CHAPTER III

MODELLING TOOL

In this section, the steps of the MIKE SHE model are described in details and its mathematical formulation is outlined. Furthermore the hydrological components of the model used in this study are described and their mathematical basis is presented.

3.1 HYDROLOGICAL DESCRIPTION

MIKE SHE simulates all the processes in the land phase of the hydrologic cycle, as stated in DHI (2004). Precipitation, falling from the atmosphere as snowfall or rainfall, is partly intercepted by vegetation and building structures. The intercepted precipitation is stored and later evaporated or passed to the soil surface. A significant amount of rainfall, reaching the soil surface, evaporates back to the atmosphere. Depending on the air temperature, the snow accumulates on the soil surface at temperature below 0 ^{o}C, while rainfall infiltrates through the unsaturated zone. When the top layer of the unsaturated zone becomes saturated, there is surface ponding and eventually overland flow begins when all the surface depressions are filled. The infiltrated water in the unsaturated zone can be stored, evaporated, taken up by plant roots and transpired through the leaves, or percolated down to the saturated zone. The overland water flows along the surface topography, evaporates and infiltrates on the way, eventually reaching streams, rivers and other surface water bodies. The groundwater also contributes to streams and rivers as a base flow, while water in rivers and streams infiltrates back into the saturated zone as recharge (Danish Hydraulic Institute, 2004).

3.2 MATHEMATICAL DESCRIPTION

The modular structure of MIKE SHE model composed of several module. These include a Water Movement module for hydrology (WM), an Advection/Dispersion of Solutes (AD) module for water quality, a Soil Erosion (SE) module for sediment transport, as well as others such as Dual Porosity (DP), Geochemical Processes (GC), Crop growth and Nitrogen processes in the root zone (CN), and IRrigation (IR). The Water Movement module of MIKE SHE has several components, each describing a specific physical process. These include evapotranspiration/interception, overland/channel flow (OC), unsaturated zone (UZ), saturated zone (SZ), snowmelt, and exchange between aquifer and rivers. Figure 3.1 gives a schematic representation of the MIKE SHE model.

The hydrological processes are described mostly by physical laws (laws of conservation of mass, momentum and energy). The 1-D and 2-D diffusive wave Saint Venant equations describe channel and overland flow, respectively. The Kristensen and Jensen methods are used for evapotranspiration, the 1-D Richards‘s equation for unsaturated zone flow, and a 3-D Boussinesq equation (Boussinesq, 1904) for saturated zone flow. These partial differential equations are solved by finite difference methods, while other methods (interception/evapotranspiration and snowmelt) in the model are empirical equations obtained from independent experimental research (Danish Hydraulic Institute, 2004). The FRAME component enables components having different time steps to run in parallel and to exchange information (Abbott et al., 1986b).

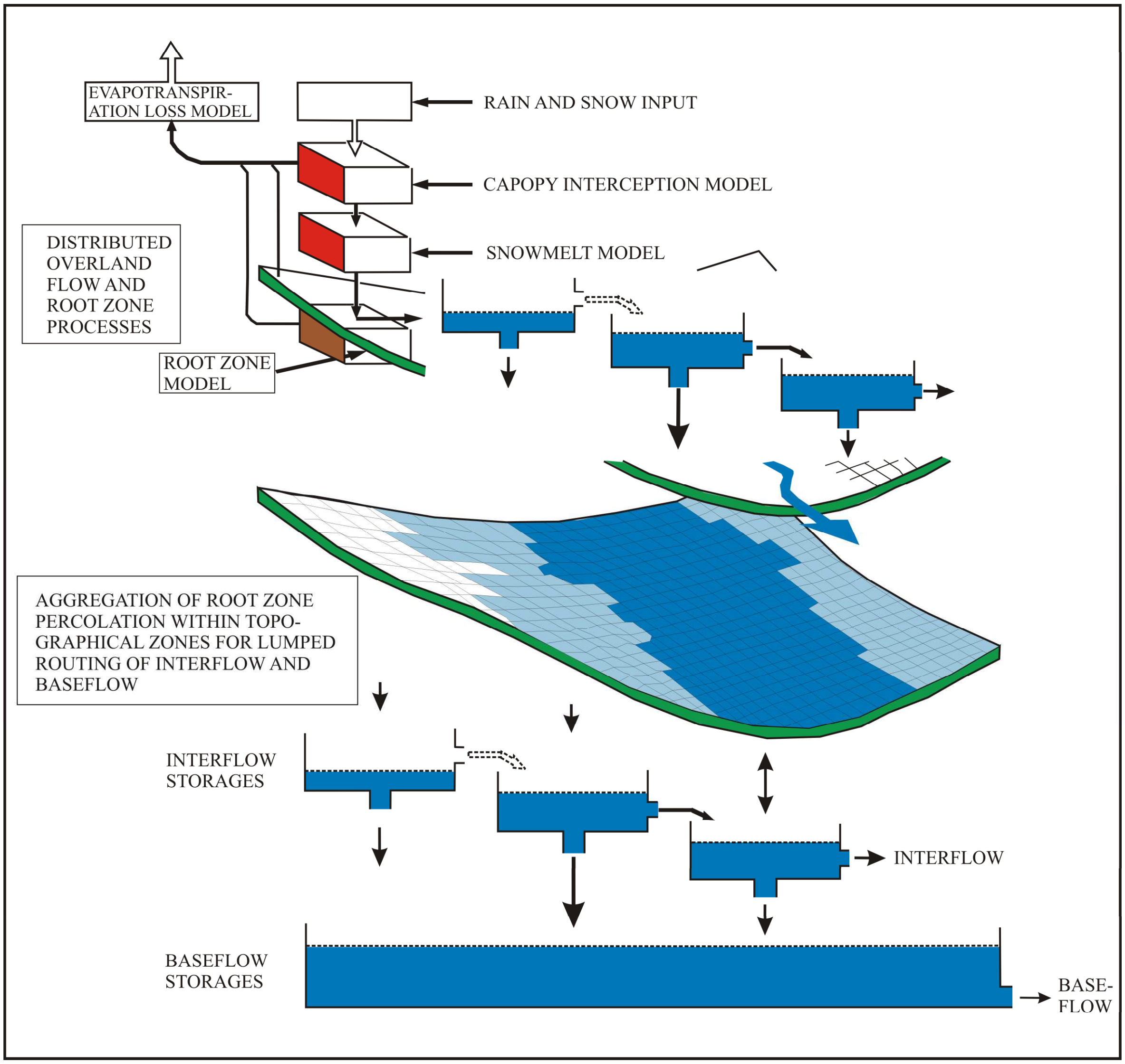

FIGURE 3.1
Schematic Representation of MIKE SHE Model (Modified after Refsgaard and Storm, 1995).

3.2.1 Interception and evapotranspiration components

The interception component determines the net amount of rainfall reaching the ground, the canopy storage and evaporation from the canopy. The interception storage capacity depends on the vegetation type, its stage of development and density, rainfall intensity as well as other climatic conditions (Abbott et al., 1986b). The evapotranspiration component calculates the amount of water that evaporates from the soil and water surfaces, and that transpires through the leaves. The latter is controlled by root zone water availability, aerodynamic transport conditions and plant physiological factors, and it varies both spatially and temporally. The processes in the interception/evapotranspiration component are shown in Figure 3.2. The model provides two methods for determining interception and evapotranspiration: (i) the Kristensen-Jensen method and (ii) the Rutter model/Penman-Monteith equation. In this study, the first method was used.

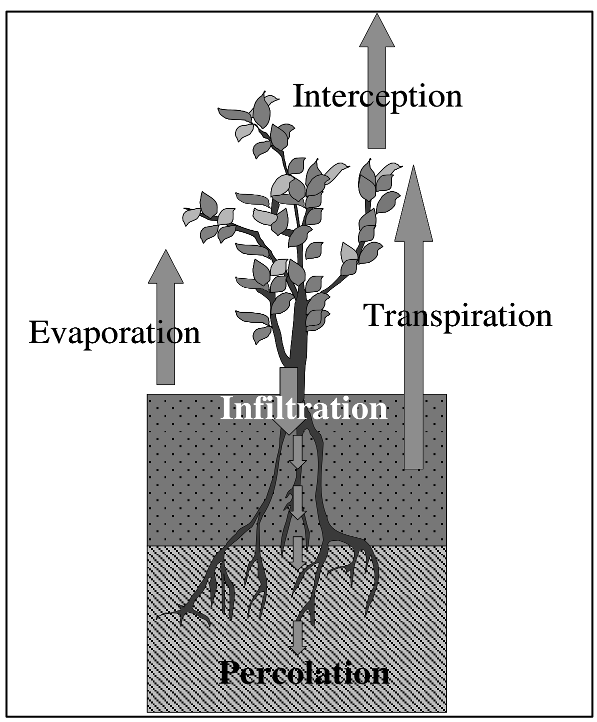

FIGURE 3.2
Schematic Diagram of Interception and Evapotranspiration

(a) Kristensen and Jensen method

The processor of MIKE SHE calculates the actual evapotranspiration and actual soil water content in the root zone using a modified code based on empirical equations which were derived by Kristensen and Jensen (1975). The temperature is always assumed to be above 0^{o}C. Thus maximum interception storage capacity of vegetation, I_{max} (mm), can be defined as:

$$I_{max} = C_{int}\, LAI \tag{3.1}$$

where

C_{int} is the interception coefficient, defining the interception storage capacity of the vegetation (mm) with the typical value of 0.05 mm.

LAI is the leaf area index ($m^2\, m^{-2}$).

Evaporation from the canopy storage, E_{can} (mm), for a sufficient amount of intercepted water, is given by:

$$E_{can} = \min\,(I_{max}, E_p\Delta t) \tag{3.2}$$

where

E_p is the potential evapotranspiration rate (mm hr^{-1})

Δt is the time step duration for the simulation (hr)

Actual Plant transpiration, E_{at} (mm) is determined as:

$$E_{at} = f1(LAI) \cdot f2(\theta) \cdot RDF \cdot E_p \tag{3.3}$$

where

$f_1(LAI)$ is a function based on the leaf area index,

$f_2(\theta)$ is a function based on the soil moisture content, and

RDF is a root distribution function.

The LAI function is given by:

$$f1(LAI) = C2 + C1 \cdot LAI \tag{3.4}$$

where

C_1 and C_2 are empirical parameters with usual values of 0.3 and 0.2, respectively.

The soil moisture function is given by:

$$f_2(\theta) = 1 - \left(\frac{\theta_{FC} - \theta}{\theta_{FC} - \theta_W} \right)^{\frac{C_3}{h_P}} \tag{3.5}$$

where

θ_{FC} is the volumetric moisture content at field capacity ($m^3\ m^{-3}$),

θ_W is the volumetric moisture content at the wilting point ($m^3\ m^{-3}$), is the actual volumetric moisture content ($m^3\ m^{-3}$)

C_3 is an empirical parameter (mm/day), based on soil type and root density where a value of 20 mm/day is used in MIKE SHE.

The root distribution function is given as:

$$RDF_i = \frac{\int_{z1}^{z2} R(z)\partial z}{\int_{0}^{L_R} R(z)\partial z} \tag{3.6}$$

where

$R(z)$ is the root extraction, calculated as:

$$\log R(z) = \log R_o - AROOT \cdot z \tag{3.7}$$

where

R_o is the root extraction at soil surface (m),

AROOT is a parameter describing root mass distribution (m^{-1}), where the typical value used is 0.25 m^{-1}

z is depth below the ground surface (m).

Soil evaporation, E_s (mm), is given by:

$$E_s = E_p \cdot f_3(\theta) + (E_p - E_{at} - E_p \cdot f_3(\theta)) \cdot f_4(\theta) \cdot (1 - f_1(LAI)) \tag{3.8}$$

where

f_3 and f_4 are a function of soil moisture content.

$$f_3(\theta) = \begin{cases} C_2 & \theta \geq \theta_w \\ C_2 \dfrac{\theta}{\theta_w} & \theta_r \leq \theta \leq \theta_w \\ 0 & \theta \leq \theta_w \end{cases} \tag{3.9}$$

where

C_2 is the empirical parameter with typical value of 0.2.

$$f_4(\theta)=\begin{cases} \dfrac{\theta-\dfrac{\theta_w+\theta_{FC}}{2}}{\theta_{FC}-\dfrac{\theta_w+\theta_{FC}}{2}} & \theta\ge\dfrac{\theta_w+\theta_{FC}}{2} \\ 0 & \theta<\dfrac{\theta_w+\theta_{FC}}{2} \end{cases} \tag{3.10}$$

The f_1(LAI) function and E_{at} are zero in the absence of vegetation, and evaporation from the soil occurs only from the upper node of the unsaturated zone.

3.2.2 Overland and channel flow component

Overland flow, influenced by topography, flow resistance, evaporation and infiltration along the path, occurs when the rainfall rate exceeds the infiltration rate, resulting in surface ponding and eventually surface water flow. There are two methods for determining the overland flow which includes (i) the diffusive wave approximation of the St. Venant equations and (ii) simplified overland flow routing. The MIKE SHE uses the first method and also considers the interaction with other processes, such as evaporation, infiltration, tile drains, and drainage into the channel network.

(a) Diffusive wave approximation of St. Venant equations

Diffusive wave approximation of the St. Venant equations is derived from the fully dynamic St. Venant equations, wherein the last three terms of the momentum equations are neglected in order to reduce the fully dynamic equations' complexity. The continuity equation (Equation 3.11) and momentum equations (Equations. 3.12 and 3.13) allow the simulation of significant variation in overland flow depth between neighbouring cells as well as that of backwater conditions.

$$\frac{\partial h}{\partial t}+\frac{\partial (uh)}{\partial x}+\frac{\partial (uh)}{\partial y}=i \tag{3.11}$$

where

h is the flow depth above ground surface (m)

u is the velocity (m s^{-1}) in the x-direction

v is the velocity (m s^{-1}) in the y-direction

i is the net input over overland flow (m s^{-1})

The momentum equations are:

$$\left.\begin{aligned} S_{fx} &= S_{ax}-\frac{\partial h}{\partial x} \\ S_{fy} &= S_{ay}-\frac{\partial h}{\partial y} \end{aligned}\right\} \qquad (3.12)\ (3.13)$$

where

S_f are the friction slopes (-) in the x and y directions

S_o are the slopes of the ground surface (–) in the x and y directions.

Using the diffusive wave approximations of the St. Venant equations and Manning's equations, one obtains:

$$vh = K_x\left(-\frac{\partial z}{\partial x}\right)^{\frac{1}{2}} h^{\frac{5}{3}} \tag{3.14}$$

$$vh = K_y\left(-\frac{\partial z}{\partial y}\right)^{\frac{1}{2}} h^{\frac{5}{3}} \tag{3.15}$$

where

uh and vh are discharge per unit length along the cell boundary in x- and y- directions respectively [m^2 s^{-1}]

k_x and k_y are Manning M or Stickler coefficient in x- and y- directions, respectively.

Flow across any boundary between grids, from equations (3.14) and (3.15), is given by:

$$Q = \frac{k\Delta x}{\Delta x^{\frac{1}{2}}}\left(Z_u - Z_D\right)^{\frac{1}{2}} h_u^{\frac{5}{3}} \tag{3.16}$$

where

h_u is the depth of water that can freely flow into the next cell (actual water depth minus detention storage, mm)

Z_u and Z_D are the maximum and minimum water levels, respectively (mm).

The modified method of Gauss Seidel is applied for the numerical solution. Depending on the condition i.e. infiltration, recharge or evaporation, water is added or removed to the ponded water in the model grid at the beginning of every overland flow time step. During iteration, since the flow equations are explicitly defined, overland flows are reduced in some situations to avoid internal water balance errors and divergence of the solution scheme. Henceforth, outflow should be:

$$\sum \lfloor Q_{out} \rfloor \leq \sum Q_{in} + I + \frac{\Delta x^2 h(t)}{\Delta t} \tag{3.17}$$

where

Q_{in} is the sum of inflows rates ($m^3\,s^{-1}$)

I is ($i\Delta x^2$) which is the net input into overland flow in each grid ($m^3\,s^{-1}$)

3.2.3 Unsaturated zone components

The flow in the unsaturated zone is assumed to be vertical. The model provides three options to calculate flow: (i) full Richard‘s equation, (ii) a simplified gravity flow and (iii) a simple two-layer water balance method for shallow water tables. The full Richard‘s equation was used in this study.

(a) Richard’s equation

The pressure head-based Richard’s equation (Richard, 1931), based on Darcy’s law (Darcy, 1856) and continuity equation, assumes the soil matrix to be incompressible and soil water to be at constant density:

$$C\frac{\partial\Psi}{\partial t}=\frac{\partial}{\partial z}\left(K\frac{\partial\Psi}{\partial t}\right)+\frac{\partial K}{\partial z}-S \tag{3.18}$$

where

C is the soil water capacity (mm^{-1}),

ψ is the pressure head (mm),

K is the saturated hydraulic conductivity ($mm\ s^{-1}$),

Z is the gravitational head (mm), and

S is the root extraction sink term (s^{-1}).

The Richard's equation (Richard, 1931) is solved numerically using the finite difference implicit approximation method, associated with the Gauss-Seidal iteration formula, thus removing the stability and convergence problems due to heterogeneous soil properties. The unsaturated zone is defined by an upper boundary (ground surface) and a lower boundary (groundwater table). Whenever there is a constant head on the surface, such as ponded water the upper boundary is considered as a Dirichlet boundary otherwise in case there is a constant head such as rainfall a Neuman boundary is applied to the surface. The lower boundary is generally a pressure boundary, but is a zero flux boundary when the water table falls below the impermeable bed, such that there is an upward flux in the lower part of the profile. The initial conditions set up by the model are hydrostatic conditions, defined by an equilibrium soil moisture-pressure profile, with no flow. The sink term in the Richard's equation is the root extraction due to transpiration in the upper part of the unsaturated zone, which is the actual transpiration for the entire root zone.

(b) Coupling of unsaturated zone to the saturated zone

Coupling is required to enable water table fluctuation, especially in shallow soils. The unsaturated zone (UZ) and saturated zone (SZ) are explicitly coupled to optimize the time steps used. The explicit interaction is solved by an iterative mass balance procedure that conserves mass for the entire column by considering outflows and source/sink terms in the saturated zone. Mass balance errors normally occur when:

(1)- water table level is kept constant during the unsaturated zone time step

(2)- an incorrect specific yield, S_y, is used in the saturated zone.

The coupling is limited to the entire unsaturated zone and the uppermost calculation layer of the saturated zone. If the water table is below the bottom of the first SZ calculation layer, the UZ module treats the bottom of SZ calculation layer one as a free drainage boundary or a zero-flux boundary (Richard‘s equation). However, several geological layers can be specified within calculation layer number one if the lower levels of the SZ calculation layers are explicitly defined.

3.2.4 Saturated zone components

There are two methods for determining the flow in the saturated zone: (i) 3-D finite difference method and, (ii) linear reservoir method, where the first method was applied in the model set-up.

(a) 3-D Finite Difference Method

In this method, the saturated flow is defined by the 3-dimensional Darcy equation (Darcy, 1856) and equation of continuity, and it is solved by an iterative implicit finite difference technique. The two solvers provided by this method are preconditioned conjugate gradient and successive over-relaxation solution techniques, which differ somewhat in the formulation of potential flow and sink/source terms. The preconditioned conjugate gradient was chosen as the solution technique in this model simulation. The SZ interacts with other components of MIKE SHE using their boundary flows implicitly or explicitly, as sources and sinks. The governing 3-D partial differential equation is given as:

$$\frac{\partial}{\partial x}\left(K_{xx}\frac{\partial h}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_{yy}\frac{\partial h}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial h}{\partial z}\right)-Q=S\frac{\partial h}{\partial t} \tag{3.19}$$

where

K_{xx}, K_{yy}, and K_{zz}	are the hydraulic conductivity along the x, y and z axes [mm s^{-1}]
h	is the hydraulic head (mm)
Q	is the source/sink term (s^{-1})
S	is the specific storage coefficient (m^{-1})

The peculiarities of the equation are that:

(1)- it is non-linear for unconfined flow

(2)- the storage coefficient is not constant and changes from a specific storage coefficient for confined conditions to a specific yield for unconfined conditions.

(b) The PCG (Preconditioned Conjugate Gradient) solver

The potential flow terms, based on Darcy's law (Darcy, 1856), are given as:

$$Q = \Delta hC \tag{3.20}$$

where

h is the piezometric head difference (mm), and

C is the conductance ($m^2\,s^{-1}$).

The horizontal conductance is calculated from the harmonic mean of the horizontal conductivity and the geometric mean of the layer thickness, while the vertical conductance is the weighted serial connection of the hydraulic conductivity, calculated from the middle of one layer to the middle of another layer. For dewatering conditions in SZ cells, where the bottom cell becomes dewatered, a correction term is added to the right-hand side of the finite difference equation, using the last computed head. The correction term is:

$$q_c = Cv_{k+½}(h_{k+1} - z_{top,\,k+1}) \tag{3.21}$$

where

C_v is the vertical conductance (m^2s^{-1}),

z layer thickness (m)

k+1 is number of node

The storage capacity is calculated by

$$\frac{\Delta w}{\Delta t} = \frac{S2\left(h^{n} - Z_{top}\right) + S1\left(Z_{top} - h^{n-1}\right)}{\Delta t} \tag{3.22}$$

where

n is time step,

S1 is the storage capacity at the start of the iteration at time step n, and

S2 is the storage capacity at the last iteration.

The boundary conditions of the saturated zone can be subject to

(1)- Dirichlet's conditions based on hydraulic head

(2)- Neumann's conditions based on gradient of hydraulic head, or

(3)- Fourier's conditions based on head dependent flux.

In MIKE SHE, the drainage flow is calculated as a linear reservoir and is controlled by the height of water table above the drain depth and the specified time constant. However, drainage flow occurs only in the top layer of the saturated zone layer and when water table is above the drain depth. With the PCG solver, the drain flow is added directly in the matrix calculations as a head dependent boundary, and is solved implicitly as:

$$q = (h - Z_{dr})C_{dr} \tag{3.23}$$

where

h is head in the drain cell (m),

Z_{dr} is the drainage level (m), and

C_{dr} is the drain conductance or time constant (m^2s^{-1})

The exchange of saturated zone flow and overland flow is calculated implicitly using the Darcy equation, with continuously updating of the overland water depth:

$$Q = \Delta h C^{\frac{1}{2}} \tag{3.24}$$

where

$C^{\frac{1}{2}}$ is the conductance from surface level to the middle of the top calculation layer ($m^2\,s^{-1}$)

In case of full contact or reduced contact between overland and saturated zones, the conductance used in the Darcy equation is different for each case. The initial conditions applied for the saturated zone can be constant or distributed over the model domain, while the initial conditions in the boundary cells are kept constant during the simulation (Danish Hydraulic Institute, 2004).