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Unified Framework for Water Balance and Hydrologic Simulation: Part I – Theoretical Development

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Abstract: In this paper a unified framework is proposed to dovetail water balance model into a hydrologic simulation model. The additive and depletive nature of process operations, including the requirement for feedback and retraction, are discussed. The need to breakdown lumped processes into constituent elemental processes for water balance is discussed. The development of storage-process interaction matrix and its convergence towards water balance model are presented. The formulation of WAPROS model and its capability to generate storage-based water balance, process-based water balance, storage-level closure error, model-level closure error and water balance ratios, besides other hydrologic processes are outlined. The distinctions between model error and simulation error and the effects of interactions between them are also highlighted. A hierarchy of errors 'simulation error - model error - storage closure error' is proposed for error handling in simulation modelling. In this paper, theoretical development of unified framework is explained.

Keywords: *water balance model, hydrologic simulation, model closure, closure error, model error, simulation error, hierarchy of errors, water balance ratios*

1. Introduction

The hydrologic cycle is the pictorial representation and the water balance equation is the numerical representation of hydrologic processes at a macro level. The hydrologic cycle shows more number of processes and depicts how these are logically interlinked. Not all these processes can actually be measured in the field. The water balance equation comes out with a small number of processes that can be measured or estimated. The equation balances the hydrologic inputs, outputs and changes in storages quantitatively. This water balance equation denotes the macro level quantity balancing at the watershed scale and it is different from the micro level mass balance equation of a process.

The beauty of the water balance equation, whose concise depiction hides its complexity, makes hydrology a more fascinating study. Though the concept looks simple, it is very difficult to quantify the hydrologic storages and processes and to balance them in an open system [5]. Hence, recourse is made from measured water balance to modelled water balance. It is suggested that the water balance equation itself is also a model [6].

The water balance component may even be considered as an accounting procedure imposed on the model, to keep track of changes in all the hydrologic processes and storages continuously. Figuratively, this can be considered accounting for every drop of water in the model. This may answer the question of what happened to one mm of rainfall received in the watershed. Heightened error in balancing indicates that the model is less stringent in accounting for the quantity of water within the model. These common and fundamental queries answered by the water balance model make it a popular concept among hydrologists and common man. Despite the difficulties faced, the elusive part of water balance continues to be challenging and captivating.

Hydrologic processes are classified into additive and depletive processes based on the nature of their effects on storage. This helps in formulating lumped processes as constituents of elemental processes and in deriving two types of water balance equations. The error inherent in closing water balance is called model error and its relevance to simulation error is discussed. For the purpose of enhanced error handling in simulation modelling, a hierarchy of errors (simulation error – model error – storage closure error) is being proposed. A simple presumption or a declaration that water balance is taken care of in the model by default will not suffice. The use of mass balance equations for modelling the processes will not automatically absolve the model from water balance closure problem and model closure errors.

This study proposes a unified framework for water balance and hydrologic simulation. This unified framework has been utilized to develop a WAPROS (Watershed Processes **S**imulation) model, which is a lumped, deterministic, hourly simulation model. The procedure used to relate both water balance and hydrologic simulation and the techniques employed to formulate WAPROS model are described in this paper as Part-I. This model is being applied to a real watershed, Ebbanad in the Nilgiris of Tamil Nadu, and the results are presented in a companion paper as Part-II. The terms water balance and water budget, though technically different, are considered synonyms within this paper. The expression, water balance model always refers to the submodel, since the primary model is the hydrologic simulation model.

2. Hydrologic Cycle

The hydrologic cycle, also known as 'water cycle', represents the continuous and never-ending circulation of water on earth. It describes the movement of water between the biosphere, atmosphere, lithosphere, and hydrosphere. The term cycle refers to the cycling of water in different phases, emphasizing water in motion in time-rate dimension. Globally, hydrologic cycle operates as a closed system, and the total amount of water within the cycle remains constant but its temporal distribution among the various storages and processes continuously changes. The hydrologic cycle is well understood to be operational in a fully closed system. When this concept is applied to a watershed, which is an open system, it presents difficulties in the estimation and verification of hydrologic components. Hence the applicability of hydrologic cycle is generally restricted to larger dimensions of space and time, i.e., at regional or global and annual or decadal scale. Water balance equation is used to study hydrology at smaller scales of space and time.

3. Global Water Balance

The water balance equation is a mathematical representation of the hydrologic cycle, indicating the quantities handled by different processes. At the global scale, this water balance equation remains constant and the component values indicate the long-term averages of the hydrologic processes. At the global scale, the components of water balance (WB) equation cannot be exactly quantified, but can only be estimated and its accuracy depends more on the prevalent technology. Sometimes the components are measured at some lower scales and extrapolated. The hydrologic cycle, in time-rate unit, can be represented as:

$$P(t) = Q(t) + ET(t) + \Delta S(t),$$

where P is the precipitation, Q is the runoff, ET is the evapotranspiration and S is the storage.

The annual water balance equation at the global scale accepts annual averages of long-term estimates or observations; the storage position is considered to be unchanged at the start of every year in the long term and ΔS is assumed to be zero. It can be represented as:

$$\overline{P} = \left[\overline{Q} + \overline{ET} + \overline{\Delta S}\right] = \left[\overline{Q} + \overline{ET} + \left(\overline{S_c} - \overline{S_o}\right)\right], \text{ where,}$$

$\overline{S_c}$ = Average storage at close of the year,

$\overline{S_o}$ = Average storage at start; and $\left(S_{o+1} = S_c\right)$;

The long term average makes, $\left(S_{o+1} = S_o\right)$ and $\left(\overline{S_c} - \overline{S_o}\right) = \overline{\Delta S} \Rightarrow 0$; and the Global WB equation becomes $\left[\overline{P} = \overline{Q} + \overline{ET}\right]$.

4. Experimental Water Balance

The water balance studies undertaken on the field entail actual measurement of the processes and this may be called Field water balance studies or Experimental water balance studies. Normally such studies are undertaken to arrive at the annual water balance at the experimental sites. In real world situations, the hydrologic process that cannot be quantified is estimated as a residual after forcing a balance. Traditionally, there was no direct way of measuring actual evapotranspiration, so errors in long term measured water balances tended to be assigned to the evapotranspiration term, despite the fact that rainfall inputs, discharge outputs and changes of storage are not always accurately measured [4]. Here the water balance equation is inverted as an estimation equation for ET:

$$ET = (P - Q - \Delta S)$$

Penman pointed out that measurement of storage is extremely difficult and wanted to get all the other terms in the balance with sufficient accuracy to enable storage to be estimated by difference [23]. It is often pointed out that the residual is not just a filler to close the balance equation and it contains estimation errors of all other variables. Hence, measurement of all the processes of interest in the water balance equation is necessitated, to arrive at the closure error (E) by measurement [4]. Then the annual water balance equation becomes:

$$P = (ET + Q + \Delta S + E).$$

4.1. Short Term Water Balance

The component values of global WB equation are fixed and the values will get updated as and when the estimation technology improves. But this water balance equation can be contrived to operate under reduced scales of space and time, which makes it more dynamic, attractive and popular. The adaptation from hydrologic cycle to the water balance equation helps to advance the hydrologic studies at watershed and daily scales. Mean water balances may be computed for any season or month; but these have distinctive characteristics and they are called as current or operational water balances [28].

The process representation changes from time-rate units (L^3T^{-1}) in hydrologic cycle to volumetric quantity units (L^3) in the water balance equation. In this paper, the water balance components are expressed in units of mm (L), representing average depth of water (L) over the watershed area (L^2).

At short time scales, the averages are replaced by the summation values, ΔS becomes non-zero and resurfaces again in the small scale water balance equation. It has been suggested to include change in water storage to the right side of the equation [21]. As the groundwater storage and hence the base flow can vary considerably from year to year, the often-applied assumption that the overall system returns to the same state of storage each year becomes invalid, which emphasizes inclusion of all terms even in a long-term water balance equation [30].

It has been suggested to include evapotranspiration and change of soil water storage to complete the water balance equation over shorter time intervals [3]. The water balance equation can then be written as:

$$P = [Q + ET + \Delta S], \text{ where } \Delta S = (S_c - S_o),$$
$$S_c = \text{Storage at close of the term},$$
$$S_o = \text{Storage at start of the term}.$$
$$\text{In the short term, } (S_c \neq S_o) \text{ and } \overline{\Delta S} \neq 0; \text{ and}$$
$$\text{the Short term WB equation becomes},$$
$$\sum P = [\sum Q + \sum ET + \Delta S]$$

When the error component is incorporated, the short-term water balance equation becomes:

$$\sum P = [\sum Q + \sum ET + \Delta S + \sum E].$$

Beven admits that we cannot currently close the water balance strictly by measurement and calls the closure problem metaphorically as the Holy Grail of Scientific Hydrology, connoting that the solution might be out there somewhere in principle, but may be impossible to find [5]. It indicates that the closure problem by measurement is now unattainable, due to limitations of current measurement techniques in estimating the components of water balance. However it is affirmed that we can verify it theoretically at the catchment scale and it is hence possible to model the water balance with an estimate of closure error [4]. But modelling water balance components through simulation will be arduous and challenging. Though many hydrologic simulation models are available for simulating the runoff efficiently, they neither compute all the components of WB nor provide comprehensive WB equation.

5. Modelled Water Balance

So far, water balance by measurement or estimation has been discussed. Normally the water balance equation contains rainfall, channel flow, evapotranspiration and change in storage components. Besides rainfall, evapotranspiration component is sum of evaporation from interception, upper soil layer, depression storages, transpiration from plants, etc.; channel flow component is sum of runoff, base flow, interflow, etc.; and change in storage component is sum of changes in storages such as upper soil layer, lower soil layer, ground water, etc. Hence, channel flow, evapotranspiration and change in storage components can be considered only as aggregated processes. These processes cannot be categorised as independent processes. The constituent processes may be called basic processes, elemental processes or independent processes. The aggregated processes may be called macro-level processes, dominant processes or lumped processes. The lumped process does not represent a single process, even though it is often incorrectly presumed to be a single process. This differentiation of processes is useful in subsequent discussions.

The field water balance closure is handicapped by infeasibility of measuring lumped processes accurately. The attempt to attain the model water balance closure is again handicapped by difficulties in simulating the lumped processes. One way out of this difficulty is to simulate the required constitutive processes and aggregate them to arrive at the values of the respective lumped processes. Or, at any point in time:

Lumped process = Sum of elemental processes; and

$$ET = ET_1 + ET_2 + ET_3 + ET_4 + ..m.. = \sum_1^m ET_i ;$$
$$Q = Q_1 + Q_2 + Q_3 + Q_4 + Q_5 + ..n.. = \sum_1^n Q_j ;$$
$$\Delta S = \Delta S_1 + \Delta S_2 + \Delta S_3 + ...p..... = \sum_1^p \Delta S_k ;$$
$$E = E_1 + E_2 + E_3 + E_4 + E_5 + ...p.... = \sum_1^p E_k ;$$

The summation of elemental processes to arrive at the values of lumped processes over the whole period of simulation can be written as: $\Sigma\Sigma ET_i$, $\Sigma\Sigma Q_j$, and so on. Now the Short Term Water Balance Equation for N number of days can be written as:

$$\sum_1^N P = \Big(\sum_1^N \sum_1^m ET_i + \sum_1^N \sum_1^n Q_j + \sum_1^N \sum_1^p \Delta S_k + \sum_1^N \sum_1^p E_k\Big).$$

When a single storage is considered,

$$\sum_1^N \Delta S_1 = \sum_1^N (S_{1,c} - S_{1,o}) = \sum_1^N (S1_c - S1_o)$$
$$= (S1_c - S1_o)_1 + (S1_c - S1_o)_2 + ...(S1_c - S1_o)_N ;$$

Here 'c' and 'o' indicate closing and opening balances respectively.

While modelling storages, the balances are updated from period t to t+1, and the closing balance at period 't' is carried over as opening balance at 't+1'. Due to this carrying over of balances:

$$S1_{o,2} = S1_{c,1}; \text{ and } S1_{o,a+1} = S1_{c,a};$$
$$\sum_1^N \Delta S_1 = (\Delta S_1 + \Delta S_2 + ... + \Delta S_N)$$
$$= (S1_{c,1} - S1_{o,1} + S1_{c,2} - S1_{o,2} + ... + S1_{c,N} - S1_{o,N})$$
$$= (S1_{c,1} - S1_{o,1} + S1_{c,2} - S1_{c,1} + ... + S1_{c,N} - S1_{c,N-1})$$
$$= (S1_{c,N} - S1_{o,1}) = (S1_{cb} - S1_{ob}) = \Delta S_1 \text{ ; and}$$
$$\text{for all storages, } \Big(\sum_1^N \sum_1^p \Delta S_k\Big) = \Big(\sum_1^p \Delta S_k\Big);$$

The summation of changes in a storage over the period of simulation is equivalent to the difference between the balance at the start and the balance at the end of simulation; or simply it is equal to the difference between the closing balance and the opening balance of the storage for the whole period of simulation.

Similarly for the error component,

$$\text{for all errors, } \left(\sum_1^N \sum_1^p E_k\right) = \left(\sum_1^p E_k\right);$$

Now the Short Term Modelled Water Balance Equation becomes:

$$\sum_1^N P = \left[\sum_1^N \sum_1^m ET_i + \sum_1^N \sum_1^n Q_j + \sum_1^p \Delta S_k + \sum_1^p E_k\right]$$

This is the fundamental equation in hydrology, that can be applied at any scale [7]. This approach requires structuring the model to suit both simulation of watershed hydrology and modelling of the water balance equation. In other words, the hydrologic model is planned to simulate all the elemental processes and to deliver the lumped process values to generate the modelled water balance equation.

5.1. Scales of Water Balance Model

The measurement-based water balance equation reckons the process values usually at the annual scale, which are now being modelled as annual water balance models. Budyko hypothesized a differential approach to annual water balance, resulting from competition between available water and energy, which are related to precipitation and potential evapotranspiration respectively [9]. There are also Horton's, and L'vovich's approaches, called functional approaches to annual water balance as these reveal functioning of the catchments [27]. These approaches are also called as Darwinian or eco-hydrological in nature.

The monthly water balance models have been employed to generate monthly water balance data directly, without going through complete simulation, or without estimating the elemental processes. The most familiar monthly water balance model was developed by Thornthwaite, which was later revised by Thornthwaite and Mather in 1947-57, for climatic classification. The monthly water balance models were widely used due to their simple structure and a small number of parameters [33]. But the estimates of annual potential evapotranspiration of many stations in India based on Thornthwaite's formula were observed to be underestimates in winter and overestimates in summer [22]. The Thornthwaite's method is criticised since it does not account for vegetative effects and its biggest shortcoming is the minimum time division, the month, which creates a situation where end-of-the-month precipitation appear as runoff in the following month, a delay that may be unacceptable in the modelled water balance [8]. As the method employs only temperature and latitude, it has been further criticised as one of the most misused empirical equations generating inaccurate estimates of evapotranspiration. Few hydrologists believe that the Thornthwaite formula should no longer be used for estimating water balances [24]. Despite the unpopularity of the Thornthwaite climate classification, its underlying water balance model continues to be useful [17]. Now there is renewed interest in using Thornthwaite's method of monthly water balance.

The monthly and long-term models are useful for regional climate estimation and classification, but these are not successful for scenario development as they ignore the important soil and vegetation factors. The long-term models work on the 'effect-to-cause' relationship or they are 'response based' or 'diagnostic', whereas the simulation models work on the 'cause-to-effect' relationship, or they are 'stimulus based' or 'prognostic'. The simulation models are preferred for scientific and logical predictions. Hence, the long-term water balance models may be considered to work on a reverse mode, especially to get rid of problems and criticisms with parameterisation. This may be analogous to the concept of 'doing hydrology backward' [18]. It has been pointed out that when compared to monthly water balance models, land surface models carry the potential to estimate hydrological partitioning accurately and thus streamflow [16].

Simulation of daily and hourly data to get the water balance equation is the most recommended procedure to tide over the aforementioned problems, but complexities do get multiplied. The smaller the basin area, the more complicated is its water balance and shorter the time interval, the more precise are the requirements for computation of the water balance components, which result in a complex water balance equation that is difficult to close with acceptable errors [28]. The error associated with the timing of predicted streamflow becomes progressively larger as we move from annual to daily timescales. Clearly, model sensitivity and complexity need to increase as the timescales decrease [1].

5.2. Effect of Neglect of Components

The practice of neglecting a few components from consideration in the water balance equation for the sake of reducing complexity or for estimating it as a residual is found to cause more errors in the estimates of other components. Contrary to expectations, this practice has not resulted in reduction of overall errors. In one experiment, it was found that the annual water balance error was 12 mm, or 2.1% of the recorded precipitation, which might include errors in unmeasured water balance elements [28].

It is observed that omission of changes in storage caused 5% error in water balance and suggests that while ΔS can be ignored in annual budgets during average years, it cannot readily be ignored in more extreme years [15]. The change in soil water storage was measured and found to vary from -18 to +100 mm per water year, leading one to conclude that this component could not be neglected [10]. Neglecting deep groundwater losses and change in water storage are reported to result in overestimation of ET [31]. It is also cautioned that value of undetermined elements of the water balance and the measurement errors could pass on to subsequent seasons and become measured components of the water balance equation [28].

5.3. Effect of Estimation from Residual

When the estimates or measurements of water balance components are error-ridden, the residual may reflect the bucket having values of neglected components, along with unknown errors. The error part is also variously interpreted and assigned to a convenient neglected component to balance the equation. In one case, water balance model error of 12% was attributed annually to groundwater recharge [32]. In another case, the error of –45.8 mm/year in water balance closure had been ascribed to systematic underestimation of rain gauges by 5-10% and the residual was added to the rainfall [14].

When the unbalanced part or residual of the water balance equation is assigned to the un-estimated component, the WB equation error is suppressed and the estimate becomes unreliable. When the WB residual was taken as the value of evapotranspiration, the figures would balance exactly and a zero error was reported [29]. It has also been reported that estimation of ET as water balance residual tends to underestimate peak evaporation rates in summer and overestimate the troughs in winter [15]. It is pointed out that estimate of a component as a residual for lack of adequate data is subjected to large errors, owing to transfer of errors to other components [12]. Hence, the procedure of adopting residual value in WB equation, for a hydrologic process may have to be dispensed with.

6. Water Balance Model Processes

The earlier shown Short-term Water Balance Equation is conceptually and numerically accurate. But from a modelling point of view, it is found that this equation is not operationally workable. We could see that the elemental processes are only identified and listed, but not linked. These processes act as the agents of being the ‘cause’ as well as ‘the caused’. A continuous simulation model requires a continuous and unbroken string that links all the storages and processes, and permits generating the required data for the water balance equation.

6.1. Process Identification and Linkage

Evapotranspiration is a lumped process, aggregated from the elemental processes such as evaporation from soil, transpiration from crops, etc. Evaporation from soil cannot go on its own forever, unless the soil is replenished with moisture. This requires infiltration of water into the soil mantle, but for which again the source of water has to be identified and linked. It may also be intriguing to see now that the most familiar soil-water process, namely infiltration, has not been discussed so far while formulating the water balance equation. Infiltration is again a dominant lumped process, constituted by a separate group of elemental processes such as infiltration of rain, infiltration from runoff, infiltration from depressions, etc. Infiltration also triggers other elemental processes like transpiration, percolation, interflow, etc. Infiltration is an important hydrologic process that links many of the storages and the processes, and yet does not figure in the water balance equation. Hence, infiltration may be categorized as the dominant latent process, or an intra-watershed triggering process.

6.2. Additive and Depletive Processes

When we consider the lumped processes in the long-term water balance equation, it can be seen that all the processes on the RHS are depletive processes that when added up equates the additive process, i.e. rainfall, on the LHS. But when we consider the elemental processes at the short-term water balance model, the set of just depletive processes will not suffice to develop the model. For example, evaporation requires soil moisture in the upper layer, which is dependent on infiltration from rainfall or runoff. Here infiltration acts as an additive process on soil upper layer and evaporation acts as a depletive process. Percolation is a depletive process for the upper layer and it is an additive process for the lower layer. Similarly, evaporation is a depletive process on the upper layer and it is an additive process to lumped evapotranspiration process. Infiltration depletes rainwater or runoff and adds water to the upper layer. Besides the two-way effects discussed above, a peculiar fact of competitive abstraction on storage is also prevalent; for example, percolation is a depletive process that drains water from upper layer and it competes with evaporation which depletes water from the same upper layer.

From this discussion, it can be seen that same elemental process acts as an additive process on one storage and as a depletive process on another storage. Each process requires two storages, one as a source and another as a sink. Hence, the elemental processes are to be categorised again as additive processes and depletive processes and their interactions with different storages are to be properly linked.

7. Process Interactions and Feedback

There are a few hydrologic storages, which are capacity restrained or the upper limits are bound; that is these storages cannot hold whatever quantity of water that comes in from addition processes; the quantity in excess over the capacity is allowed as surplus flow and the surplus flow is also to be tracked for addition in other storage; the surplus rule for a storage shall define the capacity limit and the destination storage for its surplus. Similarly, two soil storages have lower limits at wilting points and these two storages cannot allow the entire quantum of demand from the depletion processes; here the quantity to be depleted shall have to be reduced with suitable feedback specification. Storages with lower bound at zero level also exhibit similar constraints on processes. These problems can be illustrated as: a process P depletes p1 quantity from storage S1 and moves it to add to storage S2, but S2 allows only p2 quantity (p2 < p1) and the feedback should correct p1 and S1, or else error will crop in; similarly a depletive process Q estimated to deplete q1 from storage S3 will be restrained and permitted to deplete only q2 from S3 (q2 < q1) and this feedback should alter q1.

When more than one addition or depletion processes are acting on one storage, the issue becomes even more complicated depending on the allowability at that point of time. When several addition processes are acting on an already filled storage, no input from any of the processes will be allowed in and all the processes are to be pushed back or surplussed; when a similar condition is imposed on a partly-filled storage, the allowability is to be decided based on the prioritized preferences and the pushback quantities are to be estimated using a different logic. If the pushback is infeasible, the storage shall resort to surplussing of excess flow to another predefined storage, in which case allowability and infeasibility problems in the next storage will have to be addressed. These conditions will create differences between depletion and addition quantities which should be reconciled to bring a zero difference. The modelling experience shows that this feedback and correction issue is a major source of model error.

8. Model Closure Error

When modelling the water balance component, it is also important to generate values for all the processes by utilizing the model, without resorting to estimation of any process as a residual. Hence, a residual-free simulation is strongly recommended for proper appraisal of the water balance component. While doing so, the water balance component of modelling should be completed with zero or a meagre balancing error and attainment of this condition is called as 'model closure'. The model error that remains unbalanced is taken as WB closure error.

When these issues are not resolved logically and numerically, errors will creep in and will propagate through all the storages and processes, throughout the simulation period. The lower limits of storages, if not properly ensured, will permit generation of positive fluxes, by becoming negative storages, which will be very difficult to locate, unless specifically searched for. This is analogous to pumping from an empty well. It should also be noted that storage closure error in one storage will trigger errors in other storages and will ultimately result in uncontrolled model error. These problems will get aggravated during automatic calibration of the model which has only a single objective of maximizing the value of the efficiency criterion. Hence, suitable safeguards are necessary to account for feedback conditions and to prune the error at time-step scale to avoid propagating errors in simulation. When there are uncontrollable and significant water balance errors, the model is said to have been not closed and the calibration or evaluation of such model will not be meaningful.

It is commonly believed that use of mass balance equations of processes will absolve the model of this kind of closure problem. Unfortunately, even the most fundamental equation in hydrology is subjected to significant errors in each of its terms [7]. The partial differential equations (PDE), acting as continuity and mass balance equations, could not be used as such in a model since those equations have to be discretized under some numerical procedures for use in the model, with concomitant errors. Linearization of nonlinear equations may also add to simulation woes. Further these PDEs are feed forward equations and cannot handle the feedback or pushback routines. Hence, estimation of model error as narrated here shall have to become an integral part of simulation, and a starting point for model evaluation.

8.1. Model Error and Simulation Error

Simulation error is considered to contain algorithmic error, which is measured as the difference between simulated and observed values. For the sake of clarity, the term 'Model error' is used for closure error or water balance error, since this error is resident within the model; and the term 'Simulation error' for evaluation error, since this error is linked with the application of the model. The terms WB error and Model error are synonyms, but the usage of WB error may be misinterpreted to preclude applicability to those models which do not generate WB values. The model error includes: truncation error, overflow error, overdraft error, omission error, unbalanced error, algorithm error, restrained quantity error, accounting error, carry-over error, etc. This model error is largely due to avoidable mistakes in the coding, prioritisation of processes, etc. and shall have to be restricted to the minimum. The estimate of model error does not require any comparison with observed data. The simulation error relates to error in matching the observed data, which is due to imperfect process descriptions that can never be mimicked due to persisting knowledge gap in fully understanding hydrologic phenomena.

The model error is latent and resident in the model and it will always be a part of the model evaluation error. This error is reported implicitly with simulation results. Any model error, if undetected, will compound model evaluation error. For example, when the simulated flow from a model is substituted for observed flow, a re-run of the model will produce a perfect matching, with zero simulation error. This does not mean that the model is perfectly closed, with zero model error and storage closure errors. There is every likelihood that model error and closure errors will be present, but not reported or compensated.

Reduced model error due to compensation effect is likely to have error propagation in many processes. The direction of the model error, positive or negative, will impact evaluation error differently, depending on the model being over-predictive or under-predictive. Hence, the model error or WB error should be estimated by the model and it should be minimised, before embarking on calibration and evaluation. Model evaluation values, without an estimate of model error, is quite likely to mislead.

9. Hydrologic Model with Water Balance

The aforementioned discussions form the basis for the perceptual model of WAPROS. These ideas are transformed into a flow chart and the flow chart is re-examined to ensure: (i) that the storages and the processes are linked as strategized; (ii) that the planned elemental processes can be simulated; (iii) that the values of elemental processes when added up produce the required lumped processes; and (iv) that the full collection of components, processes and storages abides by the requirements of water balance modelling. Now it is again verified whether the chart and the flow can permit both hydrologic simulation and water balance modelling; if not, the entire procedure is repeated till the desired process flow is reached.

9.1. WAPROS Model Formulation

The scales of space and time to be adopted in the model are critical to formulation of a model. It has been planned to develop a model for watersheds of area100-10,000 ha with hourly time steps, in order to catch the peaks and fluctuations in channel flow. The watersheds do not filter out fluctuating responses to high-intensity, short-duration storms. A basin or catchment that is much larger in size filters out high frequencies and fluctuations of flow regime, as the averaging process is more effective when the watershed size increases [11]. The daily simulation models when applied to small watersheds mask the peaks and troughs and produce averaged flows. Hence, the hourly simulation model for a small or medium sized watershed shall have to be more sensitive than that for a large basin. This culminated in the development of WAPROS, an acronym for Watershed Processes Simulation Model.

A top-down approach has been advocated as a model building procedure, which can be described as ‘start with the simplest possible model and increase model complexity at progressively smaller scales’ [19] and it has been reformulated subsequently [2] [25] [26]. This top-down approach is duly followed at every stage of WAPROS model development.

9.2. WAPROS Modelling Framework

WAPROS uses the inventory-based simulation modelling approach, which is considered an appropriate methodology for generating the water balance equation. This inventory-based modelling is at times also labeled a reservoir method, a bucket method or a book-keeping method. The model architecture consists of different inventory units, each representing a watershed storage component. These storages are linked with each other by different additive and depletive processes. Each inventory unit has its own maximum storage capacity, minimum storage capacity, incoming process rate, outgoing process rate, prioritization of incoming and outgoing processes, surplus overflow rules, etc. For practical purposes, this approach may be treated as a modification of the system dynamics model [20].

9.3. WAPROS Model Components

The simulation model considers the following components, storages and processes of the watershed:

A	Components	Watershed physiography, climate and rainfall, soils, groundwater, forest and vegetation
B	Storages	Interception, soil detention, surface detention, structural detention, soil upper layer, soil lower layer, overland water storage and groundwater
C	Processes	Interception, soil detention, surface detention, structural detention, infiltration, percolation, macropore flow, variable source area flow, inter-flow, base-flow, evapotranspiration, overland flow and channel flow

9.4. WAPROS Model Structure

WAPROS is developed with the objective of dovetailing water balance into the hydrologic simulation model. The unified framework that brings together both water balance and hydrologic simulation in WAPROS is explained with storage-process interaction matrix as shown in Table 1. The matrix shows the details of storages and processes handled in the model and also indicate how each storages is influenced by different addition and depletion processes. It may be noticed that a few storages handle more number of addition processes than depletion processes, while others handle more number of depletion processes than addition processes.

9.5. Water Balance Equations in WAPROS Model

The water balance equations for all storages are given in Table 2. The water balance equation for one storage at any point of time is:

$$OB\ (i, j) + AP\ (i, j) - DP\ (i, j) = CB\ (i, j) \qquad (1)$$

where, OB (i, j+1) = CB (i, j) and so on.

The equation for sum of all storages at a point of time is:

$$\Sigma\ OB\ (i, j) + \Sigma\ AP\ (i, j) - \Sigma\ DP\ (i, j) = \Sigma\ CB\ (i, j) \qquad (2)$$

When summing up the values of all storages and the respective processes, the intra-flux values get cancelled and the equation becomes:

$$\Sigma OB(i,j)+\Sigma RF(i,j)-\Sigma ET(i,j)-\Sigma Q(i,j)=\Sigma CB(i,j)+\Sigma e \quad (3)$$

The equation for sum of all storages for the entire period of N days (for hourly simulation) becomes the water balance equation for the model:

$$\Sigma OB(1,1) + \Sigma\Sigma RF(i,j) - \Sigma\Sigma ET(i,j) - \Sigma\Sigma Q(i,j) = \Sigma CB(N,24) + \Sigma e;$$

$$\Sigma OB(1,1) + \Sigma\Sigma RF(i,j) - \Sigma\Sigma ET(i,j) - \Sigma\Sigma Q(i,j) - \Sigma CB(N,24) - \Sigma e = 0;$$

$$\Sigma\Sigma RF(i,j) - \Sigma\Sigma ET(i,j) - \Sigma\Sigma Q(i,j) - [\Sigma CB(N,24) - \Sigma OB(1,1)] - \Sigma e = 0;$$

$$\Sigma\Sigma RF(i,j) - \Sigma\Sigma ET(i,j) - \Sigma\Sigma Q(i,j) - \Sigma \Delta S - E = 0 \quad (4)$$

This is the popular form of water balance equation commonly reported. The storage balance equations when summed up with OB and (-) CB gives the Water Balance equation. Here, the error term E is Σ e, which is sum of errors of all storages. The negative errors of a few storages may compensate and mask the positive errors of other storages. Hence it becomes imperative to estimate the errors of individual storages explicitly to determine the actual value of error E. Rearranging the terms of the equation mentioned above,

$$\Sigma\Sigma RF(i,j) = \Sigma\Sigma ET(i,j) + \Sigma\Sigma Q(i,j) + [\Sigma CB(N,24) - \Sigma OB(1,1)] + \Sigma e$$

$$\Sigma OB(1,1) + \Sigma\Sigma RF(i,j) = \Sigma\Sigma ET(i,j) + \Sigma\Sigma Q(i,j) + \Sigma CB(N,24) + \Sigma e \quad (5)$$

Considering that errors are present in the storage balance, and then the WB equation of storage 'x' becomes:

$$OB_x(1,1) + \Sigma\Sigma AP_x(i,j) - \Sigma\Sigma DP_x(i,j) = CB_x(N,24) + e_x; \quad (6)$$

The arithmetic or calculated Closing Balance of a storage CBC will be:

$$OB_x(1,1) + \Sigma\Sigma AP_x(i,j) - \Sigma\Sigma DP_x(i,j) = CBC_x. \quad (7)$$

Subtracting the equation (6) from (7),

$$e_x = [CBC_x - CB_x(N,24)] \text{ and } \Sigma e_x = E \quad (8)$$

Where, e_x is the closing error of storage x and E is the model error, or model closure error. Every modeller shall strive to bring this error as close to zero as possible. Here CBC_x is calculated from lumped values as a one-time estimate, while CB_x is a simulated value by the model through whole iterations of carrying over of balances. The difference between the two closing balances indicates the storage closure error. The nature of restrained depletive processes due to less storage in the source and that of constrained additive processes due to filled storage in the sink and the consequent feedback corrections are the potential causes of storage closure error.

The column (vertical) sum of all storages in Table 1 result in the following two equations, called Storage-based water balance equation and Process-based water balance equation for the model:

Storage based Water Balance (S):

$$\Sigma OB + RF = ET + Q + \Sigma CB + E \quad (9)$$

Process based Water Balance (P):

$$\Sigma OB + \Sigma AP = \Sigma DP + \Sigma CB + E \quad (10)$$

It can be seen that equation (3) derived from short-term water balance principles, and the equation derived from WAPROS matrix are one and the same, signifying that hydrologic simulation and water balance are successfully unified. Now we have three estimates of error (E) from three equations (8), (9) and (10) and all three estimates of E shall have to be equal; or else, the highest difference between E's may be called the Error in closure, which is to be minimized.

In WAPROS, the water balance component is embedded in the model and the Storage-based water balance and the Process-based water balance equations are generated from within the model.

Such a model shall be so built and compiled to produce a document (file) showing the water balance and the closing balance details of all the storages in a simulation explicitly. It is noticed that most causal models assume that these balances are met *de facto*, while it is actually not so [7]. A simple presumption or a declaration that water balance is taken care of in the model by default, will not suffice. Instead, water balances and errors will have to be generated by the model.

9.6. Hierarchy of Errors in Modelling

For long, we have been obsessed with only simulation error in hydrologic modelling. Many evaluation criteria have been used on the presumption that it is the final residual between simulated data and observed data. By bringing in the model closure procedure, model error is introduced as a subset of simulation error and its numerical and directional effects on simulation error are considered significant. Now, the model error is recognised as a lumped error, whose constituents are identified as storage closure errors. The values and directions of storage closure errors influence the value and direction of model error, which in turn determines the reliability of estimate of simulation error. Now a two-stage downward analysis of error is proposed.

9.7. WAPROS Model Inputs

The model requires 30 watershed data, one hourly rainfall data file and one daily temperature file for simulation and one hourly observed flow data file for evaluation. Six input data into the model are treated as parameters: thickness of soil upper-layer, thickness of soil lower-layer, initial average soil moisture content, overland flow extraction coefficient, base flow recession coefficient and channel routing coefficient.

These parameters are physically related, and represent effective values averaged over the watershed.

When the physical parameters employed in the model are effective ones, they control transfer functions at the scale of application [13]. Since WAPROS is a lumped model and the model parameters are effective values, scale problems are not considered.

10. Water Balance Component Ratios

There are two aspects in water balance studies: the first is equating the aggregated values of inputs and outputs; and the second is getting meaningful interpretations from ratios of the subcomponents of WB. The ratios can be classified as: (i) general purpose ratios (in %), and (ii) long term climate ratios (in fractions) depending on the type of data employed and the purpose for which those are used. The ratios of water balance data will be useful: (i) for climate classification, (ii) for characterising the hydrologic status of the region or watershed, (iii) for supplying unmeasured or missing data, and (iv) for assessing the impact of changes in the watershed.

11. Conclusion

The unified framework dovetails water balance equation into the hydrologic simulation in WAPROS model, which is developed as a lumped, deterministic, hourly simulation model. The extension of concepts from hydrologic cycle, to water balance by measurement, water balance by modelling and hydrologic simulation is described in detail. The details of storages and processes handled, and how these are linked in the formulation of WAPROS model is explained. The model closure procedure and estimation of model closure error are described. The distinction between model closure error and simulation error are clarified. A hierarchy of errors from 'simulation error - model error - storage closure error' in simulation modelling is proposed. The necessity for resolving error in every storage at time-step level is also explained.

In this paper, theoretical development of unified framework is explained. The model is applied to a real watershed and the results of simulation, modelled water balances, status of all storages and closure errors are presented in a companion paper as Part-II.

References

[1] Atkinson S E, Woods R A and Sivapalan M (2002), Climate and landscape controls on water balance model complexity over changing timescales, Water Resources Research, Vol. 38(12), pp. 50-67.

[2] Bai Y, Wagener T and Reed P (2009), A top-down framework for watershed model evaluation and selection under uncertainty, Environmental Modelling & Software, Vol. 24, pp. 901–916.

[3] Beven K J and O'Connell P E (1985), General report on water balance computation techniques. New Approaches in Water Balance Computations (Proceedings of the Hamburg Workshop, August 1983). IAHS Publ.no.148. 41-46.

[4] Beven K (2001), On hypothesis testing in hydrology. Invited Commentary. HP Today. Hydrological Processes, Vol.15, pp. 1655–1657.

[5] Beven K (2006), Searching for the Holy Grail of scientific hydrology: 'Qt =H (S, R, dt)A' as closure. Hydrology and Earth System Sciences, Vol.10, pp. 609–618.

[6] Beven K and Westerberg I (2011), On red herrings and real herrings: disinformation and information in hydrological inference. Invited Commentary. HP Today. Hydrological Processes, Vol. 25, pp. 1676–1680.

[7] Beven K (2012), Causal models as multiple working hypotheses about environmental processes, Comptes Rendus Geoscience, Vol. 344, pp. 77–88.

[8] Black P E (2007), Revisiting the Thornthwaite and Mather Water Balance. Journal of the American Water Resources Association (JAWRA), Vol. 43(6), pp.1604-1605.

[9] Budyko, M I., *Climate and Life*, Volume 18. International Geophysics Series. Academic, San Diego, Calif., 1974. P 508.

[10] Chauvin G M, Flerchinger G N, Link T E, Marks D, Winstral A H and Seyfried, M S (2011), Long-term water balance and conceptual model of a semi-arid mountainous catchment. Journal of Hydrology, Vol. 400, pp. 133–143.

[11] Chow VT, Introduction and Runoff. In V.T. Chow (Ed). *Handbook of Applied Hydrology*. McGraw Hill, 1964.

[12] Flerchinger G N, Cooley K R, Hanson C L and Seyfried M S (1998), A uniform versus an aggregated water balance of a semi-arid watershed, Hydrological Processes, Vol. 12, pp. 331-342.

[13] Hatton T J, Salvucci G D and Wu H I (1997), Eagleson's optimality theory of an eco-hydrological equilibrium: quo vadis? Essay Review. Functional Ecology, Vol. 11, pp. 665–674.

[14] Hogstrom U and Larsson I (1968), Studies on the water balance of a small natural catchment area in southern Sweden, Tellus XX, Vol. 4, pp. 633-641.

[15] Hudson, JA. (1988), The contribution of soil moisture storage to the water balances of upland forested and grassland catchments, Hydrological Sciences Journal, Vol. 33(3), pp. 289-309.

[16] Hurkmans R T W L, Moel H de, Aerts J C J H and Troch P A (2008), Water balance versus land surface model in the simulation of Rhine river discharges, Water Resources Research, Vol. 44, pp. 1-14.

[17] Keim B D (2010), The lasting scientific impact of the Thornthwaite water–balance model, The Geographical Review, Vol.100 (3), pp. 295–300.

[18] Kirchner J W (2009), Catchments as simple dynamical systems: Catchment characterization, rainfall-runoff modeling, and doing hydrology backward, Water Resources Research, Vol. 45, pp.1-34
[19] Klemes V (1983), Conceptualization and scale in hydrology, Journal of Hydrology, Vol. 65, pp. 1-23.
[20] Lee J (1993), A formal approach to hydrological model conceptualization – Hydrological Sciences Journal, Vol. 38(5), pp. 391-401.
[21] L'vovich, M I (1974) *World water resources and their future.* English translation by the American Geophysical Union. Edited by Raymond L. Nace. Mysl'P.H., Moscow. P.415.
[22] Padmanabhamurty B, Satyanarayana Rao C V Vand Dakshinamurti J (1970), On the water balances of some Indian stations, Journal of Hydrology, Vol. 11, pp. 169-184.
[23] Penman H L (1955), Components in the water balance of a catchment area. Quarterly Journal of the Royal Meteorological Society, Vol. 81(348), pp. 280–284.
[24] Roderick M L, Hobbins, M T and Farquhar G D (2009), Pan Evaporation Trends and the Terrestrial Water Balance. II. Energy Balance and Interpretation. Geography Compass, Vol. 3(2), pp. 761–780.
[25] Savenije H H G (2009), HESS Opinions "The art of hydrology". Invited contribution, EGU Henry Darcy Medal award, Hydrology and Earth System Sciences, Vol. 13, pp. 157–161.
[26] Sivapalan M, Bloschl G, Zhang L and Vertessy R (2003), Downward approach to hydrological prediction, Hydrological Processes, Vol. 17, pp. 2101-2111.
[27] Sivapalan M, Yaeger M A, Harman C J, Xu X and Troch P A (2011), Functional model of water balance variability at the catchment scale: 1. Evidence of hydrologic similarity and space-time symmetry, Water Resources Research, Vol. 47, pp.1-18.
[28] Sokolov A A and Chapman, T G, *Methods for water balance computations: An international guide for research and practice*. UNESCO, 1974. P 127.
[29] Tang D Y and Ward R C (1982), Aspects of evapotranspiration and the water balance in a small clay catchment, 1967-75. Weather, Vol. 37(7), pp. 194-201.
[30] Tomasella J, Hodnett V, Cuartas, L A Nobre, A D, M J Waterloo and S M Oliveira (2008), The water balance of an Amazonian micro-catchment: the effect of inter-annual variability of rainfall on hydrological behaviour, Hydrological Processes, Vol. 22, pp. 2133– 2147.
[31] Tomer M D and Schilling K E (2009), A simple approach to distinguish land-use and climate-change effects on watershed hydrology, Journal of Hydrology, Vol. 376, pp. 24–33.
[32] Waichler S R, Wemple B C and Wigmosta, M S (2005), Simulation of water balance and forest treatment effects at the H.J. Andrews Experimental Forest. Hydrological Processes, Vol. 19, pp. 3177– 3199.
[33] Xu C Y and Singh V P (1998), A Review on Monthly Water Balance Models for Water Resources Investigations. Water Resources Management, Vol.12, pp. 31–50.

Table 1.*Storage - process interaction matrix for WAPROS model*

No	Hydrologic storages	OB	Addition processes (AP) (+)				Depletion processes (DP) (-)					CBC	CB	Error
		(1,1)	AP1	AP2	AP3	AP4	DP1	DP2	DP3	DP4	DP5	(i, j)	(N,24)	(N,24)
1	Interception – ic	OBic	RFic				EVic		SSic			CBCic	CBic	Eic
2	Soil Detention - so	OBso		OLso			EVso	IFso	SSso			CBCso	CBso	Eso
3	Surface Detention-su	OBsu	RFsu	OLsu			EVsu	IFsu	SSsu			CBCsu	CBsu	Esu
4	Structural Detention- st	OBst	RFst	OLst			EVst	IFst	SSst			CBCst	CBst	Est
5	Soil Upper Layer- ul	OBul	RFul	IFol	IFso IFsu IFst	SSic	EVul PTul	PCul	SSul	INul		CBCul	CBul	Eul
6	Soil Lower Layer- ll	OBll			PCul	SSul	PTll	PCll	SSll	INll		CBCll	CBll	Ell
7	Ground water -gw	OBgw	RFmp		PCll	SSll				BFgw SSgw		CBCgw	CBgw	Egw
8	Overland Flow -ol	OBol	RFol		SSso SSsu SSst			IFol	OLso OLsu OLst	OLcs		CBCol	CBol	Eol
9	Channel Storage - cs	OBcs	RFim RFvs	OLcs	BFgw SSgw	INul INll					Qcs	CBCcs	CBcs	Ecs
	Sum	OB	RFab				ET				Q		CB	E1
10	Rainfall – RF		RFm					RFab						Erf
A	Sum= Water Balance (S)	ΣOB	RFm				ET				Q		ΣCB	E
B	Sum= Water Balance (P)	ΣOB	ΣAP1	ΣAP2	ΣAP3	ΣAP4	ΣDP1	ΣDP2	ΣDP3	ΣDP4	Σ DP5		ΣCB	E

(im = impervious area flow; mp = macropore flow; vs = variable source area flow; m = modelled; ab = abstracted)

Table 2. *Water balance equations for storages in WAPROS model*

No	Hydrologic storages	Water balance equations
1	Rainfall – RF	RFic + RFsu + RFst + RFul + RFmp + RFol + RFim + RFvs = RFab
2	Interception - ic	OBic + RFic - EVic - SSic = CBic
3	Soil detention - so	OBso + OLso - EVso - IFso - SSso = CBso
4	Surface detention-su	OBsu + RFsu + OLsu - EVsu - IFsu - SSsu = CBsu
5	Structural detention- st	OBst + RFst + OLst - EVst - IFst - SSst = CBst
6	Soil upper layer- ul	OBul + RFul + IFol+ IFso + IFsu + IFst + SSic - EVul - PTul - PCul - SSul - INul = CBul
7	Soil lower layer- ll	OBll + PCul + SSul - PTll - PCll - SSll - INll = CBll
8	Ground water -gw	OBgw + RFmp + PCll+ SSll - BFgw - SSgw = CBgw
9	Overland flow -ol	OBol + RFol + SSso+ SSsu + SSst - IFol - OLso - OLsu- OLst - OLcs = CBol
10	Channel storage - cs	OBcs + RFim+ RFvs + OLcs + BFgw + SSgw + INul + INll - Qcs = CBcs

[Footnote: Storages 1 to 6 are capacity restrained, having surpluses from storages as SS; EV = Evaporation; PT = Plant Transpiration; IF = Infiltration; PC = Percolation; rainfall is not a typical storage and not having carry over procedure, but included in the matrix to account for error in rainfall abstractions (ab), and Erf = (RFm – RFab)].