The SIMPEL soil water models

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www.hydrology.uni-kiel.de/simpel/
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- www.openoffice.org
All models are wrong. Some of them are useful.

(George Box 1979)
1 Structure and Preliminary Notes

This documentation contains the following parts based upon each other: First the basic model (single layer storage model) is discussed, then different versions are introduced which are all derived from the basic model.

Changes or new versions of the models are available via internet
I also send them as CD via mail or e-mail.
Older and more simplified versions are also available, sometimes they are better suited for education.

1.1 Fields of application

On principle SIMPEL-models are applicable for 95% of all soils. Compared to other, more complex models the following components are not included:

- lateral flow, surface runoff when exceeding infiltration capacity.

Therefore the SIMPEL-models will not give reliable results under the following conditions:

- lateral inflow and runoff (sloping surfaces)
- heavy soils with low infiltration capacity and surface runoff
- high temporal resolution (> daily values)

In other ways there is not much that can go wrong with using SIMPEL models as...

...SIMPEL-Models cover the low end of hydrologic computing.
1.2 Revision history

- 1986: First version
- June 2003: moving web server to www.hydrology.uni-kiel.de/simpel
- June 2003: change data format to OpenOffice
- June 2003: inclusion of runoff module with unit-hydrograph for training purposes
- April 2004: improvement of documentation for unit hydrograph
- January 2006: English translation by Heike Pfletschinger
- February 2006: adding the wetland version
- Spring 2006: inverse modelling added, quality measures added (Nash-Sutcliffe)
- Summer 2008: added screenshots in English, minor corrections
- Spring 2012: update of documentation and screenshots
1.3 **Simpel in a minute**

- Download from: [http://www.hydrology.uni-kiel.de/forschung/projekte/simpel/](http://www.hydrology.uni-kiel.de/forschung/projekte/simpel/)
- Available free of charge under the Creative Common Licence
- Including dataset of 15 years from Bornhöved (Schleswig-Holstein/ Northern Germany)

**Type of model**

- One-dimensional soil water model (bucket-type)
- Implemented as Excel-Spreadsheet
- Evaporation calculated with German DVWK-methods

**Versions of the model**

- Basic model with Haude-evaporation, all in one file
- Version with separate files
  - Input files (input_evaporation.xls)
  - Calculation for evaporation (toolbox_evaporation.xls)
  - Soil water model (simpel2.xls)
- Version with surface runoff and Unit-Hydrograph
- Calculation of nutrient transport with measured substance concentrations in the soil water

**Suitable for**

- Calculation of the water balance on light and medium soils

**Not suitable for**

- Sloping surfaces (no lateral runoff in the basic version)
- Sites with capillary rise in the root zone (not implemented, try wetland version)
- Simulations with high temporal resolution (storage models are well suited for daily fluctuations)
1.4 Express setup of a new catchment

This chapter shows the overloaded educator and/or scientist you how to setup a simple run in 5 minutes.

1.4.1 Mandatory steps:

- Copy precipitation time series and climate data including the date column to `input_evaporation.xls` (Worksheet: `input_time series`)
- Select method for evaporation in `toolbox_evaporation.xls`, adjust crop coefficients (Worksheet: `crop_evaporation`) and adjust transfer of evaporation data to the simple model (Worksheet: `SIMPELevaporation`)

or (if you have an evaporation data set)

- copy potential evaporation (e.g. pan evaporation) to `simpel2.xls`, Column C

In case you want to compare measured and modelled runoff;

- copy the measured values (use dimension “mm”) to the comparison worksheet in `simpel_uh.xls`

Now you should have the first results for your climate, using the predefined LAI-Values, soil physical parameters and Unit-Hydrograph coefficients. You may not have a calibrated model, but at least a localized version ready for the students.

1.4.2 Fine Tuning

The next step is to fine tune the parameters which can be measured or taken from textbooks or personal imagination:

- soil physical data in the simulation worksheet (`simpel.xls` and `simpel_uh.xls`)
- modify infiltration limit (column M in worksheet `bucket_model`) and
- analyse measured runoff and compute the unit hydrograph for your catchment
- Leaf area index (start and end of vegetation)

1.4.3 Frequent errors

If the spreadsheet shows you error messages, try to find to the first occurrence of the error. The causes for the most frequent errors are:

- width of column is not adjusted (not a real error, but confusing for beginners)
- missing values and text fields in input data (sometimes coded as text or “ “ (space))
- check soil physical parameters for plausibility (is FC and Start_Reduction > pWP)
2 Basics

The simplest method for calculating the areal water balance is to use the climatic water balance, i.e. the
difference between precipitation and potential evaporation. It gives a rough estimation without saying
much about the actual evaporation as it does not include any buffer properties of the soil.

The most accurate water balance is achieved by using a simulation model based on Darcy resp. Richards
equation and a physically based method for calculating evaporation. These models are accurate but need
high effort for training, parametrization and data collection.

A practical solution can be using so called bucket models as they are used in large scale models (e.g. global
climate models). They simulate the soil water content of sites without groundwater in the root zone with
simple and generally available data and can be established with low effort. As indicated by the name,
bucket or storage models calculate the water balance within different layers of the soil which are treated
like a water bucket. (see system structure in Fig. 1). The most simple case only takes the root zone into
account. Hydrologic models normally work with interception storages (leave resp. plant, litter in forests),
one or more soil storage and a groundwater storage.

Fig. 1 shows the model structure. The storages are leaves, litter, soil and groundwater. Input data are
precipitation, potential evaporation, areal leaf index and soil physical parameters. Output is given as flow
between the reservoirs, actual evaporation as the sum of interception, evaporation and transpiration,
infiltration to the groundwater and surface runoff.

Leaf and litter storages are implemented as simple overflow storage devices. They are calculated by taking
the actual storage content, adding precipitation and subtracting evaporation. When the balance exceeds
storage capacity, the surplus flows to the next storage (e.g. from leave to litter). This happens as well
when the demands for evaporation cannot be reached within the actual storage.
The disadvantage of this simple approach is that a downward flow only occurs when field capacity is exceeded. It is therefore possible to get no flow to the groundwater during the summer months even if the soil water content reaches almost field capacity. To get more realistic results in such a case a non-linear function is used to generate a flow from the rooted zone dependent on soil water content even with unsaturated soils. For soil storage in this model an approach after Glugla is chosen.

3 System Structure

The model is written in “Microsoft Excel”, it runs on versions from Office 97 on. A version for LibreOffice is planned. The technical model structure depends on the model version. Earlier versions contained everything in one file. The newest version separates input, calculation for evaporation and the soil water model to enable the combination of different input files, e.g. for different soils and crops. The files are separated into:

- Input evaporation.xls (time series and static input values)
- Toolbox evaporation.xls (calculation of evaporation, ETp)
- Storage model(s) (soil hydrology simulation, e.g. SIMPEL2.xls)

Figure 2 shows the worksheets of one spreadsheet file (soil water model) with the following modules:

- storage model containing the model
- interception capacity sub model to calculate the interception capacity based on LAI
3.1 Input Data

3.1.1 Input evaporation data

All input data for evaporation are compiled in the file input_evaporation.xls, some methods might only need parts of it.

The data sets are:

- time series (daily climatic data)
- static input values (geographical position etc.)
- plant parameters for Penman/Monteith
- LAI time series
- long term monthly mean values (only needed for Thornthwaite)

The following time series can be entered (Fig. 3):
• T: daily mean air temperature (°C)
• SD: duration of sunshine (h) to calculate global radiation
• Rg: global radiation (J cm⁻²), alternative to sunshine duration
• Rf: air humidity daily mean (%)
• U: wind velocity daily mean (m s⁻¹)
• T14: air temperature at 2pm (°C) - only for Haude-evaporation
• Rf14: relative air humidity at 2pm (%) - only for Haude-evaporation

Figure 3: Input time series for calculating evaporation
### Static Input data for the different formulas

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### EPIC Input Parameter

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Figure 4: Input of static parameters

Figure 5: Input of LAI time series
The Leaf Area Index (LAI) has to be entered as time series as shown in Fig. 5. Time spans between the measurements can be chosen freely. For the simulation LAI data are converted to daily values via linear interpolation (see chapter 3.3.1 “model of leaf interception” on page 39 for details).

Fig. 4 shows the static input parameters used for global radiation (maximum sunshine duration for net radiation). Albedo and crop height are needed to calculate the energy balance and resistances. All other values relate to the Penman/Monteith method and are adopted from the EPIC documentation. They are discussed in more detail in chapter 3.2 on page 21ff.

![Figure 6: Input Thornthwaite coefficients](image)

The coefficients shown in fig. 6 are only needed for the Thornthwaite method. The data sets can be found in meteorological reference tables or in the database of the GHCN (Global climate historical network, http://www.ncdc.noaa.gov/ghcnm/).

### 3.1.2 Soil physical input

Soil physical data are separated from evaporation data to be able to calculate water balances of different soil profiles with the same potential evaporation.

The input fields can be found in the spreadsheet “soil water model” oder “storage model” (fig. 7). The input values are resumed in tab. 1. They can be measured in a laboratory, but they can also be found in soil science reference maps, textbooks or other references for pedotransfer functions.
Table 1: Soil physical parameters of the model

<table>
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<th>Parameter</th>
<th>Value</th>
<th>Remark</th>
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<td>Field capacity</td>
<td>25</td>
<td>in vol.-% in the root zone</td>
</tr>
<tr>
<td>Permanent wilting point</td>
<td>10</td>
<td>in vol.-%</td>
</tr>
<tr>
<td>Start reduction</td>
<td>15</td>
<td>in vol.-%, start reduction from ETp to ETa, see fig. 26</td>
</tr>
<tr>
<td>Depth of root zone</td>
<td>100</td>
<td>in cm (depth of soil column)</td>
</tr>
<tr>
<td>Capacity leaf interception</td>
<td>2</td>
<td>Max. capacity of the plant canopy in mm with fully developed leaves (max. LAI)</td>
</tr>
<tr>
<td>Min. cap.</td>
<td>0.1</td>
<td>Minimum capacity (stem and branches during winter) with LAI=0 (in mm)</td>
</tr>
<tr>
<td>Coeff. c</td>
<td>150</td>
<td>Empirically determined after Glugla</td>
</tr>
<tr>
<td>Lambda</td>
<td>0.001</td>
<td>Empirically determined after Glugla</td>
</tr>
<tr>
<td>Capacity litter layer</td>
<td>1</td>
<td>Interception capacity of the litter layer in forests (mm)</td>
</tr>
<tr>
<td>Initial value litter layer</td>
<td>0</td>
<td>in mm</td>
</tr>
<tr>
<td>Initial value soil storage</td>
<td>20</td>
<td>in vol-%</td>
</tr>
<tr>
<td>drying factor litter</td>
<td>2</td>
<td>Part of the water content that can evaporate within one day (see chapter 3.3.2 “model of the litter layer”)</td>
</tr>
</tbody>
</table>
3.2 Toolbox Evaporation

All methods for potential or non-stressed evaporation (ETp) are summarized in the file Toolbox_Evaporation.xls. The separation from the input data has the advantage that a change or test of an evaporation formula is possible without a change of the input data. It requires only the change of name of the linked file (in Excel: Edit → Links → Source → Modify).

To reduce the complexity for education, there is also single file version containing only the Haude method to calculate evaporation.

The full-featured, 3-file versions include the following evaporation methods:

- Haude
- Penman, simplified according to Wendling
- Penman Original
- Makkink
- Thornthwaite
- Blaney Criddle
- Turc
- Penman/Monteith

If not mentioned otherwise, all equations, methods etc. are taken from the German DVWK-guideline (DVWK 1995) which sets the standards for the calculation of evaporation (and other hydrologic computing procedures).
In this documentation we show mainly the worksheet formulas and not the mathematical equations. For more complex formulas, forms are shown to make the plain cell formulas easier to understand.

The transfer of the calculated evaporation to the soil water model (link of spreadsheets) is not carried out from the worksheet of the different methods, but from a separate worksheet called “SIMPEL-Evaporation”. Therefore all information about calculation of evaporation stays traceable within the spreadsheet and the methods for evaporation can be changed without affecting the references to evaporation in the soil water worksheet.

Calculation of evaporation according to Penman/Monteith is taken from the EPIC-model as this model uses daily values and is relatively widespread. An implementation of the new FAO method is planned for the near future.

### 3.2.1 Temporary variables

Many equations for evaporation rely on the same input data and use the same parameters – mostly for calculating the radiation budget and humidity. These parameters and some intermediate steps are summarized in a separate worksheet (temp_vars) as shown in fig. 8.

![Figure 8: Temporary variables for evaporation](image)

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3.2.1.1 Sunshine duration and global radiation

Sunshine duration and global radiation are displayed in the first columns in fig. 8. Column B calculates the Julian day (1-365) from the date given in column A.

Column C calculates the temporary variable needed for the astronomically possible sunshine duration and extraterrestrial radiation (eq. 2).

Columns D and E calculate sunshine duration (SD, eq. 1) and extraterrestrial radiation (Re, eq. 3) as a function of date and geographical position.

\[
S_0 = 12.3 \sin (\zeta) \cdot (4.3 + (\varphi - 51.0)6) \\
\zeta = 0.0172 \cdot JT - 1.39 \\
R_0 = 245 \cdot (9.9 + 7.08 \sin (\zeta) + 0.18 \cdot (\varphi - 51.0) \cdot (\sin \zeta - 1))
\]

RG = global radiation (J·cm\(^{-2}\))
R\(_0\) = extraterrestrial radiation (J·cm\(^{-2}\))
S\(_0\) = astronomically possible (maximum) sunshine duration (h)
S = measured sunshine duration (h)
JT = Julian Day (1 to 365)
\varphi = latitude (52 for Kiel)

If data for global radiation is not available it can be computed from measured sunshine duration according to the Angström-equation (column F).

\[
F2: = +E2 \cdot (0.19 + 0.55 \cdot [\text{input_evaporation.xls}] \text{input_time_series'!$C2/D2})
\]

The final value for global radiation is located in column G. Measured values are used as far as they are available. In case of missing data, global radiation is computed from sunshine duration.
3.2.1.2 Humidity

In columns H to M of fig. 8 temporary variables of humidity are calculated. The dependent variables for these calculations are relative humidity (column H) and mean air temperature (column I). The saturation vapor pressure of air (hPa) is calculated in column J according to the following equation:

\[ e_s = 6.11 \cdot e^{\frac{17.62 \cdot T}{243.12 + T}} \]  

\( J2: = 6.11 \times \exp\left( \frac{17.62 \times I2}{243.12 + I2} \right) \)

Vapor pressure is calculated from relative humidity (H2) and saturation vapor pressure (J2) according to the following equation:

\[ S2: = J2 \times (1 - \frac{H2}{100}) \]

For the different versions of the Penman equation, a non-dimensional function of temperature is used (column L):

\[ L2: = \frac{2.3 \times (I2 + 22)}{(I2 + 123)} \]

In column M the specific enthalpy for evaporation is calculated, which is the radiant energy needed to evaporate 1mm of water (temperature dependent).

\[ M2: = 249.8 - 0.242 \times I2 \]

3.2.2 Calculating crop evaporation

Most evaporation formulas produce results for a standard cover, normally short, well watered lawn. This value has to be adjusted to the other crops with crop-coefficients. Only the Haude and the Penman/Monteith method do consider different crops.
### Figure 9: Crop-coefficients

<table>
<thead>
<tr>
<th>Month</th>
<th>M. Grassland</th>
<th>W. Wheat</th>
<th>W. Barley</th>
<th>M. Barley</th>
<th>W. Rye</th>
<th>Oat</th>
<th>Sugar Beet</th>
<th>Potato</th>
<th>W. Rapeseed</th>
</tr>
</thead>
<tbody>
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### Haude coefficients

<table>
<thead>
<tr>
<th>Month</th>
<th>Dryland</th>
<th>Grass</th>
<th>Vegetation</th>
<th>Workshop</th>
<th>Sugar Beet</th>
<th>Grass --&gt; Vegetation</th>
<th>Sugar --&gt; Workshop</th>
<th>Grass --&gt; Workshop</th>
<th>Sugar --&gt; Workshop</th>
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<td>0.10</td>
</tr>
</tbody>
</table>

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There are two worksheets in SIMPEL toolbox_evaporation for the conversion of ETp: crop-coefficients (fig. 9) and conversion of the time series (crop evaporation, fig. 10). The coefficients are adopted from the German DVWK-guideline. In case of a missing monthly value the coefficients are adopted from converted Haude-coefficients with the difference between the Haude-coefficient for grassland and the specific crop plant. As this method is quite simple, these factors are highlighted in red color in the worksheet. Fig. 10 shows the general layout for the conversion: date (A), initial evaporation value (ETp-grassland, column B). Columns D to K give the potential evaporation for the different crops. To transfer potential evaporation values to the soil water module make sure to link this worksheet instead of the original method in the “Simpel-Worksheet”, where the soil water model is looking for the evaporation values.

3.2.3 Thornthwaite method
The calculation according to Thornthwaite is a very old and widespread in practice. For Germany, it does not give reasonable results.

The calculation is split in two parts: calculation of the coefficients (fig. 6) and of evaporation (fig. 11).
Evaporation is calculated according to the following equation:

\[ E_{TP} = 0.533 \left( \frac{S_0}{12} \right) \left( \frac{10 - T}{J} \right)^a \]  

\[ J = \sum_{Dec}^{Jan} \left( \frac{T}{5} \right)^{1.514} \]  

The coefficients \( J \) (eq. 7) and \( a \) (eq. 6) are based on monthly mean values. Whenever temperatures are negative, values of \( E_{TP} \) also become negative and are set to 0 automatically.

### 3.2.4 Turc method

This method is mainly used in France and the Mediterranean region. Global radiation (fig. 12, column C) is calculated according to the previous described method from sunshine duration or given as a measured value. Column E contains the coefficient (in Germany for most parts 1), column F holds the uncorrected \( E_{TP} \) values, in column G all values \(<0.1\) are set to 0.1.
with

\[ \text{if } RF < 50 : \quad C = 1 + \frac{(50 - RF)}{70} \]  \hspace{1cm} (9)

\[ \text{if } RF \geq 50 : \quad C = 1 \]

\[ \text{ET}_p = 0.0031 \cdot C \cdot (R_g + 209) \cdot \frac{T}{(T + 15)} \]  \hspace{1cm} (8)

\[ \text{EP}_p = (8.128 + 0.457 \cdot T) \cdot \frac{S \cdot 100}{S_{\text{year}}} \]  \hspace{1cm} (10)

3.2.5 Blaney-Criddle method

The Blaney-Criddle formula is often used in irrigation management. In Germany, the best results can be obtained with the modified version of Schrödter (1985). \( \text{ET}_p \) is calculated from temperature and maximum daily sunshine duration. This method is done without a calculation of the total sum of annual sunshine duration \( (S_{\text{year}}) \), the corresponding values are taken from a table shown in fields G11 to H20 in fig. 13. Results \( (\text{ET}_p) \) can be found in column D. For a comparison of the two versions, the sums of the whole period are computed in cell F2 and F3. Similar to the method according to Turc negative values are set to 0.
3.2.6 Makkink method

This method originating from the Netherlands is a version of the Penman method, much like the Wendling formula. The cell formula is shown in the editing line in fig. 14. Calculation of evaporation is derived directly from the temporary variables.

\[ ET_p = \frac{s}{(s + y)} \cdot \left( C_1 \cdot \frac{R_G}{L} + C_2 \right) \]  

Figure 13: Calculating evaporation according to Blaney-Criddle
3.2.7 Wendling

Another version from Makkink respectively Penman is the method according to Wendling. By introducing a so called coastal coefficient \( f_K \) it is specifically adapted to coastal regions.

\[
ET_p = \frac{(R_G + 93 \cdot f_K \cdot (T + 22))}{150 \cdot (T + 123)}
\]  

(12)

Figure 14: Calculating evaporation according to Makkink

Figure 15: Calculating evaporation according to Wendling

3.2.8 Penman
The Penman method is – despite a revised version (Allen et al. 1998) - worldwide the best known method and should be used whenever possible. The version which is introduced with this documentation is slightly simplified and resembles the method recommended by the FAO for agricultural aims. \( g(T) \) is the non-dimensional function of temperature as introduced in chapter “Humidity” 3.2.1.2.

\[
ET_p = g(T) \cdot \left( \frac{0.6 \cdot R_g}{L} + 0.66 \cdot (1 + 1.08 \cdot U) \cdot (1 - \frac{R_f}{100}) \cdot S_R \right) \quad (13)
\]

### 3.2.9 Penman/Monteith for coniferous woodlands

This undocumented method is adopted from Jochen Schmidt especially for coniferous woodlands – it will be removed in future versions.

Table 2: Parameter for calculating evaporation according to Penman/Monteith for coniferous woodlands

<table>
<thead>
<tr>
<th>Column</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Date (input data)</td>
</tr>
<tr>
<td>B</td>
<td>Day of the year (input data)</td>
</tr>
<tr>
<td>C</td>
<td>Global radiation (input data)</td>
</tr>
<tr>
<td>D</td>
<td>Air temperature (input data)</td>
</tr>
<tr>
<td>E</td>
<td>Relative humidity (%) (input data)</td>
</tr>
</tbody>
</table>
| F      | Conversion global radiation from $J/cm^2$ to $W/cm^2$  
         \[ = C2/\text{Penman Monteith}'11SIMP6 \] |
| G      | Max. possible radiation (copied from temporary variables, calculated) |
| H      | $rg/r0 [J/cm^2] = C2/G2$ |

Figure 16: Calculating evaporation according to Penman
3.2.10 Penman/Monteith – EPIC version

The following method is taken from the EPIC-model (version 5.3, Williams et al. 1983, Williams 1995). The whole model and documentation is available via internet (http://www.brc.tamus.edu/epic/). The advantage of the EPIC method is its applicability and parameterization for most agricultural crops. It is implemented in SIMPEL in a way that all single equations are traceable. Dimensions of the original documentation are retained (e.g. kPa instead of hPa).

As the documentation is not accessible offhand like the DVWK-guideline the basic equations are illustrated in more detail in a table together with the formulas.

Simplifications and changes
- atmospheric pressure (eq. 56) and therefore as well the psychrometric constant (eq. 55) are set to a constant (equation 56)
• Albedo for covered soils is not calculated based on biomass but derived from the LAI

For a better understanding of all components of the Penman/Monteith equation they are all displayed in fig. 17 – it is recommended to make a colored printout. It can also be found in bigger size on the CD.

Table 3: Variables and their derivation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Variable and their derivation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input values</strong></td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>Temperature (time series)</td>
</tr>
<tr>
<td>LAI</td>
<td>Leaf area index (time series)</td>
</tr>
<tr>
<td>CO₂</td>
<td>Carbon dioxide level in the atmosphere in ppm (constant, input data)</td>
</tr>
<tr>
<td>V</td>
<td>Daily mean wind speed in m s⁻¹ at 10m height (time series, converted from 2m values)</td>
</tr>
<tr>
<td>PB</td>
<td>Barometric pressure (kPa, constant)</td>
</tr>
</tbody>
</table>
| LAIₜₜ₁ | LAI when soil cover = 1 (constant)  
This value is needed to calculate the Albedo for the surface. EPIC derives the albedo from biomass. As these data is not available in SIMPEL this value is estimated from LAI. |
| RAMX   | Maximum possible solar radiation (time series, calculated in 3.2.1.1) |
| ea     | Saturation vapor pressure (time series) |
| ed     | Vapor pressure (time series) |
| bv     | Coefficient for adjustment – origin is not documented in EPIC, in SIMPEL adopted from the EPIC-parameters |
| p₁     | Parameter ranging from 1.0 to 2 (eq. 71), for calculating crop resistance, coefficient for adjustment – origin not documented |
| CHT    | Crop Height (m), (constant) |
| RA     | Solar radiation in MJ m⁻² (time series, calculated by sunshine duration or measured) |
| VPDₑ   | Threshold vapor pressure deficit (kPa), adopted from EPIC-parameter files |
| g₀     | Leaf conductance |
| ABP    | Albedo plants |
| ABS    | Albedo soil |
| **Calculated values** | |
| VPD    | Vapor pressure difference (kPa) |
| δ      | Slope of saturation vapor pressure curve  
δ = (\( \frac{e_a}{t + 273} \)) ⋅ (\( \frac{6791}{T + 273} \) − 5.03)  (14) |
| γ      | Psychrometer constant, in the model calculated from atmospheric pressure, here set to a constant as atmospheric pressure  
γ = 6.6 ⋅ 10⁻⁴ ⋅ PB  (15) |
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
</table>
| $G$ | Soil heat flux (is given as a formula in the documentation, in the model it is set to 0). \[
G = 0.12 \cdot (\frac{T_i - T_{i-1}}{3} + \frac{T_{i-2} + T_{i-3}}{3}) \] (16) |
| $AD$ | Air density in gm$^{-3}$ \[
AD = 0.01276 \cdot PB \quad 1 + 0.0367 \cdot T \] (17) |
| $FV$ | VPD correction factor \[
FV = 1 - (b_v \cdot (VPD - VPD_s)) > 0.1 \] (18) |
| $g_0^*$ | Leaf conductance in ms$^{-1}$ \[
g_0^* = g_0 \cdot FV \] (19) |
| $SC$ | Soil cover index, differing from the model it is calculated from the LAI \[
SC = \min (1; \frac{LAI}{LAI_{SCI}}) \] (20) |
| $Z0$ | Crop displacement height \[
Z0 = 0.131 \cdot CHT^{0.997} \] (21) |
| $ZD$ | Surface roughness parameter in m \[
ZD = 0.702 \cdot CHT^{0.979} \] (22) |
| $AR$ | Aerodynamic resistance \[
AR = \frac{6.25 \cdot (\ln(\frac{10 - ZD}{Z0}))^2}{V} \quad \text{for unvoered soils} \quad AR = \frac{350}{V} \] (23) |
| $CR$ | Canopy resistance \[
CR = \frac{p_1}{LAI \cdot g_0^* \cdot (1.4 - (0.00121 \cdot CO_2))} \] (24) |
| $HV$ | Latent heat of vaporization in MJkg$^{-1}$ \[
HV = 2.5 - (0.0022 \cdot T) \] (25) |
| $AB$ | Albedo \[
AB = AB_p \cdot (1 - SC) + AB_s \cdot SC \] (26) |
| $RAB$ | Net outgoing long wave radiation in MJm$^{-2}$ for clear days \[
RAB = 4.9 \cdot 10^{-9} \cdot 0.34 - (0.14 \cdot \sqrt{\epsilon_d} \cdot (T + 273))^4 \] (27) |
| $h_0$ | Net radiation in MJm$^{-2}$ \[
h_0 = RA \cdot (1.0 - AB) - RAB \cdot \left(\frac{0.9 \cdot RA}{RAMX} + 0.1\right) \] (28) |
| $E_p$ | Potential Evaporation \[
E_p = \frac{\delta \cdot (h_0 - G) + \frac{86.7 \cdot AD \cdot VPD}{AR}}{HV \cdot (\delta + \gamma \cdot (1 + \frac{CR}{AR}))} \] (29) |
\[HV = 2.5 - (0.0022 \cdot T)\]
\[\delta = \left(\frac{e_a}{T + 273}\right)\left(\frac{6791}{T + 273} - 5.03\right)\]
\[h_{oi} = RA_i \cdot (1.0 - AB_i) - RAB_i \left(\frac{0.9 \cdot RA_j}{RAMX_j} + 0.1\right)\]
\[\gamma = 6.6 \cdot 10^{-4} \cdot PB\]
\[G = 0.12 \cdot \left(T_i - \frac{T_{i-1} + T_{i-2} + T_{i-3}}{3}\right)\]
\[RAB_i = 4.9 \cdot 10^{-9} \cdot 0.34 - (0.14 \cdot \sqrt{e_d}) \cdot (T_i + 273)^4\]
\[f(V) = 2.7 + 1.63 \cdot V\]
\[E_p = \frac{\delta \cdot (h_0 - G) + 86.7 \cdot AD \cdot VPD}{AR} \cdot HV \cdot \left(\delta + \gamma \cdot \left(1 + \frac{CR}{AR}\right)\right)\]
\[AD = \frac{0.01276 \cdot PB}{1 + 0.0367 \cdot T}\]
\[AR = \frac{6.25 \cdot \left(\ln\left(\frac{10 - ZD}{Z0}\right)\right)^2}{V}\]
\[Z0 = 0.131 \cdot CHT^{0.997}\]
\[ZD = 0.702 \cdot CHT^{0.979}\]
\[CR = \frac{P_1}{LAI \cdot g_0^* \cdot (1.4 - (0.00121 \cdot CO_2))}\]
\[g_0^* = g_0 \cdot FV\]
\[FV = 1 - (b_v \cdot (VPD - VPD_i)) \geq 0.1\]

*Figure 17: Derivations of equations for calculating evaporation according to Penman/Monteith (for further explanations refer to tab. 3)*
Table 4: Columns in the spreadsheet (for specifications for equations refer to the EPIC documentation)

<table>
<thead>
<tr>
<th>Column</th>
<th>Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Date (input data)</td>
</tr>
<tr>
<td>B</td>
<td>Wind velocity (input data)</td>
</tr>
<tr>
<td>C</td>
<td>Mean air temperature (input data)</td>
</tr>
<tr>
<td>D</td>
<td>Global radiation in MJ/m² (input data or copied from temporary variable and calculated)</td>
</tr>
<tr>
<td>E</td>
<td>relative humidity (% input data)</td>
</tr>
<tr>
<td>F</td>
<td>LAI (input, interpolated to daily values)</td>
</tr>
<tr>
<td>G</td>
<td>Saturation vapor pressure: ea (kPa, Gl. 25.52), (copied from temporary variable and calculated) =+temp_vars!J2/10</td>
</tr>
<tr>
<td>H</td>
<td>Vapor pressure: ed (kPa, eq. 25.53): =+G2*E2/100</td>
</tr>
<tr>
<td>I</td>
<td>Latent heat of evaporation (MJ/kg, eq. 25.51): =2.5-0.0022*$C2</td>
</tr>
<tr>
<td>J</td>
<td>Slope of saturation vapor pressure curve (eq. 25.54) =+((G2/(C2+273)))*(6791/(C2+273)-5.03)</td>
</tr>
<tr>
<td>K</td>
<td>RAB net outgoing long wave radiation in MJ/m² for clear days =4.9*(10^-9)<em>(0.34-0.14</em>SQRT(H2))*(C2+273)^4</td>
</tr>
<tr>
<td>L</td>
<td>RAMX (adapted from sunshine and converted, eq. 25.60 and 25.61) =+temp_vars!E2/100</td>
</tr>
<tr>
<td>M</td>
<td>AD (air density, eq. 25.67): =0.01276*$AC$13/(1+0.0367*C2)</td>
</tr>
<tr>
<td>N</td>
<td>Crop Height, calculated from maximum height and LAI daily value =+G2/max_lai*crop_height</td>
</tr>
<tr>
<td>O</td>
<td>ZD (eq. 25.69): =0.702*N3^0.979</td>
</tr>
<tr>
<td>P</td>
<td>Z0 (eq. 25.68): =0.131*N3^0.997</td>
</tr>
<tr>
<td>Q</td>
<td>AR (25.67 and 70) aerodynamic resistance, second part of if-condition for times without vegetation =IF(F2&gt;0;6.25*LN((10-O2)/P2))^2/B2;350/B2</td>
</tr>
<tr>
<td>R</td>
<td>VPD (kPa): =+I2-J2</td>
</tr>
<tr>
<td>S</td>
<td>FV (equ. 25.73): =MAX(1-Bv_EQ73*(R2-limit_Vpd);0.1)</td>
</tr>
<tr>
<td>T</td>
<td>g0* (equ. 25.73): =+leaf_conductance*S2</td>
</tr>
<tr>
<td>U</td>
<td>Canopy resistance: =+p1_eq71/F2<em>T2</em>(1,4-0.00121*co2content)</td>
</tr>
<tr>
<td>V</td>
<td>EA (formula soil cover) =1-MIN(1;F2/LAI_full_cover)</td>
</tr>
<tr>
<td>W</td>
<td>Crop albedo: =Albedo*(1-V2)+(albedo_soil*V2)</td>
</tr>
<tr>
<td>X</td>
<td>ho (radiation balance) =+D2*(1-W2)-K2*(0.9*D2/L2+0.1)</td>
</tr>
<tr>
<td>Y</td>
<td>G: soil heat flux (temporarily set to 0 as in the model): 0.00</td>
</tr>
<tr>
<td>Z</td>
<td>Numerator of evaporation formula (eq. 25.65) =+J2*(X2-Y2)+86.7<em>M2</em>R2/Q2</td>
</tr>
<tr>
<td>AA</td>
<td>Denominator of evaporation formula (eq. 25.65) =(I2<em>J2+$AC$14</em>(1+U2/Q2))</td>
</tr>
<tr>
<td>AB</td>
<td>ETp (eq. 25.65) =+Z2/AA2</td>
</tr>
</tbody>
</table>
Fig. 18 shows the static input values from the file `input_evaporation`. They are adopted from the EPIC parameter files and their values have to be copied to the main input area (column A) as seen on the right hand side of the table.

The calculation of evaporation is shown in fig. 19 and 20. The columns correspond to the definitions in tab. 4. Input data are copied to the right hand side of fig. 20 for control.

**Figure 18: Input area static parameter for calculation according to Penman/Monteith**

**Figure 19: Calculation according to Penman/Monteith part one (columns A-X)**
3.2.11 HAUDE

Compared to the previous described methods the HAUDE-evaporation needs different input data:

- relative humidity: $f$ in % at 2pm
- Temperature: $T$ in °C at 2pm
- Haude-coefficient (dependent on crop and month)

$$ET_p = f \cdot (e_{s14} - e_{a14})$$  \hspace{1cm} (30)

The Haude-coefficient $f$ is dependent on the cultured crop and the month. The different coefficients are listed in a table in the spreadsheet (fields I3:N15 in fig. 21).
The coefficients for column C are directly taken from the table for coefficients (J3-N15). Therefore crop (H2) and month (B, is calculated from the date) must be given. Possible values for crops are: “spruce”, “grassland”, “wheat”, “sugar beet” and “corn”. When adding new crops, both the table and the command (column C) have to be extended. The crops have to be put in alphabetical order.

3.3 Soil water model

3.3.1 Leaf interception model

Interception (evaporation of precipitation from leaf surfaces) depends on the abundance of leaves. Therefore it is necessary to obtain the vegetation storage capacity which is usually calculated based on the Leaf Area Index (LAI). In the model this is done by the sub-model LAI_time_series in the “toolbox_evaporation” spreadsheet (Fig. 22). Here daily LAI-values are computed from the irregularly scaled time series of the Leaf Area Index (LAI_time_series) from input_evaporation. Minimum data needed is the start of the growth period, time of maximum LAI and harvest or cutting time.
With the LAI values and maximum capacity given in the input_evaporation-spreadsheet (data input refer to chapter 3.1.1, fig. 5, p. 16) the daily time series of the LAI is calculated by linear interpolation of the irregular time series. The contents of the columns are shown in Table 5.

Table 5: Interpolation of leaf area index (LAI)

<table>
<thead>
<tr>
<th>Column</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Date (adopted from bucket model)</td>
</tr>
<tr>
<td>B</td>
<td>Index: row number from which initial value is transfered</td>
</tr>
<tr>
<td>C</td>
<td>Initial value: lower interpolation value of LAI</td>
</tr>
<tr>
<td>D</td>
<td>Final value: upper interpolation value LAI</td>
</tr>
<tr>
<td>E</td>
<td>Start date: date of lower interpolation value</td>
</tr>
<tr>
<td>F</td>
<td>Finish date: date of upper interpolation value</td>
</tr>
<tr>
<td>G</td>
<td>value: LAI for given date (column A), calculated by linear interpolation with values given in column C and D.</td>
</tr>
</tbody>
</table>

The effective interception capacity (balance sheet bucket_model) is based on LAI and the maximum storage capacity.

3.3.2 Model of the litter layer/surface layer

The uppermost soil compartment is of special interest in ecosystems because it dries faster than the lower layers underneath due to its direct contact with the atmosphere. This is especially important for the litter layer (respectively the O-horizon) in forests which has a different texture than the mineral soil. Different studies showed that the drying of this layer as shown in fig. 24 can be calculated by simple equations. In the model the drying is controlled by the "litter reduction factor" (cell Y14, fig. 7, chapter 3.1.2 on p 19) which specifies the maximum evaporation expressed as part of the water content. Therefore, a factor 2 indicates that within each step of calculation a maximum of half of the storage capacity can evaporate.
The resulting drying curve is displayed in the worksheet “litter” and in fig. 23. In Fig. 24 you can see a measured curve from our own experimental site, a beech forest near Bornhöved in Schleswig-Holstein.

**Figure 23: Desiccation curve litter layer**

**Figure 24: Measured desiccation curve**
3.3.3 Basic soil water model

In the worksheet soil water model the water fluxes in the are calculated based on climate, potential evaporation and soil parameters. The single steps are documented in the following table:

**Table 6: Columns of the bucket model**

<table>
<thead>
<tr>
<th>Column</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Input data</strong></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Date</td>
</tr>
<tr>
<td>B</td>
<td>Precipitation</td>
</tr>
<tr>
<td>C</td>
<td>Evaporation (taken from the “SIMPEL_evaporation” worksheet)</td>
</tr>
<tr>
<td><strong>Leaf interception</strong></td>
<td></td>
</tr>
<tr>
<td>D</td>
<td>Interception storage capacity +MinLAI+[toolbox_evaporation.xls]LAI_time_series!G2*bucket_model!$Y$24</td>
</tr>
<tr>
<td>E</td>
<td>Maximum interception (restricts maximum evaporation from the interception bucket to bucket size or ETp) +MIN(C4;$D4)</td>
</tr>
<tr>
<td>F</td>
<td>Temp. result, water balance: precipitation – evaporation by interception from the leaves +B4-E4</td>
</tr>
<tr>
<td>G</td>
<td>Remaining precipitation, deletes negative precipitation values from column F +MAX(0;F4)</td>
</tr>
<tr>
<td>H</td>
<td>Remaining ETa: passed on to litter layer +MIN(0;F4)+C4-E4</td>
</tr>
<tr>
<td><strong>Litter interception</strong></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>Maximum interception, analog to column E, including function of desiccation. Maximum litter evaporation results from the lower value of the remaining evaporation and (litter bucket content+precipitation)/desiccation factor: +MIN(H4;MIN($Y$11;(K3+G4))/$Y$14)</td>
</tr>
<tr>
<td>J</td>
<td>Water balance: bucket content of previous day + precipitation – interception from bucket: +K3+G4-I4</td>
</tr>
<tr>
<td>K</td>
<td>Contents of litter bucket: +IF(J4&gt;$Y$11;$Y$11;MAX(0;J4))</td>
</tr>
<tr>
<td>L</td>
<td>Remaining precipitation, passed on to soil: +MAX(0;J4-K4)</td>
</tr>
<tr>
<td>M</td>
<td>Remaining ETa, passed on to soil, negative values are cut off: +MIN(0;J4)+H4-I4</td>
</tr>
<tr>
<td><strong>Soil water balance</strong></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>Balance: bucket previous day + precipitation: =R3+L4</td>
</tr>
<tr>
<td>O</td>
<td>Calculation of actual evaporation dependent on the soil bucket (see below) +IF(N4-$Y$19;M4;M4*(N4-$Y$19)/($Y$19-$Y$17))</td>
</tr>
<tr>
<td>P</td>
<td>New Balance: =+N4-O4</td>
</tr>
<tr>
<td>Q</td>
<td>Seepage to groundwater according to Glugla</td>
</tr>
</tbody>
</table>
A basic variable for the soil water model is the soil water content (SWC) at “Start of Reduction” (WC_SR, Cell Y5). This is the point, where soil water becomes limiting and plants cannot transpire at full ETp (ETa-ETp). The values for the linear reduction function decrease from 1 (between starting point of reduction and field capacity) to 0 (at the permanent wilting point) as illustrated in fig. 26.
Because the calculation of $ET_a$ is one of the basic algorithms, we repeat the basic steps (Column O):

\[
\begin{align*}
\text{if } SWC & \geq WC_{SR} \text{ then } ET_a = ET_p \\
\text{if } SWC & < WC_{SR} \text{ then } ET_a = ET_p \times \frac{SWC}{WC_{SR}}
\end{align*}
\]

3.4 Surface Runoff

From summer semester 2003 on SIMPEL is used for the lecture “Hydrological Extremes”, which introduces students to runoff, hydrographs etc. For the practical part of this lecture, SIMPEL is modified to be able to model unit-hydrograph and surface runoff.

Unit-hydrograph (UH) is defined as the specific hydrograph that is generated by 1mm effective precipitation. This effective precipitation is the part of the precipitation remaining for runoff after subtracting interception evaporation. Fig. 27 shows the process: from 1 mm precipitation a hydrograph is produced which (no seepage to deeper layers) should reproduce 1mm total sum of runoff. The hydrograph is specific for a specific area. The calculation of the UH-coefficient is done with statistical methods from single events or longer periods of discharge. The measured runoff is correlated with the delayed effective

Figure 26: Ratio of actual to potential evapotranspiration ($ET_a/ET_p$) dependent on the available soil water content, adopted from ERNSTBERGER 1987.
precipitation of the specific period and a multiple regression is applied. Regression coefficients are the coefficients from the UH (for further information see Dyck 1995 or other textbooks on hydrology).

The calculation of discharge using UH is done according to the following equation:

$$Q_t = k_t \cdot N_t + k_{t-1} \cdot N_{t-1} + k_{t-2} \cdot N_{t-2} + \ldots + k_n \cdot N_{t-n}$$

with

- $Q_t$: discharge at time $t$
- $N_t$: effective precipitation
- $k_i$: coefficient of the unit-hydrograph

The approach implemented in SIMPEL is not a pure UH approach but a combined method! SIMPEL uses the UH approach only for calculation from the surface runoff whereas the original method considers the total runoff. Seepage from groundwater which is roughly equivalent to the base flow in rivers, is always calculated with the soil water model.

The basic steps in the model (see diagram fig. 1) are:

- precipitation falls on the canopy
- calculation of interception
- remaining precipitation falls to the ground and is divided into infiltrating water and surface runoff. The infiltration limit is calculated in column M. It can be a constant value or a function where infiltration depends on the soil water deficit.

Figure 27: Sketch of Unit-Hydrograph
In column V the effective surface runoff is calculated following a simple scheme:

- Bucket overflow is transferred directly to the surface runoff
- Precipitation exceeding the infiltration limit is also transferred to runoff
- Discharge is taken as input for the unit-hydrograph within the worksheet “discharge” and is calculated separately from the soil water.

Calculating steps are in detail (see fig. 28):

**Column M**

*Input of maximum infiltration (fixed value), can be substituted by a function of the soil bucket*

**Column O** (infiltrating precipitation):

\[ = \text{IF}(L4 > M4; M4; L4) \]

If after subtracting interception (L4) precipitation is bigger than maximum infiltration (M4), the infiltrating precipitation (O4) equals maximum infiltration capacity (M4), otherwise it equals precipitation (L4).

**Column V** (surface runoff):

\[ = \text{IF}(S4 > AC17; S4 - AC17 + (L4 - O4); (L4 - O4)) \]

If the balance (S4) is greater than storage capacity of the soil (AC17), surface runoff (V4) equals the difference between soil storage capacity and the balance plus the precipitation that is not infiltrated to the soil (L4 - O4), otherwise surface runoff equals the difference between precipitation underneath the canopy and infiltration to the soil (L4 - O4).

**Figure 28:** Bucket model with separated discharge

3.4.1 Calculating runoff with the unit-hydrograph
The real calculation of the runoff is done in the worksheet “discharge” as shown in fig. 29. Column B contains precipitation, column C surface runoff from the bucket model, column D discharge from the (slower) soil water bucket (seepage to the groundwater). In column E a curve from the surface runoff is calculated from the unit-hydrograph that is shown in the fields G2 to H16. In the cells E2 until E16 the coefficients are built up. From cell E16 on the cell formula can be copied. Columns F and G contain year and month for data analysis in the following worksheets. Actually, the models works with a daily time scale which is quite coarse for flood-modeling where mostly hourly values are used.

3.4.2 Analysis of the discharge hydrograph

Figure 30 shows two approaches to analyze the calculated values. In the upper half frequencies of the discharges and other time series are calculated. Class limits are in column A and can be chosen freely, but have to be arranged ascending. When changing the frequency distribution (cells B2:E13), the tips in the Excel-Help for array/matrix-functions should be noticed. Another possibility for analysis are pivot-tables as shown in the worksheet “discharge_annual” where a annual summary is shown.
3.5 Output

The output of the model contains time series, balances, check values and one graph showing the time series of some variables. It is no problem to define more graphs or pivot-tables. The output in time series are: actual evaporation, interception, discharge and water content for each storage element. Control values and balances are shown in tab. 7.

Table 7: Check values and balances (see fig. 2)

<table>
<thead>
<tr>
<th>Sums/ Totals</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>P</td>
<td>922</td>
<td>Total precipitation</td>
</tr>
<tr>
<td>ETp</td>
<td>484</td>
<td>Total potential evaporation</td>
</tr>
<tr>
<td>ETa</td>
<td>259</td>
<td>Total transpiration and evaporation</td>
</tr>
<tr>
<td>ETa leave</td>
<td>97</td>
<td>Total leaf interception</td>
</tr>
</tbody>
</table>
### 4 Versions of the model

After several requests there are now some variations of the model available. To keep the basic model convenient and usable the other versions are not integrated in it. They are provided in separate versions so nobody has to handle parameters that are not available. The disadvantage for the programmer lies within the administration, documentation and enhancement of multiple versions.

The different available variations are as follows:

- **wetlands**: calculates groundwater level in wetlands as a function of potential evaporation, a reduction from ETp to ETa does not occur
- **four layers with and without free root distribution**: splits the soil bucket into four layers of variable thickness, enables the calculation of flow from and into different horizons
- **linkage with matter flux**: links measured concentrations to the calculated water flows
- **a second wetland version with an accounting procedure for groundwater storage.**

#### 4.1 Four-layer model

The four-layer model was developed for the need of acquiring flows within individual horizons to calculate e.g. matter loads or water content. The basic structure of the model does not differ from the original version. The only difference is the splitting of the soil bucket into several layers.
4.1.1 Water uptake by the roots

The water uptake by the roots can be calculated according to two different algorithms that are available in two different worksheets:

- there is no root profile provided, the simulated soil column is defined as totally rooted, the total amount of water is available for the plants.
- a root profile is provided that regulates the amount of uptake when the water content of the soil is less than that of the start of reduction.

4.1.2 Input parameter

The only difference for the input parameter compared to the original model is that physical soil parameter have to be entered for four horizons (fig. 31). The total depth is summed up and results in the length of the simulated soil column. If calculations are done with root distribution, the fraction of root mass in the soil layer upon the total root mass has to be indicated (row 7 in fig. 31). The value for the last horizon is calculated automatically resulting in a total sum of 1.

![Figure 31: Input for the four-layer model with root distribution](image)

4.1.3 Output
Additional to the output of the one-layer model a worksheet is predefined that lists the simulation results of each horizon (water content, inflow, discharge, evaporation, calculation of soil moisture) in a table and as graph.

![Figure 32: Table of simulation results for each horizon](image)

D:\ms\My Dropbox\simpel\Simpel_English_20120124.odt - 01/25/2012 13:50:46 - 51
4.1.4 Calculation of soil moisture

Figure 33: Graph of simulation results for each horizon
The calculation of the soil water balance for each layer in column N to AN is done analog to the prior explained single bucket:

Initially inflow and potential evaporation are adopted from the upper horizon. Potential evaporation is converted to actual evaporation in dependence to the soil water content (refer to fig. 26). The remaining evaporation (as far as present) is taken to the next horizon. In case of overflow the discharge passes on calculated according to Glugla when WC < FC.

4.1.5 Root extraction

Uptake of the soil water by the plant roots can be simulated with two different methods: with and without given root profile.

4.1.5.1 Without root profile

When there is no root profile given the draining of the soil water bucket takes place top down over the whole soil profile analog to the method when calculating ETa: amounts that are not withdrawn in the actual horizon are passed on to the next layer.

4.1.5.2 With root profile

Is the fraction of roots (standardized to 1, refer to output) given the former explained method is modified. Two cases can be distinguished:
- actual water content >=FC, calculation as shown above
- actual water content <= FC, minimum between (ETa × fraction of roots) and maximum possible withdrawal is taken. This gives a more constant course of the desiccation of the soil. However the sum of ETa does barely change.

The appropriate cell formula (from cell O4) is:
or
If actual water content > WC when reduction starts then
\[ \text{ET}_a = \text{ET}_p \]
otherwise
use the smaller of the following values:
\[ \text{ET}_a = \text{function of soil water content in the original model} \]
\[ \text{ET}_a = \text{potential evaporation} \times \text{root fraction} \]

There are advantages and disadvantages in both methods. Which one of them is better suited cannot be decided yet. Generally, the simulation with root profile produces a more constant desiccation, deeper soil layers are cited earlier to cover water demand.

### 4.2 Wetland with capillary rise

As SIMPEL contains no module for capillary rise the calculation of the water balance from sites affected by groundwater (mires, moist grassland) is not possible, but some simplifications can help. The basic structure of the wetland model is as follows: a one-dimensional extract (soil column) of a wetland is hydrologically made up of pore volume filled with water (aquifer) and an unsaturated zone. Depending on evaporation and precipitation the proportion of the two zones to each other changes as the groundwater table rises and sinks. The discharge to the river depends on the difference of the water level between river and groundwater in the soil column.

#### 4.2.1 Input data

Unlike the basic SIMPEL the following additional values are needed:
- Pore volume to calculate the groundwater content
- Water level of the river (assumed to be a constant)
- Bending factor river indicates which parts of the water level difference can flow from groundwater to the river
- Profile depth of the whole soil (groundwater and unsaturated zone)
- Initial value of the groundwater level

#### 4.2.2 Calculation scheme

The calculation scheme with the relating formulas from column I on is shortly illustrated. Up to column I the basic model is used. Reduction of evaporation does not occur. Thus, \( \text{ET}_a \) always equals \( \text{ET}_p \) so that the calculation of evaporation has got far more significance! Mistakes in the calculation of evaporation are
therefore penetrating the end result without compensation by the soil bucket which often cuts high ETP-values to more realistic ETA-values.

In this case the actual cell is number 4, reference to row 3 therefore mean the value of the day prior to the one calculated. The input area (cells AA etc.) is shown in figure 35.

Table 8: Calculation scheme of the wetland model

<table>
<thead>
<tr>
<th>Column</th>
<th>Formula</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>G4-H4</td>
<td>Water balance of remaining quantities P and ETP</td>
</tr>
<tr>
<td>J</td>
<td>=IF(I4&gt;0; (1-V3)/$AA$12<em>U3/10; V3</em>U3/10/$AA$12)</td>
<td>Defines the maximum intake and release from unsaturated soil bucket</td>
</tr>
<tr>
<td>K</td>
<td>=IF(I4&gt;0; MIN(J4;I4); MAX(J4;I4))</td>
<td>Defines the real intake or release from the soil bucket</td>
</tr>
<tr>
<td>L</td>
<td>=+T3+K4</td>
<td>New content of soil bucket</td>
</tr>
<tr>
<td>M</td>
<td>=+I4-K4</td>
<td>Water balance, adds directly to or from the groundwater</td>
</tr>
<tr>
<td>N</td>
<td>=+Q3+M4</td>
<td>New content groundwater (mm)</td>
</tr>
<tr>
<td>O</td>
<td>=+N4/$AA$3*10</td>
<td>New level groundwater (cm)</td>
</tr>
<tr>
<td>P</td>
<td>=IF(O4+$AA$14; (O4+$AA$14)/10*$AA$22/ $AA$13; 0)</td>
<td>Discharge to river</td>
</tr>
<tr>
<td>Q</td>
<td>=+N4-P4</td>
<td>GW-content reduced by discharge</td>
</tr>
<tr>
<td>R</td>
<td>=+Q4/$AA$3*10</td>
<td>GW-level</td>
</tr>
<tr>
<td>S</td>
<td>=+(R4-R3)/10*$AA$4</td>
<td>Difference GW-level to the day before</td>
</tr>
<tr>
<td>T</td>
<td>=+L4-S4</td>
<td>New soil content (unsaturated zone), assuming that when water level changes soil is filled up to FC</td>
</tr>
<tr>
<td>U</td>
<td>=+$AA$7-R4</td>
<td>Height of unsaturated zone</td>
</tr>
<tr>
<td>V</td>
<td>=((T3/(U3/10))-$AA$5)/ $AA$21</td>
<td>Water content soil column as part of the available WC</td>
</tr>
</tbody>
</table>

Figure 35: Input area wetland model
4.3 Calculation of nutrient loads

The multiple-layer version of the model was extended with a module to calculate fluxes of nutrients. Unlike the other versions LOADS.XLS demands a significantly higher effort for data collection and interpretation. Therefore it is normally only useful for scientific purposes. The additional worksheets are:

- input of concentrations (conc horizon 4),
- calculation of daily values and loads (load horizon 4) and
- the summary in weekly, monthly or yearly values in a pivot-table (pivot horizon 4).

4.3.1 Input data

Additional to the inputs for the model with root distribution the matter concentrations in the soil water (e.g. nitrate) have to be measured. The measurement interval is normally one week, an example is shown in fig. 36. Daily values are generated with linear interpolation (fig. 37)

![Figure 36: Input area for measured loads in leachate](image)
4.3.2 Calculation scheme

For calculating daily values with the dates given the two values closest together with the wanted value in between are searched (column F and G fig. 37). With linear interpolation the value of the actual day is calculated (column H). With this value and the discharge calculated for the horizon the load (column I) can be calculated. The remaining columns (J, K and L) are needed to build weekly, monthly and yearly sums on the basis of a pivot- table (fig. 38).

Figure 37: Interpolation area for measured loads in leachate
4.3.3 Suggestions for modifications

4.3.2.1 Multiple horizons and matter

In most scientific projects not only one substance in one horizon, but several substances in multiple horizons are measured.

To adapt the model for these cases the following steps have to be done:

- selection of the three worksheets for fluxes calculation (Input, Pivot and Load) at the lower boundary
- right mouse button -> Copy -> OK
- if necessary rename and fit the name to the new matter respectively the depth
- enter the new concentrations, new calculations are done automatically
4.3.2.2 Changing interpolation

The linear interpolation of the concentrations in between two measurements is sometimes risky. Another opportunity is not to interpolate but take the values from either D or E. Which method to take depends on the measured concentrations. The following versions are possible:

- punctual values for a particular day (one single sample)
- continuous sampling over the whole timespan
- sampling governed by tension (detracted amount dependent on soil water tension)
- sampling on several days in the timespan

This problem exceeds the aims of this documentation. For more information on this topic you can contact Claus Schimming at the Ecology Center Kiel (claus-s@ecology.uni-kiel.de).

4.4 Wetland with groundwater balance

Northern Germany is a very flat region. When we tried to model a flat catchment (Kielstau, located near Flensburg), we found that the difference between measured and modelled discharge had systematic errors. Fig. 39 shows the two versions and the measured runoff. In autumn, the values of the original version are too high. It seems that there is a systematic error linked to the seasons. To improve the quality of the models we added an additional groundwater storage with an unconventional approach.

![Figure 39: Comparison of measured discharge, original SIMPEL-Version and the wetland version](image)
To optimize the model, we introduced an additional variable, the fraction of wetland. This fraction is characterized by the following characteristics:

- ETa of wetland is always equal to ETp (no reduction)
- if there is not enough available soil water to reach ETp, the needed amount is taken from a separate groundwater storage which gets a negative balance.
- if the ground water balance is negative, percolation from the soil column is not given to the groundwater but is used to fill up the deficit from summer.

Figure 40: Comparison of basic (upper part) and wetland (lower part) version
Table 9: Wetland formulas

<table>
<thead>
<tr>
<th>Col.</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q</td>
<td>$q_4 = \text{IF}($P4&gt;$\text{Start_Reduction};1;($P4-$\text{Perm._Wilting_point})/($\text{Start_Reduction}-\text{Perm._Wilting_point}))$</td>
</tr>
<tr>
<td>P4</td>
<td>Water balance (actual water content)</td>
</tr>
<tr>
<td>X</td>
<td>$=\text{IF}(AE3&gt;0;\text{MIN}(W4*0.9;AE3);0)$</td>
</tr>
<tr>
<td>AB</td>
<td>$=+(W4-X4)+AB3-AC4$</td>
</tr>
<tr>
<td>AC</td>
<td>$=\text{IF}(AB3&gt;0;\text{IF}(AB3*\text{GW_constant}&gt;AB3;AB3;+\text{GW_constant}*(AB3/\text{GW_init_value})^{\text{GW_Power_Coeff.}});0)$</td>
</tr>
<tr>
<td>AD</td>
<td>$=+C4*\text{Wetland_part}*(1-Q4)$</td>
</tr>
<tr>
<td>AE</td>
<td>$=+AE3+AD4-X4$</td>
</tr>
</tbody>
</table>

Figure 41: New input parameters for the wetland model
4.5 Inverse modelling

We normally use in modelling a set of fixed input parameters to fit a measured and modelled data set as close as possible using. For “inverse” modelling, we use modelling as a tool to “measure” input variables. We can e.g. use soil water models to estimate the soil water tension.

4.5.1 Built-In functions for inverse modelling

Excel and other spreadsheets have two functions suitable for inverse modelling: Goal seek and Solver. Goal seeker is a very simple method without limit of the input variables. Solver is more suitable, because you can limit the range of variables. It makes sense e.g. to limit the depth of the root zone to reasonable values between 0.3 and 0.8 m.

4.5.2 Applications

Inverse modelling requires some modifications of the worksheets: you have to define a goal variable and several input variables and their ranges. Because this definition is highly specific, we did not include it in the original worksheets.

As an example, we used the modified wetland spreadsheet from chapter <wetland model>. There are some papers indicating that the evaporation of wetlands is much higher than calculated with conventional evaporation methods. Values in literature are up to 1.3 of potential ETp. We wanted to check these assumptions with an inverse modelling run of the model. As input data for the optimization, we has the modelled and measured discharge. The criterion for optimization was the Nash-Sutcliffe index. In the worksheet, we introduced a new factor for evaporation. A factor for 1.3 would e.g. means that real evaporation is set to 1.3 times the original value. Figure 42 shows the main screen of the solver worksheet. The goal function is the Nash-Sutcliffe index with a goal value of 1. The variables are located in cells h18-h27, the window below contains the boundary conditions, e.g. a root depth between 40 and 100 cm. It is highly advisable to keep the number of the variables as low as possible. First because it extends calculation time and second because the probability of side effects grows higher.

<table>
<thead>
<tr>
<th>Cell</th>
<th>Content</th>
</tr>
</thead>
<tbody>
<tr>
<td>A115</td>
<td>Wetland fraction: Fractions of wetland in the whole catchment (0..1)</td>
</tr>
<tr>
<td>A116</td>
<td>GW storage start: Initial value of storage content in groundwater, serves also as a base line for groundwater calculation</td>
</tr>
<tr>
<td>A117</td>
<td>GW constant:</td>
</tr>
<tr>
<td>A118</td>
<td>GW Power Coeff.</td>
</tr>
</tbody>
</table>
4.6 Quality indicators

Based on a worksheet of Oliver Schmitz (oschmitz@hydrology.unikiel.de)

Whether the approximation of measured and modelled data is good is not a trivial question and depends largely on the goal if the modelling project. Sometimes it is only sufficient to have a correct monthly water balance, sometimes daily flood peaks and extremes are required. An in depth discussion of the problems related to calibration can be found in xxxxx. In practice, several methods are used to compare measured and simulated values. They belong to two classes: comparison of sums and differences and statistical measures like correlation and the Nash-Sutcliffe index. The indicators of the first type are sums and the deviations of single values (Average error, mean square error). They enable a comparison of total amount, but are not very sensitive to deviations in extreme values.

Last not least, a visual comparison of the two data sets is always useful. and can reveal systematic deviations (e.g. seasonal errors) which are not detected with statistical methods.

Figure 42: Optimization of Parameters (xxx replace by english version)
4.6.1 Definitions

The following indicators are calculated:

Average Error:

$$AE = \overline{P} - \overline{O}$$

Nash-Sutcliffe Index (similar to correlation, varies between $-\infty$ and 1):

$$NS = 1 - \frac{\sum_{i=1}^{N} (O_i - P_i)^2}{\sum_{i=1}^{N} (O_i - \overline{O}_i)^2}$$

Root mean square error

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} (P_i - O_i)^2}{N}}$$

Mean absolute error

$$MAE = \frac{\sum_{i=1}^{N} |P_i - O_i|}{N}$$

Other coefficients are either trivial sums or documented elsewhere (see, e.g. the built-in helpfile for information about regression coefficients).

4.6.2 Implementation

The worksheet error.xls can be downloaded from the website. It is prepared to handle one observed and up to ten predicted data sets with up to 10 000 values. If your data set contains more than 10 000 values first select and copy the formulas in the columns Y to AH and add as much rows as you need (up to 55 000) before you insert your data set.

There is no error checking while you are inserting data. So ensure that:

- you only insert data in the columns A to L (column A is only for convenience, not used for calculations)
- your data meets the country's specific settings (corresponding decimal separators)
- no null values or strings occur in your data
- the amount of observed data equals the amount of input data

Figure 44 shows the input section of the worksheet with one column filled with simulated values (column C). The observed values (B) and the date column (A) can be linked to another model, thus it it can be easily
integrated into the SIMPEL system. Figure 43 shows the right side of the worksheet with the results section. Actually, only one column is filled because we just added one column of modelled values.

Figure 43: Input area for error worksheet

Figure 44: Results section of error worksheet
5 Suggestions for education and training

At our institute we have mainly students from geography, agriculture and biology with a weak mathematical background. We do not teach them how to build a model, but how to use a model and how to analyse model results. The introduction to SIMPEL normally takes 1-2 hours, then they have to carry out simple sensitivity analyses and calibration exercises. The following questions can provide the students with several hours of work:

- Sensitivity of soil physical parameters: How does the field capacity influence soil water content (SWC), runoff? You can also create an index of water stress (e.g. days with SWC below a limit).
- Form of hydrograph: prepare two versions, one steep (for sealed surface) one very smooth. Watch the differences in runoff depending on the precipitation
- change the method and threshold value for infiltration into the soil.
- test different crops and formulas for evaporation
- if you have measured runoff/discharge data: let the students calibrate the models, discuss the different results and methods (e.g. same effect by changing different parameters)

6 Literature

6.1 Textbooks


- Good summary of the different evaporation formulas, unfortunately very expensive (250 US-$)


- German standard for calculating evaporation, as well on yearly and monthly basis


- The old FAO worldwide standard


- Basic literature for physical background, many equations!

Recommended, very application oriented book with Lotus/Excel worksheets, most examples are taken from North America


The best German book on this topic, unfortunately out of stock


Regularly new edited handbook, mainly suited for engineers


Old but still sound: Basics in measurement instrumentation, only available in libraries


The best book for people who want to know anything about plants dealing with climate


Highly recommended as reference, unfortunately very expensive!


Basics of heat and water transport in the atmospheric boundary layer


Good overview on most practical problems (measurements, statistics etc.)


Good overview on basics. Not very detailed but extensive. Together with SHAW 1994 best replacement of the more expensive “Handbook of Hydrology”.


Good summary, more ecological than Dyck & Peschke, out of stock


Extensive tutorial on measurements and analysis, UB: U 950 - 519,1 (Part 1), U 950 - 519,2


Better than WMO 1980: contains chapter for discharge measurements, UB 950-168, partition No.: geo 730
6.2 Articles


