Hydrologic Modeling of a Groundwater Dominated Watershed Using a Loosely Coupled Modeling Approach

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EXTENDED ABSTRACT

Since the late 1960s, hydrologic modeling focused more and more on interactions between surface and groundwater flow systems, leading to the development of integrated modeling approaches simulating flow in these two systems and the simulation of interactions between them. These interactions are of variable character as well as spatial and temporal heterogeneity.

The primary objective of this study is the application and investigation of a loosely coupled modeling approach, combining two well-known models of the United States Geological Survey, the Precipitation Runoff Modeling System (PRMS) and the Modular Finite-Difference Groundwater Flow Model (MODFLOW), in order to simulate complex hydrological processes in a mesoscale watershed. Within the scope of the hydrologic modeling groundwater recharge, the parameter unidirectionally linking the surface water and groundwater system is used to couple these two models loosely. Considering factors that have a great influence on groundwater recharge (e.g. climate, topography, soil, and land use), the potential of modeling the hydrologic system with a distributed surface water model is explored. In addition, the option of constraining the PRMS parameter determining groundwater recharge, and therefore the loosely coupled surface-groundwater model, with observed head levels only, is investigated.

This modeling approach is applied to the Esperstedter Ried basin, an ungauged, mesoscale, groundwater-dominated catchment in central Germany. The study represents a good example of problems frequently occurring in hydrologic modeling. Due to the lack of observed streamflow and surface runoff data, the calibration and validation of any hydrologic model for this watershed proves to be difficult. Furthermore, the basin features a strong surface-groundwater interaction of unknown degree.

This research paper describes the concept of an inexpensive and simple method of combining the advantages of two established hydrologic modeling approaches by using output information of the surface water model as input for the groundwater model. The basic assumption is made that groundwater recharge rates provided by PRMS are reasonable because the estimation procedure benefits from the fairly high resolution of meteorological, land use and soil parameters of the surface water model. At present, the approach presented in this paper is limited to a unidirectional coupling of the surface and groundwater model, which is only accounting for groundwater estimates provided by PRMS as input for MODFLOW; whereas possible upward movement of water, i.e. groundwater seepage to the surface is neglected. Performance and efficiency of this approach are assessed in the scope of applying the model in steady-state as well as transient mode to the Esperstedter Ried basin.

The results of this case study, which produced a number of reasonable as well as some unsatisfying simulations, demonstrate the potential of coupling a surface water model and a groundwater model to obtain more complex and accurate analyses and simulations of hydrologic systems. However, the study also shows the need for further research in regard to constraining the parameter linking both models, i.e. groundwater recharge. Furthermore, the necessity for a more dynamic and complex method of integrating surface and subsurface interactions is revealed, which accounts for downward as well as upward movement of water in the subsurface system.

1. INTRODUCTION

Traditional hydrologic modeling approaches generally concentrate on either the surface or the subsurface system. Surface water models are designed and calibrated with emphasis on surface water movement, evapotranspiration and infiltration; whereas the subsurface is commonly viewed as a simple, lumped system and groundwater processes are not physically based. Groundwater models, on the other hand, focus on obtaining exact groundwater head levels in respect to occurring stresses while surface water processes are oversimplified.

For the last three decades, a major objective of hydrologists has been the coupling of both approaches in order to model the entire hydrologic system and, furthermore, to investigate the interaction between surface and subsurface processes. Particularly basic methods of modeling surface-groundwater interactions based on numerical solutions of differential equations and a variety of integrated models have been developed since the late 1960s. Some of the first studies of surface-subsurface interactions were conducted by Smith & Woolhiser (1971), who coupled a one-dimensional flow vertical infiltration model to an overland flow model, Pinder & Sauer (1971) linked a one-dimensional streamflow model to a two-dimensional aquifer, and Freeze (1972) designed a model simulating three-dimensional transient subsurface flow as well as one-dimensional streamflow. In recent years, a number of integrated models has been developed, including SHE, MIKE-SHE, and FHM. SHE (SYSTÈME HYDROLOGIQUE EUROPÈEN) is a physically based modeling system, simulating various components of water movement (such as evapotranspiration, overland and channel flow, flow in the unsaturated and saturated zones, and many more) based on finite-difference or empirical equations. In addition to representing the entire land phase of the hydrologic cycle (interception, evapotranspiration, surface runoff, river routing etc.), MIKE-SHE also describes water movement in the unsaturated soil zone and groundwater flow. The coupled surface and groundwater model FHM, which incorporates components of the surface water model HSPF and the groundwater model MODFLOW, is another example for an integrated model.

This paper describes an alternative approach to modeling a surface-groundwater system by loosely coupling two well-established models of the United States Geological Survey, the Precipitation Runoff Modeling System (PRMS) and the Modular Finite-Difference Groundwater Flow Model (MODFLOW), which are both available free of charge on the internet. The factor unidirectionally linking both systems (i.e. the parameter coupling the surface and the groundwater model), namely groundwater recharge, is investigated regarding the performance of this loosely coupled approach. Furthermore, the possibility of constraining the PRMS parameter determining the amount of recharge into the subsurface reservoir by merely using observed groundwater head levels is assessed.

2. MODEL DESCRIPTION

2.1. The groundwater model MODFLOW

The Modular Three-Dimensional Finite-Difference Groundwater Flow Model (MODFLOW) first released by the U.S. Geological Survey in 1984, has become the most widely used groundwater model (McDonald & Harbaugh 1984) MODFLOW is a mathematical model simulating the groundwater flow through heterogeneous, porous media. In MODFOW three-dimensional groundwater flow is described by the partial-differential equation

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-W=S_S\frac{\partial h}{\partial t} \quad (1)$$

where K_{xx}, K_{yy}, *and* K_{zz} = the hydraulic conductivity along the x, y, and z axes that are assumed to be parallel to the major axes of hydraulic conductivity (L/T), h = the potentiometric head (L), W = volumetric flux per unit value representing sources and/or sinks of water (W < 0.0 for outflow of the groundwater system, W > 0.0 for inflow (T-1), *SS* = specific storage of porous material (L-1), and *T* = time (McDonald & Harbaugh 1984).

Spatial discretization in MODFLOW is achieved by considering real-world aquifers a system of grid cells which are characterized in terms of rows (i), columns (j), and layers (k). Every cell represents a unit of homogenous properties. In the current version MODFLOW-2000, the finite-difference grid is assumed to be of rectangular shape horizontally, while the vertical dimension is distorted. Temporal discretization is based on time steps, which are grouped into stress periods. The length of particular time steps is user-defined during the model setup.

In this study MODFLOW-2000 is used, which is operated in the comprehensive graphical user environment GMS (Department of Defense Groundwater Modeling System).

2.2. The surface water model PRMS

The U.S. Geological Survey's Precipitation Runoff Modeling System (PRMS), a deterministic, physical-process based watershed model was developed by Leavesley *et al.* in 1983 (Leavesley *et al.* 1983). PRMS which operates either as lumped- or distributed parameter model, is designed to analyze the dynamics and responses of a hydrologic system regarding the influence of multiple combinations of precipitation and climate as well as specific features of the study areas (e.g. land cover, soils, and topography). PRMS achieves a reasonable representation of the real-world system because the various elements of the hydrologic cycle are represented by either physical laws or empirical relationships.

The system response is investigated on different temporal and spatial scales; discretization in time is achieved by the distinction between daily mode (daily averages or total values) and storm mode (time intervals as short as one minute). Spatial heterogeneity of the system is accounted for by dividing the catchment into homogenous subunits of climate, land use and pedo-topo-geological characteristics, so-called hydrological response units (HRUs).

2.3. The Coupled Modeling Approach

The PRMS model will provide a set of parameters best suited to simulate the water balance of a catchment; furthermore, the model estimates inflow to the groundwater reservoir which is distributed in time and space. These estimated recharge values are converted on temporal and spatial scales to be incorporated into MODFLOW. The groundwater model is run both in steady-state and transient mode in order to analyze the behavior of the model to spatially and temporally distributed recharge. The link between the surface water model PRMS and the groundwater model MODFLOW is the PRMS parameter $ssr2gw_{rate}$ (coefficient to route water from to the groundwater system), which provides recharge estimates. Currently, the link between both models is unidirectional, investigating whether it is possible to provide spatially and temporally variable information on groundwater recharge by running a surface water model.

However, the coupling of both models necessitates the conversion of spatial and temporal scales. The surface system and, consequently, the estimation of recharge values are distributed in space by hydrologic response units, whereas the groundwater system operates on the basis of gridded cells (Figure 1). To define specific recharge rates for each grid cell, the proportion of area of each HRU per cell is computed; hence, the amount of recharge can be determined for every active cell in the MODFLOW grid model based on this proportion. The conversion of temporal scales needed for the transient MODFLOW simulation is performed by calculating the mean monthly amount of recharge for each HRU based on daily output of $ssr2gw_{rate}$ values. The monthly recharge values are then mapped to the appropriate MODFLOW cells based on the proportion each MODFLOW cell within each HRU. Furthermore, an average recharge value for a specific PRMS model run is computed over the entire timeframe, which specifies the recharge in form of a Type II boundary condition for a steady-state simulation.

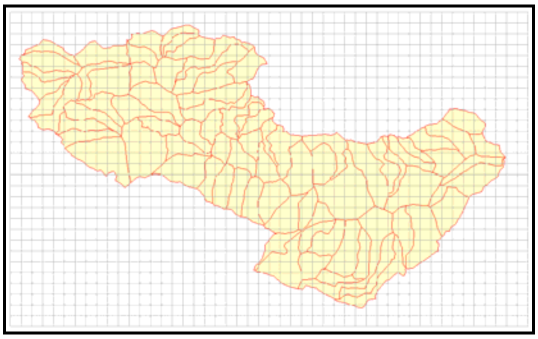

Figure 1: Schematic of the MODFLOW grid overlain by HRUs

3. APPLICATION TO THE ESPERSTEDTER RIED BASIN

3.1. Study Site

The coupled modeling approach is applied to the ungauged Esperstedter Ried basin (Germany), which covers an area of approximately 135 km². This catchment is characterized by predominantly flat, karstic terrain, a poorly developed natural stream network, and groundwater seepage to the surface. Approximately 53.0 percent of the basin area features a slope smaller than 5.2 percent; elevation ranges from a maximum of 474 m to 120 m at the flood plains.

The study site is located in a mid-latitudinal transition zone between the marine influenced climate of Western Europe and the continental influenced climate of Eastern Europe. This region, which features a long-term mean annual precipitation (P) of less than 550 mm and a mean annual potential evapotranspiration (PET) of approximately 530 mm, is characterized by sub-humid conditions. As a result of the relatively high evapotranspiration rates, which exceed the amount of rainfall from April to September, particularly the eastern part of the watershed has a negative water balance on a mean annual basis, i.e. the amount of water gained from precipitation (P) smaller than the loss into the atmosphere by evapotranspiration (ET) (P - ET < 0).

The complex aquifer system of the Esperstedter Ried catchment is characterized by joint aquifers built of mainly sandstone, siltstone, and claystone in the western part of the basin, while the flood plains in the east of the catchment feature a pore aquifer of tertiary and quaternary glacial till and fluvial gravel. Subsurface conditions in the flood plains are highly variable; there can be a maximum of five aquifers with embedded confining layers of primarily clay. An important feature of the Esperstedter Ried catchment is the Zechstein strata, which consists of paleozoic marine sediments (e.g. lean clays, dolomite, anhydrite, gypsum, mineral salt, and potash salt). Leaching and subrosion of these sediments are the cause for karst topography, and variety of karst phenomena, such as land subsidence, karstic caves, collaps sinks, and karrenfelds. Due to the geologic conditions (karstic landscape and a nearly undisturbed south-striking succession of beds) the Esperstedter Ried features a poorly developed, natural drainage network. There are a few relatively small headwaters in the western part of the basin. The watershed, however, is mainly drained by an artificial canal network consisting of two major and a system of smaller canals in the vicinity of the Esperstedter Ried wetland.

Vegetation and land use in the Esperstedter Ried basin are strongly influenced by anthropogenic factors. Approximately ninety percent of the catchment is used as farmland and pastures. The Esperstedter Ried wetland, which is fed by groundwater seepage to the surface, is one of the most important inland salt marshes in Germany, where not only reed grasslands but also a variety of salt plants, such as *Salicornia europea*, *Spergularia salina*, and *Triglochin maritium*, can be found

3.2. Available Time-Series Data

The period of study (1992 – 2000) was selected based on the availability of a time series of observed hydrological, meteorological, and groundwater head level data for the Esperstedter Ried basin. There are six precipitation and two temperature stations located in this region, for which daily precipitation and temperature records are provided by Germany's National Meteorological Service (Deutscher Wetterdienst - DWD). In addition, data on global radiation, wind force, and humidity are available.

The availability of observed groundwater data is a crucial factor for both the groundwater and the loosely coupled modeling approach. A time series of hydraulic head levels can be obtained from thirteen wells within the watershed, which provide measurements obtained by data loggers in seven and fourteen day intervals.

4. MODELING PROCEDURE

4.1. Model Setup

In this study the groundwater flow system is simplified by using the so-called aquifer viewpoint, which conceptualizes the catchment in a quasi-three dimensional approach. The governing equation for this approach is

$$\frac{\partial}{\partial x}\left(T_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T_y \frac{\partial h}{\partial y}\right) = S\frac{\partial h}{\partial t} - R + L \qquad (2)$$

where T = the components of transmissivity, S = the storage coefficient, R = the sink/source term, and L = the leakage term. In the scope of this study, model specifications are made under the assumption of an isotropic and homogenous aquifer. The groundwater system is differentiated into an unconfined and a confined aquifer, which are assumed not to interact and each one features only horizontal flow. To investigate the model performance in regard to recharge, the simplified groundwater flow system receives input only from groundwater recharge which is defined by Neumann boundary conditions (specified flux); the external boundaries are specified as zero flow conditions. Consequently, potential subsurface flow into or out of the watershed due to karst topography is assumed to be non-existent. The three-dimensional model grid is built of two layers featuring 1392 grid cells (500 m by 500 m resolution) each. Figure 2 shows the MODFLOW model grid of the Esperstedter Ried catchment.

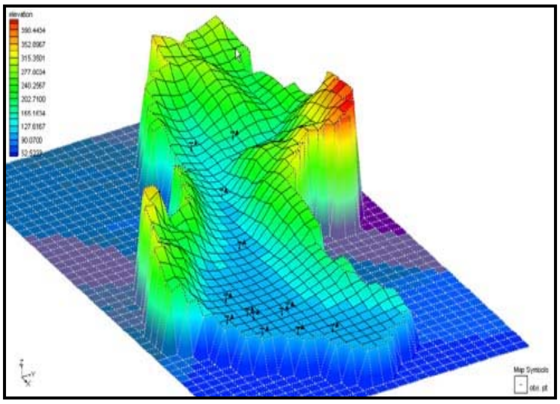

Figure 2: Model grid of the Esperstedter Ried basin (Three-dimensional view)

The groundwater recharge rate is obtained from PRMS, which features the advantages of distributed surface water models: climatic variations are accounted for by using several climatic stations to specify zones of variable precipitation and temperature; topographic factors (elevation, aspect, and slope) are also considered in these calculations. The model allows the definition of spatially and temporally variable vegetation and land use parameters as well as soil characteristics. Consequently, processes such as evapotranspiration, interception, infiltration, and surface runoff, are distributed in space and a regional water balance can be computed on short time steps (daily) or averaged on monthly or annual basis. To account for the absence of streamflow measurements, the PRMS model of the Esperstedter Ried basin is calibrated based on available climatic data, digital elevation data, and information on soils and land use; in addition, the system response is evaluated based on a base flow separation as well as a comparison to nearby basins. The base flow separation provided reasonable results and, considering physiographic differences (e.g. local variability of precipitation, topography, geology, and land use) the comparison confirms a realistic parameterization for a basin in central Germany.

4.2. Modeling Results

The first step of simulating the hydrologic system is the application of a steady-state model, which is a traditional approach to investigate the long-term system behavior of a groundwater-dominated watershed. The average amount of recharge over time of 0.1369*e-03* m/d (50 mm/yr) is derived from the PRMS model ($ssr2gw_{rate}$ 0.1). Hydraulic conductivity is calibrated based on the root mean squared error (RMSE) using the PEST utility in GMS. The optimal hydraulic conductivity value for the $ssr2gw_{rate}=0.1$ model run is 0.176 m/s, which gives a reasonable RMSE of 2.6568 and a good objective measure of $r^2 = 0.986$. However, the steady-state modeling approach is not sufficient to meet the objectives of this study and to analyze the performance of the coupled modeling approach as well as the flow system of the Esperstedter Ried. A comparison of modeling results obtained from simulations using variable amounts of recharge points to the problem of calibrating an unknown quantity with another: it is impossible to analyze the system response to varying amounts of groundwater recharge in the steady-state simulation because the model adjusts the hydraulic conductivity by increasing or decreasing it in order to account for variable flux conditions while optimizing the root mean squared error. Thus, RMSE values computed of various parameter estimation runs differ insignificantly, while recharge values can vary by several orders of magnitude. Using the steady-state mode, the recharge parameter and consequently the amount of inflow into the aquifer cannot be constrained without detailed information on aquifer properties or the actual recharge rate.

During the second step of the application, a discretization in time results in a higher complexity of transient models, which account for the change of hydrologic stresses affecting groundwater recharge and discharge (e.g. pumping, change of recharge or ET rates). In case of the Esperstedter Ried basin, the purpose of the simulation is to test a modeling approach based on an analysis of the long-term behavior of the system, which is assumed to be observable in terms of seasonal variations of flow. The capacity of an aquifer to govern the transfer of water by storing or releasing it, is an essential characteristic, which specifies whether a system features transient conditions or reaches steady-state (i.e. fluid flux is stopped and head levels stabilize). Therefore, calibrating storage parameters, namely specific storage (SS) and specific yield (SY), is crucial for transient simulations and for allowing a detailed calculation of the water budget. During the calibration process, the storage parameters are both automatically estimated using PEST and manually refined; for both parameters a reasonable range of values can be estimated based on aquifer properties. Modeling the Esperstedter Ried basin with the loosely coupled approach included multiple model runs using variable recharge and hydraulic conductivity values. The calibration process of the $ssr2gw_{rate}=0.1$ simulation results in a set of parameters (HK = 0.177, SS = 5.0*e-06*, and SY = 0.25), which feature a root mean squared error of 8.29. Figures 3 and 4 represent a comparison between a reasonable fitted (Fig. 3) and a badly fitted (Fig. 4) well.

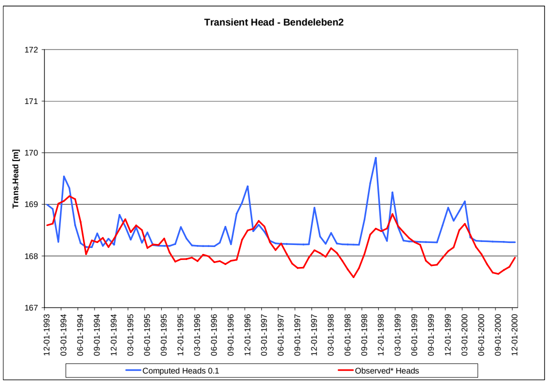

Figure 3: Transient head levels of the well Bendeleben2 (*observed graph shifted on the y-axis by a factor of 0.05 for a better comparison)

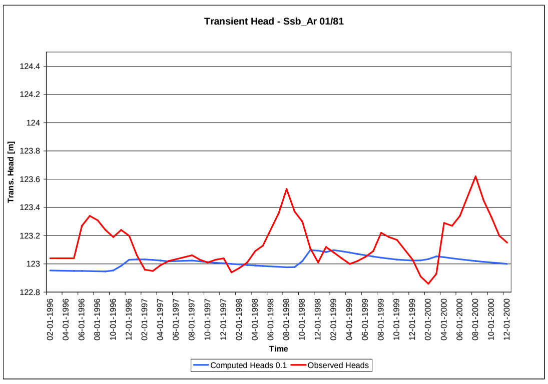

Figure 4: Transient head levels of the well Ssb_Ar 01/81

To evaluate the performance of the loosely coupled transient model regarding the problem of constraining recharge, several simulations were run using various recharge rates as well as different storage parameters. The sensitivity analysis, which ranged between $r^2 = 0.143$ and $r^2 = 0.023$, suggests that the $ssr2gw_{rate}$ parameter cannot be fully constrained. Adjustment of $ssr2gw_{rate}$ led to a simultaneous adjustment of the storage parameters with no distinct pattern emerging. This lack of pattern is most likely caused by the lack of an appropriate objective function for the calibration of transient groundwater models. The RMSE, a typical objective measure used in groundwater modeling, is not able to account for variations in time when applied to transient simulations. The r^2 metric aids in the calibration of the temporal behavior, but it is not easily integrated into a parameter estimation package such as PEST, which was used during this study. However, the r^2 metric was favored over the RMSE to distinguish between good and poor simulations.

Despite the fact that several wells correlate very well with the observed changes in head values the loosely coupled model does not suffice to simulate the complex surface-groundwater system of the Esperstedter Ried basin at the moment. However, the approach of using spatially and temporally heterogeneous PRMS recharge is promising if recharge could be constrained, for instance by streamflow data or better knowledge of aquifer properties.

5. SUMMARY AND CONCLUSIONS

The primary objective of this study was to evaluate the application of a loosely coupled modeling approach combining the Precipitation Runoff Modeling System (PRMS) and the Modular Three-dimensional Finite- Difference Groundwater Flow Model (MODFLOW).

For the calibration of the steady-state model the daily recharge estimates were averaged over time in order to simulate the long-term system response of the catchment. Due to the non-unique parameter estimation of recharge and hydraulic conductivity, recharge could not be constrained. The results of the transient simulation are distributed changes in head levels, which show that the system response can be simulated to some degree in regard to the dynamics of varying head levels in time. Since recharge values cannot be constrained in PRMS it is impossible to calibrate on one specific set of aquifer properties (hydraulic conductivity, specific yield and storage). The estimated hydraulic conductivity (0.177 m/d) as well as the storativity values (SS 0.5*e-05*, SY 0.25) represent realistic set of parameter values for the actual geologic environment of the Esperstedter Ried catchment. A visual evaluation of calculated transient head levels plotted against the observed time series shows reasonable results for several wells; the computed head values of particular wells, such as Bendeleben2 ($r^2 = 0.71$), allow for a good fit and reveal similar dynamics and amplitudes in head level changes, whereas other wells (e.g. Ssb_Ar 01/81) show poor fits and correlations ($r^2 = 0.08$). One reason for these poor fits are obviously the simplifying assumptions made when designing the model, such as the neglect of pumping and discharge of water in form of wells.

However, the range of values considered realistic in regard to the real-world system is too wide to constrain MODFLOW parameters to a level, which allows for a sufficient simulation and assessment of the actual amount of recharge. It became obvious that the adjustment of groundwater recharge led simultaneously to an adjustment of the storage parameters, with no pattern emerging. One problem is the lack of on an appropriate objective function to analyze transient groundwater models. The traditional approach of using the root mean squared error is not able to assess the temporal behavior of the model; it is limited to evaluating the actual fit between simulated and observed heads. In addition, the r^2-metric, which is not integrated into the actual MODFLOW parameter estimation process, is used because it aids the calibration and assessment of the temporal system behavior.

The reasonable simulated system dynamics at a majority of the observation points indicated the method of estimating spatially and temporally heterogeneous recharge in PRMS to be promising. However, the fact, that the calibration of the transient model achieved many times acceptable values with different amounts of recharge proves that the coupled modeling approach cannot be calibrated only on groundwater data, and emphasizes the need to constrain recharge values prior to implementing the parameter into MODFLOW.

Further research is necessary in order to investigate the interactions between both systems in more detail. One crucial factor in linking these systems has proven to be the constraint of the groundwater recharge rate, which should be considered in regard to further efforts in developing a coupled model. The results of this study confirm the need for a more dynamically integrated model, which features a bidirectional linking of the surface and groundwater model and places more emphasis on the transition zone between surface and subsurface reservoirs as well as processes, such as groundwater seepage to the surface, inflow to the aquifer from the soil zone or from interactions between streambeds and aquifers.

6. REFERENCES

Freeeze, A. (1972): Role of Subsurface Flow in Generating Surface Runoff, 1. Base Flow Contributions to Channel Flow. Water Resources Research, 8(3): 609 - 623.

Leavesley, G.H., R.W. Lichty, B.M. Troutman & L.G. Saindon (1983): Precipitation- Runoff Modelling System: User's Manual. U.S. Geological Survey Water Resources Investigations 83-4238, Denver, Colorado.

McDonald, M.G. & Harbaugh, A.W. (1984): A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model. U.S. Geological Survey, Techniques of Water-Resources Investigations, Book 6, Chapter A1, Washington.

Pinder, G.F & S.P. Sauer (1971): Numerical Simulation of Flood Wave Modification Due to Bank Storage Effects. Water Resources Research, 7(1): 63 - 70.

Smith, R.E & D.A. Woolhiser (1971): Mathematical Simulation of Infiltrating Watersheds. Hydrol. Paper, 47. Colorado State University, Fort Collins.