach has been applied successfully to explain variations in solute concentrations measured in a stream. Conceptual reservoirs with limited capacity, such as the canopy and root zone, cannot be represented as having constant concentrations. To simulate changes in solute composition in these and other hydrologic compartments in the landscape, routines from PHREEQC (Parkhurst et. al., 1999), an aqueous geochemistry model, is incorporated. PHREEQC computes final solution compositions of water masses mixed in ratios predicted by the XTOP_PRMS hydrologic model. With this addition, XTOP_PRMS was renamed the Water, Energy, and Biogeochemical MODel, or WEBMOD. The purpose of this paper is to describe the WEBMOD algorithms that simulate the reservoirs and fluxes shown in figure 1.

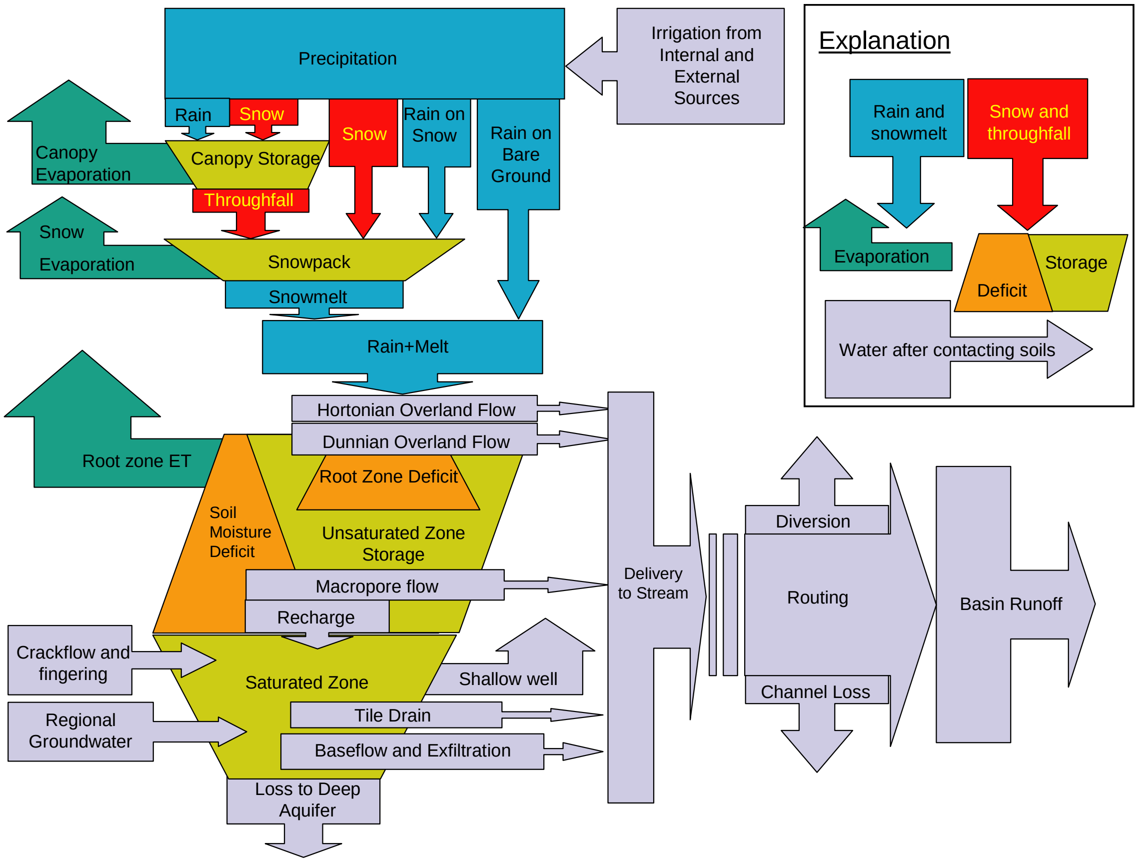

Figure 1. Reservoirs and fluxes of WEBMOD. Infiltration, transpiration and wetting of the root zone by groundwater are not shown to simplify the schematic

MODEL OVERVIEW

The Modular Modeling System (MMS) (Leavesley et. al. 1998) provides a framework to develop and couple process and input/output routines into a single model and facilitates model analysis and optimization. Eighteen modules were joined to form WEBMOD: six modules simulate storage and fluxes of water in the canopy, snowpack, hillslopes, and streams; four modules simulate distribution of temperature and energy needed to estimate potential evapotranspiration (PET); three modules track reservoir volumes and compute solute concentrations; and five modules are involved in input/output and computing statistics. File management, run-time graphics, parameter editing routines, sensitivity analyses, optimization methods, and basic variable statistics are all core functions of the MMS. The GIS Weasel (Viger et. al., 1998) provides a geographic information system interface to derive and distribute parameter values describing topography, drainage, land cover, soils, and vegetation. Vegetation is assigned both summer and winter characteristics. An individual hillslope from the hilltop down to a stream forms a unique Model Response Unit (MRU) in WEBMOD; the vast majority of parameters describing slope, aspect, vegetation, and soils are assumed homogeneous in an MRU. Topographic wetness indices are computed for each hillslope, and fluxes are simulated through the root and unsaturated zones for each index, or area of similar hydrologic behavior.

WEBMOD was designed primarily for multi-year simulations of fluxes estimated on a daily time step. Shorter time steps can be employed with daily estimates of potential evapotranspiration and snowpack processes apportioned into the sub-daily time periods. The minimum climate data needed consist of daily observations of precipitation along with minimum and maximum temperature. The form of precipitation (rain or snow), pan evaporation, and measured insolation can be used if available, but the model will generate values for these variables if they are not provided by the user. Observed streamflow and solute concentrations also may be included in the data file to evaluate and optimize model performance. Sources and volumes of irrigation or regional ground-water fluxes also may be specified for ground-water and agricultural simulations. Summary results and statistics can be printed or saved in a data file for every day, month, or year, or just once at the end of the model run.

Water and solutes enter and leave the model through top, bottom, or side boundaries. The atmosphere serves as the source for precipitation and the sink for evapotranspiration; the basin outlet is the sink for water discharged from the basin; and aquifers can act as sources and sinks. Irrigation from a shallow aquifer is considered an internal flux whereas irrigation from a deep aquifer or irrigation canal crossing the basin is considered an external input. Within the model, water moves between six interior compartments that are represented as storage volumes and saturation deficits: canopy, snowpack, three hillslope compartments (root zone, unsaturated zone, and saturated zone), and the stream (figure 1). Consistent with TOPMODEL, an individual root zone and unsaturated zone is simulated for each topographic wetness index. The wetness index reproduces thicker unsaturated zones farther away from streams and hollows and simulates variable areas of saturated land surface that are source areas for Dunnian overland flow (Beven et. al., 1979). The sum of all hillslope discharges are converted to longitudinally averaged inputs into the reach channel for each MRU and then routed to the basin outlet via the main channel. The linear routing technique (Clark, 1945) is similar to one described by Dawdy et. al. (1972) and is the same as the channel-routing method algorithm used in TMOD9502, distributed by Keith Beven at Lancaster University.

Distribution of Temperature and Precipitation

Model performance is very sensitive to measurements and estimates of fluxes of water into and out of the atmosphere. For watersheds with one meteorological station, precipitation and temperature are distributed to individual hillslopes of differing aspects and elevations using modules from PRMS (Leavesley et. al., 1983). The distributed temperatures are then used to predict the proportions of rain and snow in the precipitation. For watersheds with multiple meteorological stations, precipitation and temperatures are distributed using the XYZ methodology described by Hay and McCabe (2002). Temperatures are distributed using lapse rates, and differences in elevation and aspect.

Evapotranspiration and Canopy Interception

Day length and air temperature are used to estimate daily potential evapotranspiration using the Hamon method (Hamon, 1961). The potential evaporative demand will be removed, as available, from the canopy storage, snowpack, and soil.

On days with active evapotranspiration (summer, or growing season) and no canopy storage, WEBMOD simulates that 70% of the soil ET will be transpired to the canopy where it will be evaporated; this fraction is reduced to 10% of the soil ET during dry winter days when leaf stoma are usually closed. By including the transpiration separate from soil evaporation, nitrogen and other ions can be translocated to the canopy where they mix with rainwater to become a solute in throughfall. On days with precipitation, the canopy will store water until it exceeds the user-defined capacity; snow capacity usually exceeds rain capacity and both are a function of vegetation type and density. Vegetation types include bare ground, grass, shrubs, or trees. Only shrubs and trees are assumed to have a canopy capacity when there is snow on the ground. Both summer and winter cover types and density can be specified. The summer values become active during periods of active evapotranspiration. The user defines the earliest possible month for evapotranspiration; from that point on, maximum temperatures are summed until the total exceeds a specified level of degree days, at which point the evapotranspiration is assumed to be active until the end of a user-specified growing season. Snow in the canopy can sublimate, melt, or unload to the snowpack underneath. Snow unloads if two days pass with no new precipitation and there is still snow in the canopy.

Irrigation

Irrigation water in WEBMOD can originate from several sources. Water can be extracted from the stream, the saturated zone, or from a source external to the model boundaries. In all cases, the user provides a time series of the equivalent depth of irrigation desired for each MRU. Applied irrigation volumes are limited by available stream water, pump capacity, and screen depths. The irrigation water is combined with precipitation such that the runoff response of an irrigated watershed can be observed. Some ski areas make snow with water from surface-water diversions or ground-water wells. Snowmaking and its effect on water supply and quality is one possible WEBMOD scenario.

Snowpack

The HYDRO-17 model, developed by Anderson (1973), is used in WEBMOD to describe the accumulation and ablation of the snowpack. HYDRO-17 is a temperature index model that has a seasonally varying melt factor. A more complete energy balance is computed on days with rain on snow. Hydro-17 simulates reduced energy loadings, and resulting attenuated melt rates, for periods when snow-covered area is less than 100 percent. Snow melt, direct precipitation, and irrigation can infiltrate into the root zone.

Overland flow

TOPMODEL includes routines to simulate both Hortonian (Horton, 1939) and Dunnian (Dunne, 1970a,b) overland flow. Hortonian overland flow occurs when the rate of precipitation or snowmelt exceeds the infiltration rate of the soil. Dunnian overland flow occurs when precipitation or snowmelt occurs on a saturated soil.

WEBMOD employs a modification of the Green-Ampt infiltration model (Green and Ampt, 1911) to predict Hortonian overland flow. In the original version of TOPMODEL, soils are assumed to be homogeneous for a given hillslope; once the precipitation rate exceeds the infiltration rate, ponding occurs over the entire hillslope. This assumption was modified in WEBMOD by using a log-normal distribution to describe vertical infiltration rates for each hillslope. The same Green-Ampt routine is then used for nine soil classes, whose log-normal population is described by a median and coefficient of variation. The default coefficient of variation is 14.13 which results in an order of magnitude change with each class. By setting the coefficient to 0.0, the original TOPMODEL homogenous soils are simulated. When using any value other than 0.0, the median infiltration value describes 34.3 percent of total hillslope area, with the higher and lower infiltration values on either side of the median infiltration rate describing 23.7, 7.8, 1.2, and 0.1 percent of the area.

Variable Source Area and the Topographic Wetness Index

Rain, irrigation, and snowmelt remaining after canopy interception and overland flow are routed through the hillslope using modifications of TOPMODEL (Wolock, 1993) concepts first described in detail by Beven and Kirkby (1979) and recently critiqued by Beven (1997). Dunnian overland flow is a key component of TOPMODEL. The area of saturated soils (source areas) will vary with every time step, expanding with substantial infiltration events and shrinking as the hillslopes dry out. Therefore a storm during a wet period will generate a quicker streamflow response than an equivalent storm during a dry period.

Using gridded digital elevation model data, flow direction, flow accumulation, and slope are derived for each grid cell. The topographic wetness index can then be calculated for each cell as $\ln(a/\tan B)$, where ln is the Naperian logarithm, a is the area draining through a unit contour width from upslope, and B is the local slope. Areas with significant upslope contributing area and low slopes will have a higher topographic index than an area near the ridge tops and with higher slopes; the larger the topographic wetness index the shallower the water table is expected to be. Areas with the largest indices, usually near streams, are expected to be the wettest and may be saturated. Any precipitation or snowmelt on saturated areas will run off as overland flow as described above.

The saturation deficit is calculated for representative values of the topographic index distribution (called bins in WEBMOD) as

$$sd_i = sbar + (szm \times (TL - st_i)) \times resp\_coef \tag{1}$$

where sd_i is the saturation deficit for topographic index bin i in a given MRU; sbar is the average soil moisture deficit for the MRU; szm is a parameter describing the shape factor of the exponentially decreasing transmissivity curve for the MRU; TL is the mean topographic index for the MRU; st_i is the value of the topographic index for the bin i; and resp_coef is a time-dependent response coefficient introduced to reduce saturation deficits and surpluses at shorter time scales. Without this coefficient, daily exfiltration volumes summed from hourly time steps, described below, far exceed the volumes produced at daily time steps.

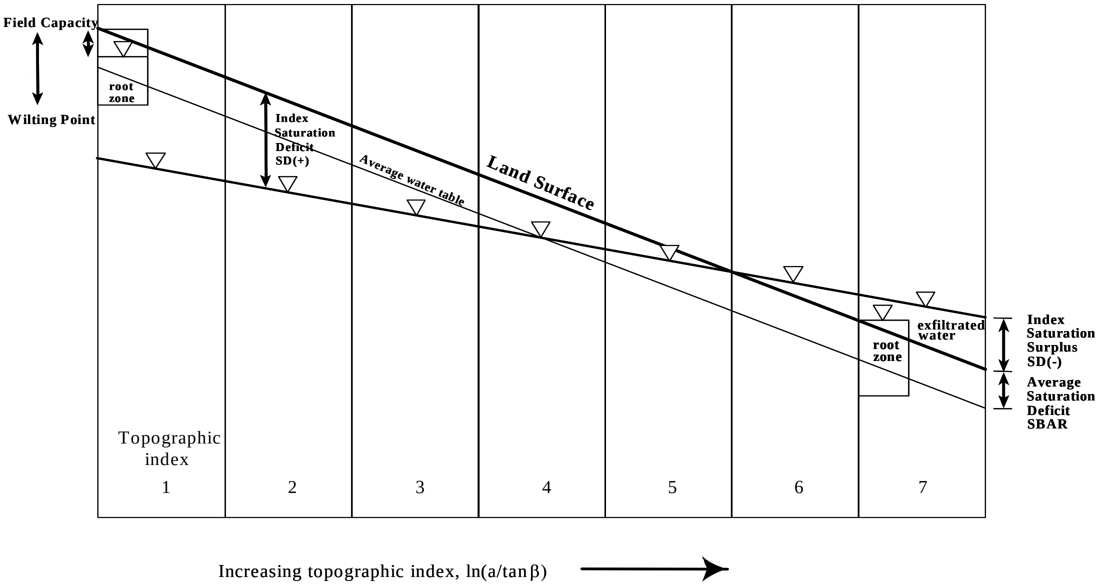

Figure 2. Variations of saturation deficits and water table with increasing topographic index. Where negative saturation deficits are predicted, WEBMOD will satisfy any root zone deficit and then collect any additional surplus as exfiltration to combine with baseflow for delivery to stream.

WEBMOD differs from the original TOPMODEL in the way negative saturation deficits are handled (figure 2). The calculated deficit, sd_i, is the maximum amount of water that can infiltrate in soils of a given topographic index (in excess of that needed to fill the root zone to capacity) before producing overland flow. In the original TOPMODEL, sd_i values less than zero (a saturation surplus, or artesian head at or above the land surface) are simply set to zero. Conceptually, this would imply that excess water is redistributed back up the slope thereby decreasing the rate that the water table would lower. Also, during periods with no precipitation in the original TOPMODEL, evapotranspiration from the root zone can produce substantial deficits even in bins with negative values of sd_i. In WEBMOD, surpluses identified by negative sd_i values are used to satisfy the root zone deficit for that bin. The amount of water transferred from the saturated zone to the root zone is equal to the hypothetical artesian head, or the root zone deficit, whichever is less, multiplied by the total hillslope area within that topographic index. Any water in excess that needed to satisfy the root zone deficit is then collected as exfiltrated water and delivered to the stream. Note that although figure 2 is not intended to be interpreted as a cross section of a hillslope, the analogy would be close if the section sliced through a converging drainage had a hollow or riparian area at the bottom. Processing of hillslope contributions to the stream begins with the saturated areas with the highest topographic indices and proceeds to the unsaturated areas with lower indices.

Unsaturated zone

The unsaturated zone is modeled as a root zone that can lose water to evapotranspiration, and a separate unsaturated zone storage that drains to become lateral preferential flow or ground-water recharge. Evapotranspiration from the root zone will occur at the potential rate when soils are at field capacity, and reduce linearly to zero when soils have dried to the wilting point.

Infiltration in excess of that needed to bring the soil moisture to field capacity and vertical preferential flow are available to the unsaturated zone storage, *suz*. The total depth of storage available for infiltration is equal to the root zone deficit plus the saturation deficit, sd_i, for each topographic index bin.

Recharge to the saturated zone, uz_i, is estimated for each topographic index bin using a simple time-delay function of

$$uz_i = (suz_i \times dt)/(sd_i * td) \tag{2}$$

where uz_i is the recharge rate to the saturated zone for the topographic index bin i during a given time step; suz_i is the unsaturated zone storage for the bin (a percentage less than or equal to the saturation deficit sd_i); dt is the time step, in hours; sd_i is the saturation deficit for the bin; and *td* is the time-delay constant, in hours per unit saturation deficit. The recharge amounts for each topographic index bin, uz_i, are area weighted and summed to yield a recharge rate to the saturated zone for the entire hillslope, quz. A fraction of the recharge may be selected for delivery to the stream via lateral preferential flow paths such as macropores, root casts, or flows along shallow lenses of impermeable layers (Piñol et. al., 1997). The amount of lateral preferential flow (or macropore flow) is computed as

$$qdf = quz \times qdffrac \tag{3}$$

where *qdf* is the amount of preferential flow delivered to the stream, *quz*, is the recharge described previously, and *qdffrac*, is user-specified proportion for each MRU. Note that this quickflow component is in addition to the one implicitly included in the exponentially decreasing hydraulic conductivity with depth (equation 4). Vertical preferential flow paths are also available that bypass the root zone or the unsaturated zone entirely. To reiterate, these flow paths are included to build models where vertical bypass is strongly supported by hydrologic or geochemical evidence.

Saturated zone

Following the standard TOPMODEL convention, saturated hydraulic conductivity is assumed to decrease exponentially with depth,

$$K_{(z)} = K_0 e^{-\frac{z}{szm}} \tag{4}$$

Where $K_{(z)}$ is the saturated hydraulic conductivity at depth; K_0 is the saturated hydraulic conductivity at the land surface; and *szm* is a shape factor. Smaller values of *szm* result in more rapid decreases in conductivity with depth. The transmissivity at the surface, T_0, is equal to the saturated hydraulic conductivity at the surface, K_0, times the shape factor *szm*. The TOPMODEL parameter T0 is equal to $ln(T_0)$. The transmissivity profile, defined by T0 (a function of K_0 and *szm*), determines the maximum baseflow discharge, *szq*, from an MRU for a given time step.

$$szq = e^{(T0+\ln(dt))-TL} \tag{5}$$

Where *szq* is maximum baseflow discharge for the MRU during a time step; T0 is the Naperian logarithm of the $T_{0;}$ dt is the time step; and TL is the mean topographic index for the MRU.

Baseflow discharge, *qb*, is calculated as:

$$qb = szq \times e^{\left(\frac{-sbar}{szm}\right)} \tag{6}$$

where szq is the maximum base flow discharge; sbar is the average soil moisture deficit; and szm is the transmissivity profile shape factor. The average hillslope saturation deficit, sbar, also is updated each time to reflect any pumping for irrigation and any gains or losses to the aquifer.

Tile Drains

Tile drains, or any preferential flow processes within the saturated zone, are simulated by specifying a threshold water table level that, when exceeded, initiates preferential discharge from the saturated zone. Preferential flows then increase linearly with a rising water table up to some maximum that reflects the effective saturated conductivity of the preferential flow system.

Channel Routing

The sum of all hillslope discharges for each MRU are converted to longitudinally averaged inputs into the reach and then routed to the basin outlet via the main channel. All river segments with similar distances away from the basin outlet are modeled as being in the same time-delay ordinate. This technique estimates flow and solute loads at the outlet and not for a specific upstream branch.. Losing rivers may be simulated by assigning a loss rate in flux per linear distance of channel (cfs/mi for example).

Geochemical simulations

The user provides initial estimates of reservoir compositions in a standard PHREEQC input file (Parkhurst et. al., 1999). Time series describing the solutes in precipitation and irrigation waters from external sources also are needed in standard MMS format (time stamp followed by space-delimited data). With each time step, fluxes and mixing ratios predicted by the hydrologic components are provided to PHREEQC which computes and stores each solution composition. There may be 100 hillslopes in a watershed model, each with a canopy, snowpack, and a thin O-horizon to mix with overland flow and a saturated zone. There is also one unsaturated zone for each topographic wetness index. The number of discrete stream segments depends on the velocity of the stream and the time step of the model. Depending on the desired level of complexity, the user can simulate and track equilibrium or kinetic reactions, sorption-desorption, ion exchange, and solid solution equilibria for any reservoir in the model.

CONCLUSION

WEBMOD is being used to simulate the processes involved with water quantity and quality in watersheds with diverse hydroclimatology, soils, and management practices (Webb et. al., 2003; Linard et. al., 2006). The simulations potentially can provide estimates of antecedent and forecasted watershed hydrology that can be used to optimize water use and water quality. And finally, WEBMOD is a valuable tool for both teaching and testing conceptual and numerical models requiring mass balance.

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