Technical document

&

User's guide

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1 Technical description

SIM (Safe Irrigation Management) is a one-dimensional, daily water balance model designed for simulating soil moisture content under specific crop, soil, irrigation management, water quality and climatic conditions. The model contains 4 modules (Figure 1): i) crop water demand and irrigation scheduling module, ii) salinity management module, iii) bacterial movement and risk assessment module and v) nutrient management module. Each module is described hereafter:

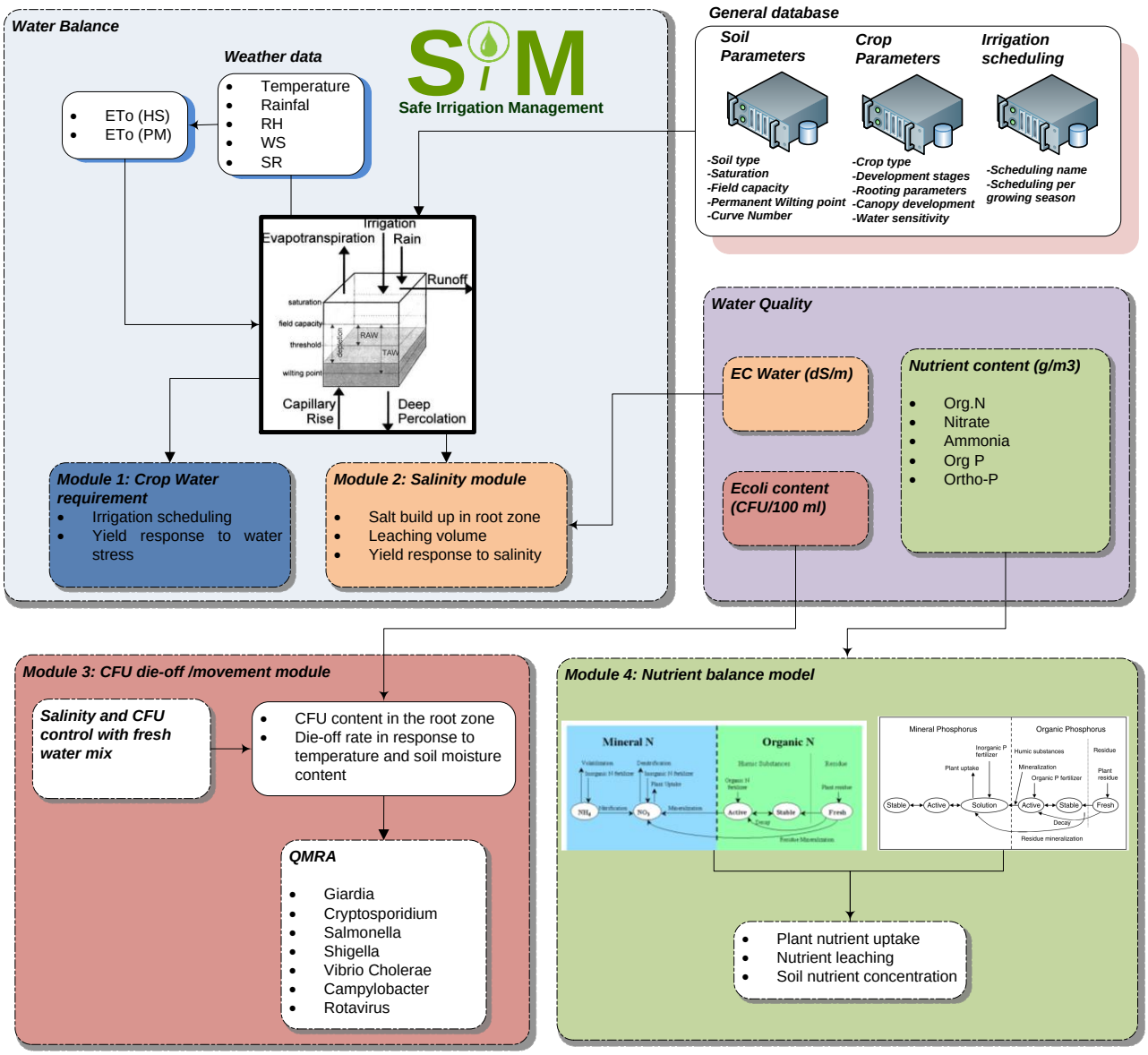


Figure 1 Flowchart summarizing SIM model operation

1.1 Module 1: Crop water demand and irrigation scheduling

SIM model simulates the net water retained in the soil as the difference between inputs (irrigation and precipitation) and outputs (evapotranspiration, runoff and drainage). Therefore, the daily soil water balance is calculated as follows:

$$\delta w = (P_i + I_i) - (Tc_i + Es_i) - (RO_i + dr_i) \qquad (1)$$

Where δw is the daily variation in soil moisture content (mm); P the precipitation (mm) at day i ; I is the water applied by irrigation (mm), T_c is the crop transpiration (mm); Es is the soil evaporation; RO is the runoff (mm) and dr is the volume of water drained below the root zone (mm).

The water balance model within SIM operates with three layers (Figure 2):

i) layer 1: the surface layer (0 – 0.15 m)

ii) layer 2: the active root zone layer (0.15 m – root depth) and

iii) layer 3: the below root zone (root depth – maximum root depth) layer.

Before plant roots reach 0.15 m, layer 2 will have zero thickness. As the plant roots grow, the boundary between layers 2 and 3 changes till reaching the maximum root depth of the crop at which layer 3 thickness become zero.

Soil water moves from upper layers to the one below only when the soil water content of the upper layer exceeds field capacity. When the 3 layers reach the field capacity, any excess of water from precipitation or irrigation will be drained off from the soil profile.

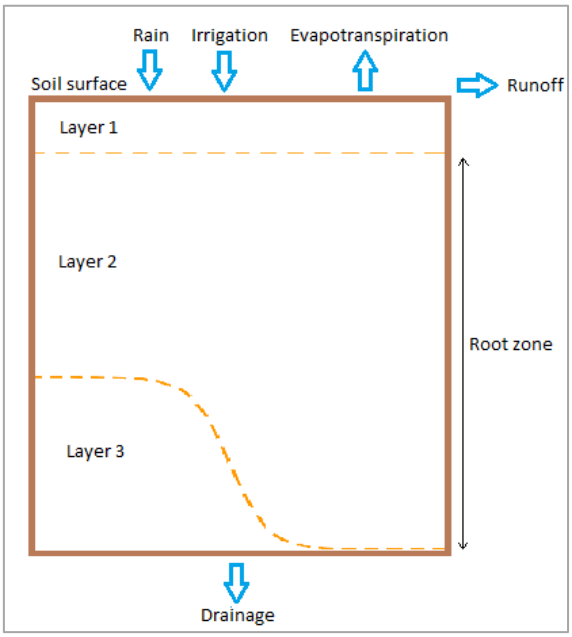


Figure 2: Overview of the soil water balance

Starting from day 1 (planting date), soil water is redistributed (eq. 1) between the three layers taking into consideration crop development stages, the evapotranspiration rate, soil water holding capacity, rainfall intensity and irrigation volume.

1.1.1 Runoff

Surface runoff occurs when rainfall or irrigation water flowing over the soil surface exceed the storage capacity of the soil and therefore its water infiltration capacity. It differs among soil types based on the relative imperviousness and is estimated using the US-SCS curve number method (USDA-SCS, 1972), as follows:

$$RO = \frac{(P - 0.2S)^2}{(P + 0.8S)} \qquad (2)$$

Where *RO* is the daily surface runoff (mm/day); *P* is the gross rainfall (mm/day); and *S* is the maximum storage capacity for the given antecedent moisture conditions (mm) estimated as described by (Hawkins et al., 1985) from the storage at dry antecedent conditions (S_i), the relative saturation (f_s) of the top 15 cm of the soil (layer 1) and two dimensionless weighing factors (W_1 and W_2) .

Hence:

$$S = S_i \times \left(1 - \frac{f_S}{f_S + \exp(W_1 - W_2 f_S)}\right) \quad (3)$$

and

$$f_S = \frac{\theta}{\theta_{sat}} \quad (4)$$

Where θ is the soil water content of the top 15 cm soil layer (layer 1) and θ_{sat} is the soil water content at saturation (mm).

The two dimensionless weighing factors (W_1 and W_2) are calculated from the curve number for dry (CN1), average (CN2) and wet (CN3) antecedent conditions (Hawkins et al., 1985; Ponce and Hawkins, 1996):

$$CN_1 = \frac{CN_2}{2.281 - 0.01281 CN_2} \quad (5)$$

$$CN_3 = \frac{CN_2}{0.427 + 0.00573 CN_2} \quad (6)$$

The corresponding maximum storage conditions for the CN_n is calculated using the following equation:

$$S_n = 250\left(\frac{100}{CN_n} - 1\right) \quad (7)$$

and accordingly,

$$W_1 = ln\left(\frac{1}{1 - {S_3}/{S_2}} - 1\right) + W_2 \quad (8)$$

$$W_2 = 2\left[\ln\left(\frac{0.5}{1 - {S_2}/{S_1}} - 0.5\right) - ln\left(\frac{1}{1 - {S_2}/{S_1}} - 1\right)\right] \quad (9)$$

1.1.2 Soil moisture content

The potential soil water holding capacity (WHC) is defined as the difference between water content at field capacity (θ_{FC}) and wilting point (θ_{PWP}). It is the amount of water that a crop can extract from the root zone, and hence it depends on the type of soil and the rooting depth (*Z*). The total available water (TAW) is calculated as follows:

$$WHC = (\theta_{FC} - \theta_{PWP}) \times 1000 \times Z \quad (10)$$

With WHC expressed in (mm); θ_{FC} *and* θ_{pwp} in ($m^3\ m^{-3}$) and q_{PWP} is the water content at wilting point ($m^3\ m^{-3}$) ; and Z in (m).

The readily available water (RAW) is a fraction of the WHC that can be easily extracted by the roots before the plant experience any water stress condition that might affect crop yield. RAW can be calculated as following:

$$RAW = p \times WHC \qquad (11)$$

Where p (dimensionless) is a crop parameter that corresponds to the fraction of WHC that can be depleted from the root zone before moisture stress occurs. Lower is the p value, more sensitive the crop is to water stress.

1.1.3 Crop development stages

The canopy cover on a particular day is determined by linear interpolation between the dates of the crop development (Emergence dates, 20% cover, maximum cover, maturity and harvest) assigned as input parameters (Figure 3). The daily root growth Δr instead is calculated using the sigmoidal root growth curve (Borg & Grimes, 1986) as following:

$$\Delta r = \left[0.5 + 0.5 \times SIN\left(3.03 \times \left(\frac{t_p}{n}\right) - 1.47\right)\right] \times (r_{max} - r_0) \qquad (12)$$

Where t_p is the number of days after planting (DAP); n is the number of days for maximum root depth (DAP); r_0 is the planting depth (m) and r_{max} is the maximum root depth (m).

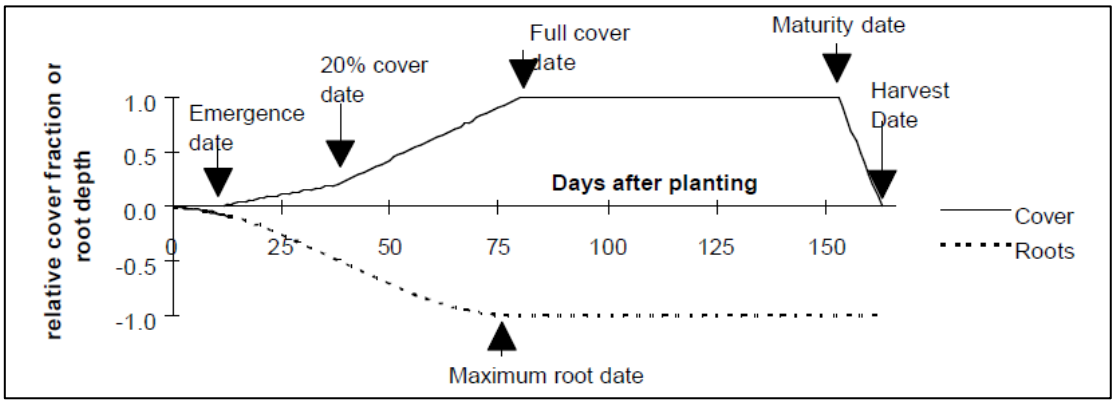


Figure 3 Crop cover and root depth development (source: Hess et al., 2000).

1.1.4 Crop transpiration

The potential crop transpiration (Tr_{max}) on any day (i) is given by:

$$Tr_{max} = ETo_i \times Kc_{max} \times (CC_i / CC_{max}) \qquad (13)$$

Where ETo_i is Reference evapotranspiration (mm. d^{-1}) at day i, Kc_{max} crop coefficient at maximum canopy cover (CC_{max}) and CCi, canopy cover at day i.

The reference evapotranspiration (*ETo*) in SIM model can be calculated using the empirical Hargreaves-Samani (1985) method or the physical FAO Penman-Monteith (Allen et al., 1998) equation depending on the weather data availability.

a) Hargreaves-Samani equation:

$$ET_O = 0.0023 \times (T_{max} - T_{min})^{0.5} \times (T_{med} + 17.8) \times RS \qquad (14)$$

Where T_{max} is the maximum air temperature (°C); T_{min} is the minimum air temperature (°C); T_{med} is the average temperature (°C) and *RS* is the solar radiation calculated from the latitude and expressed in (MJ. $m^{-2}.d^{-1}$).

b) FAO Penman-Monteith equation:

$$ET_o = \frac{0.408 \times \Delta \times (R_n - G) + [\gamma \times \left(\frac{900}{T + 273}\right)] \times u_2 \times (e_S - e_a)}{\Delta + [\gamma \times \left(1 + (0.34 \times u_2)\right)]} \qquad (15)$$

Where ET_o is the reference evapotranspiration (mm.d^{-1}); *Rn* is the net radiation at the crop surface (MJ. $m^{-2}.d^{-1}$); *G* is the soil heat flux density (MJ. $m^{-2}.d^{-1}$); *T* is the mean daily air temperature at 2 m height (°C); u_2 is the wind speed at 2 m height (m/s); e_S is the saturation vapour pressure (kPa); e_a is the actual vapour pressure (kPa); e_S-e_a is the saturation vapour pressure deficit (kPa); Δ is the slope vapour pressure curve (kPa. °C^{-1}) and γ is the psychrometric constant (kPa. °C^{-1}).

The actual plant transpiration (Tr_a) is assumed to occur at potential rate (Tr_{max}) when the soil moisture content (θ) is between the field capacity (θ_{FC}) and the RAW (θ_{RAW}) (Figure 4). For excess of water, it decreases linearly and reaches zero at saturation level (θ_{sat}) (Figure 4). Below θ_{RAW}, water in the soil becomes more bounded to the soil matrix and the plant water uptake will be slowed down linearly to reach zero at the permanent wilting point level (θ_{pwp}).

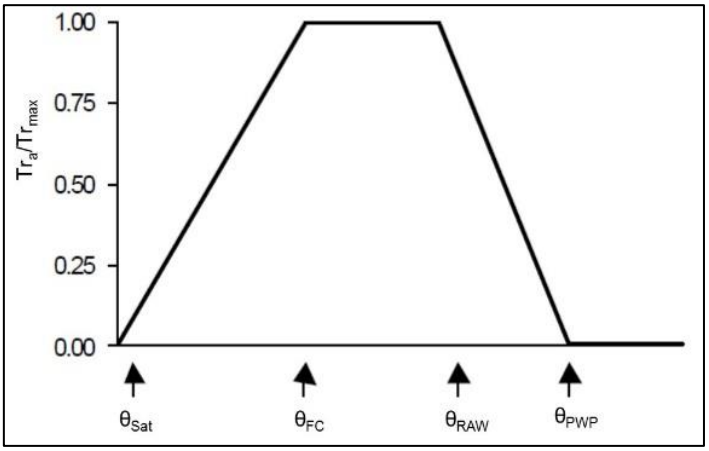


Figure 4 Relative plant transpiration as function of soil water content

1.1.5 Soil evaporation

The potential soil evaporation (*ESo*) at any day *i* occurs whenever water content in the upper 15 cm (layer 1) exceeds the reference evapotranspiration (*ETo*). Under this condition, evaporation from the soil is limited by the atmosphere or climatic conditions. Soil evaporation will then be limited by soil wetness and it slows down gradually till the moisture content in the upper 15 cm soil layer is below the permanent wilting point (PWP).

1.1.6 Water drainage

The water balance module of SIM is a three layers, one dimensional bucket model. The model is limited to the maximum root depth of the plant. Therefore, the drainage water (*dr*) is the volume of water exceeding the holding capacity of the soil at the maximum root depth. It occurs whenever the water input (rainfall / irrigation) exceeds the crop evapotranspiration and the maximum water retention capacity of the soil.

1.1.7 Irrigation management

Irrigation management is very flexible within SIM model. Users can decide to schedule irrigation automatically or apply any volume of water at any given date. For each growing stage (initial/ development / maturity and senescence), SIM user can define the timing and the amount of water to be automatically applied. Irrigation timing can be assigned as:

- Fixed irrigation interval (days)
- Fixed soil moisture deficit (mm)
- Fixed soil water depletion (% of the total WHC)
- No irrigation

Once the irrigation timing is set, users can select the volume of water to be automatically applied as i) fixed amount (mm); ii) return to fixed soil moisture deficit (mm) or iii) return to fixed soil water depletion (% of the total WHC).

Such flexibility in water application is designed to fit the agronomic / economic requirements of any given irrigated plant, technical capacity of the water application system and farmers' irrigation practices.

1.1.8 Yield reduction from water stress

The yield response factor (*Ky*) approach introduced by Doorenboos and Kassam, (1979) was used to estimate the potential yield reduction $\left(1 - \frac{Ya}{Ym}\right)$ from water stress. This approach assumes that water is the only yield limiting factor and is summarized with the following equation:

$$\left(1-\frac{Ya}{Ym}\right)=Ky\left(1-\frac{Tra}{Trmax}\right) \quad (16)$$

Where Y_a and Tr_a correspond to the actual yield and crop transpiration, respectively while Y_m and Tr_{max} are the potential yield and maximum crop transpiration attainable whenever the crop is grown under optimum water supply and stress free conditions.

1.2 Module 2 : Salinity

1.2.1 Salt balance model

Similar to the water balance, the salt model in SIM is a three layers, one dimensional profile. The initial salt content (S_0) in the soil is calculated using the electrical conductivity of the saturation extract (EC_s) at day 1 after planting. The electrical conductivity of the unsaturated soil (EC_e) at day 1 is calculated from the EC_s and from the water content (θ) of the soil compartment at planting date ($\theta = \theta_{FC}$) as following:

$$EC_e = EC_s \frac{\theta_{FC}}{\theta_{sat}} \quad (17)$$

Hence the initial salt content (S_0) is calculated as:

$$S_o = \theta_{FC} \times EC_e \quad (18)$$

Starting from a given salt content in the soil (S_0), the salt input to the system is the irrigation water while salt output is achieved through leaching by drainage water. Accordingly, the mass of salts added by irrigation water (S_I) is calculated as:

$$S_I = I \times EC_I \quad (19)$$

While the salt drained (S_d) from the system is calculated as:

$$S_d = dr \times EC_e \quad (20)$$

Where I is the depth of irrigation water applied (mm), dr is the drainage volume (mm), EC_I is the electrical conductivity of irrigation water (dS.m^{-1}) and EC_e, the electrical conductivity of the soil water (dS.m^{-1}).

Therefore the total salt in the soil (S_T) is calculated as:

$$S_T = S_0 + S_I + S_d \quad (21)$$

and the new ECe is calculated as:

$$EC_e = \frac{S_T}{\theta} \quad (22)$$

1.2.2 Effect of salinity on crop yield

The salinity effect on crop yield (Figure 5) is expressed in yield reduction factor (Y_R) using the approach adopted by Ayers and Westcot, (1989) and based on Maas & Hoffman equation, (1977) as follows:

$$Y_R = 100 - \left(\frac{100}{EC_{max} - EC_{min}}\right)(EC_e - EC_{min}) \qquad (23)$$

Where EC_e is the mean electrical conductivity of the saturated paste extracted from the root zone (dS/m); and EC_{min} is the salinity threshold below which the plant yield is not affected (dS/m) and EC_{max} the maximum electrical conductivity that can be tolerated by the plant (dS/m).

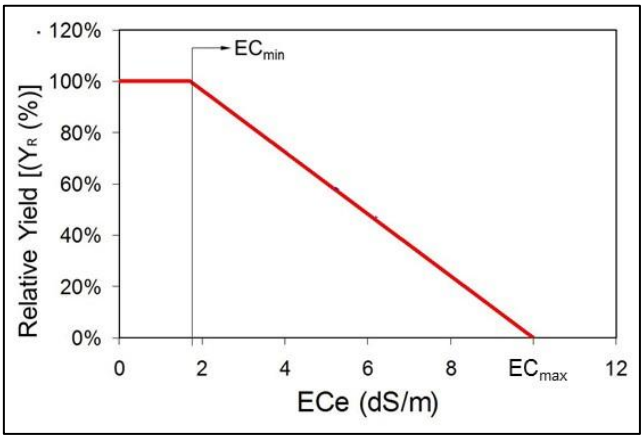


Figure 5 yield reduction as affected by salinity

1.2.3 Salinity management

To avoid the effect of salinity build up in the root zone and consequently yield reduction, SIM users can activate the salinity leaching option. This option will maintain the salinity level in the root zone below the minimum threshold by increasing the volume of water applied to leach the excess of salts by calculating a salt leaching fraction as follows:

$$LF = \frac{S_L}{S_T} \times I \qquad (24)$$

Where LF is the leaching fraction required to leach the mass S_L calculated as follows:

$$S_L = (EC_e - EC_{min}) \times \theta_{sat} \qquad (25)$$

1.3 Module3: Bacterial movement module

SIM was designed to assess crop water requirements with treated wastewater taking into consideration two main parameters: i) water salinity (dS/m) and ii) concentration of *E. coli* (cfu/100 ml).

1.3.1 E. coli die-off

The fecal indicator *Escherichia coli* is subject to die-off and leaching from the soil. *E. coli* die-off is modeled as a first order equation of exponential decay according to Chick's law (Crane & Moore, 1986) as follows:

$$N_t = N_{t-1} \times e^{-kf_T t} \qquad (26)$$

Where Nt is the number of E. coli at time step t (cfu); Nt-1 is the number of E. coli in the previous time step t-1 (cfu) (on day 1, Nt-1 = N0 which is the initial number of E. coli in the soil); k is the decay rate (days); fT is the temperature correction factor (dimensionless) and t is the time step (days). The decay rate k is function of temperature and soil moisture according to a review by Ensink & Fletcher, (2009), as reported in Styczen et al., (2010).

The soil water moisture corresponding to the values of soil moisture retention and factor m was calculated from the soil water retention curve of each soil type. Values of k were interpolated by solving the linear relationships of the die-off rate with soil suction at different temperatures shown in Figure 6 below.

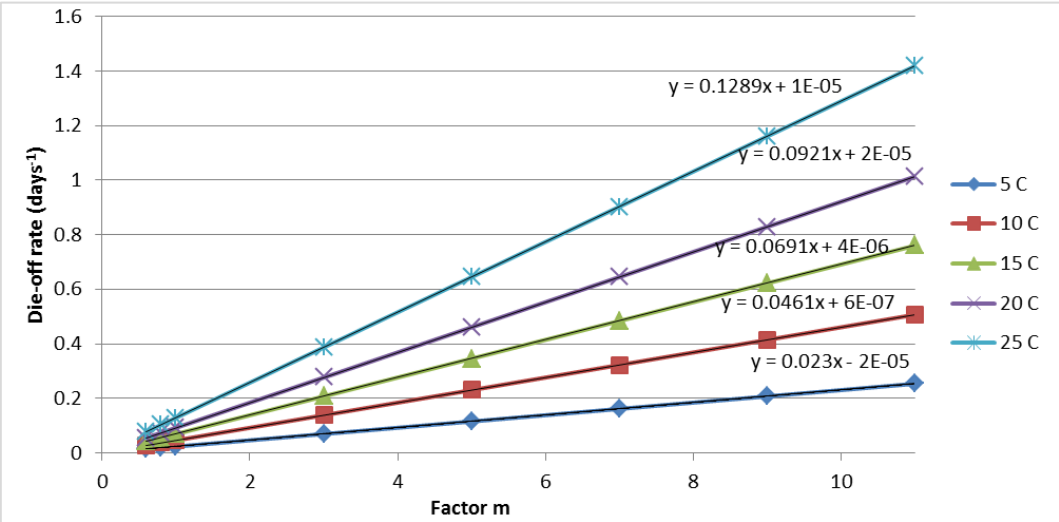


Figure 6 Die-off rate of E. coli as function of temperature and soil moisture content

Where *Soil pF* is the soil moisture retention according to the soil moisture retention curve which gives the relation between soil moisture suction and soil moisture content (dimensionless). Values of f_T were interpolated by solving the linear relationships between temperature and temperature correction factors displayed in

Table 1.

Table 1: Corresponding temperature correction factors (Styczen et al., 2010).

Temp. (°C)	**0**	**5**	**10**	**15**	**20**	**25**
f_T	0	0.25	0.5	0.75	1	1.4

1.3.2 Bacteria leaching from the soil

Leaching of *E. coli* from the root zone occurs with drainage water; therefore the model computes the amount of leached *E. coli* according to three concepts, as follows

- no leaching;
- as proportional to the total volume of drainage water;
- based on a maximum bacterial retention capacity of the soil which is founded on the microbial removal rates as maximum filtration capacity of the soil from the review by Pang, (2009).

1.3.3 Quantitative Microbial Risk Assessment Module

The risk module is based on the estimation of a daily single risk of infection of the exposed farm workers to a selection of pathogens along the growing season of the selected crop. Daily exposure is not limited to the irrigation events since farm workers could be present in the farm at any time to accomplish various and different agricultural practices. The estimation follows the Quantitative Microbial Risk Assessment (QMRA) by Haas et al. (1999) which is based on two mechanistic dose-response models, using fecal coliforms (FC) as indicator. In our case, we used *Escherichia coli* rather than FC as its origin is solely fecal, although we used FC when referring to data based on this parameter as described by Mara et al., (2007). To calculate the risk of infection of a farm worker after the ingestion of a quantity of soil, the dose-response models used were the beta-Poisson model and the exponential model, as follows:

Beta-Poisson dose-response model:

$$P_I(d) = 1 - [1 + \left(\frac{d}{N_{50}}\right) \times \left(2^{\frac{1}{\propto}} - 1\right)]^{-\propto} \qquad (27)$$

Exponential dose-response model:

$$P_I(d) = 1 - \exp\,(-rd) \qquad (28)$$

where PI (d) is the risk of infection of an individual (pppy) exposed to a single pathogen dose d (cfu/g of soil); N50 is the median infective dose (cfu/g of soil); α and r are pathogen infectivity constants (Table 2).

Table 2: Main pathogens infecting humans and the corresponding best-fit dose-response model, median infective dose and infectivity constants.

Pathogen	Best-fit model	N_{50}	α	R	Strain	Response	Reference
Bacteria							
Campylobacter jejuni	beta-Poisson	8.9E+02	1.44E-01	N.A.	A3249	Infection	Black et al., 1988
Salmonella spp.	Beta-Poisson	2.3E+04	3.13E-01	N.A.	Starin I	Infection	Haas et al., 1999
Salmonella Typhi	beta-Poisson	1.11E+06	1.75E-01	N.A.	Quailes	Disease	Hornick et al., 1970
Salmonella anatum	beta-Poisson	3.71E+04	3.18E-01	N.A.	Strain I	Disease	McCullough and Eisele, 1951
Salmonella meleagridis	beta-Poisson	1.68E+04	3.89E-01	N.A.	Strain I	Disease	McCullough and Eisele,1951
Salmonella serotype newport	Exp.	N.A.	N.A.	3.97E-06	newport	Disease	McCullough and Eisele, 1951
Shigella	beta-Poisson	1.48E+03	2.65E-01	N.A.	2457T	Positive stool	DuPont et al., 1972
Viruses		N_{50}	α	R			
Rotavirus	beta-Poisson	6.17E+00	2.53E-01	N.A.	CJN	Infection	Ward et al., 1986
Protozoa		N_{50}	α	R			
Cryptosporidium parvum	Exp.	N.A.	N.A.	0.0042	TAMU isolate	Infection	Haas et al., 1999
Giardia	Exp.	N.A.	N.A.	1.99E-02	From infected human	infection	Rendtorff, 1954

1.3.3.1 The single pathogen dose

The single pathogen dose d to which a farm worker is exposed is expressed as the amount of pathogen colony forming units per gram of soil and is calculated as follows:

$$d = N_1 \times N_P \times S_i \qquad (29)$$

Where d is the single pathogen dose (cfu/g of soil); N1 is the number of *E. coli* present in 1 g of soil; NP is the *E. coli*:pathogen ratio and Si is the quantity of daily ingested soil set by the user (g).

The user can determine the quantity of ingested soil Si and therefore decide the level of advancement of the agricultural practices, where smaller values correspond to mechanized agriculture and therefore industrialized countries and greater values correspond to developing countries or labor-intensive agriculture.

The number of *E. coli* in 1 g of soil is therefore calculated using the soil bulk density as follows:

$$N_1 = \frac{N_t}{Bd \times rmax \times 1000} \qquad (30)$$

Where Nt is the total number of *E. coli* present in the soil at day i (cfu) (subject to die-off and leaching); Bd is the soil bulk density; rmax is the maximum rooting depth (m) and 1000 is a conversion factor.

The QMRA model reads daily *E. coli* data from the '*E. coli* die-off/movement' module and generates a daily infection risk that actually indicates whether the exposed individual is above, below or at the tolerable infection risk for each of the pathogens included in the model. Therefore, and differently from the assumption made by Mara et al., (2007), the QMRA takes into account the die-off of the indicator as die-off of the pathogen when reading N1.

1.3.3.2 Daily tolerable infection risk

SIM calculates a daily threshold infection risk for every pathogen in function of the length of the growing season which determines the exposure of the farm worker in the field. The calculation follows the conversion of the tolerable infection risk to a single event infection risk used in the QMRA (WHO, 1999) to determine the required pathogen reduction. Therefore the daily tolerable (or threshold) infection risk of a pathogen is calculated as follows:

$$P_{th} = 1 - (1 - P_{ATh})^{\frac{[\frac{1}{365}]}{GS}} \qquad (31)$$

Where P_{Th} is the daily threshold of a pathogen (pppd); P_{ATh} is the annual tolerable infection risk (pppy) corresponding to a new DALY of 10^{-4} pppy (Table 3); and *GS* is the length of the growing season of a crop (days).

Table 3: Tolerable annual infection risks (WHO, 2006)

Pathogen	Annual tolerable infection risk (pppy)
Salmonella serotype newport	1.00E-01
Cryptosporidium	2.20E-01
Giardia	1.00E-01
Salmonella	1.00E-01
Schigella	1.00E-01
Campylobacter	3.10E-02
Rotavirus	7.70E-02
Salmonella typhi	1.00E-01
Salmonella anatum	1.00E-01
Salmonella meleagridis	1.00E-01

1.3.4 Risk Control

SIM can mix the wastewater used for irrigation with freshwater to maintain an infection risk target. The user can set a threshold value for *E. coli* content in the root zone. Whenever, the amount of *E. coli* in the irrigation water, calculated from the concentration of *E. coli* and the total irrigation volume, is above this threshold, the control module will calculate the volume of wastewater that would supply the threshold value of *E. coli* content and satisfy the rest of the irrigation need on the same day with freshwater.

1.4 Module4: Nutrient management module

The nutrient management module used in SIM model is the same used by SWAT model and described in details by Neitsh et al., (2005).

1.4.1 Nitrogen cycle

SIM monitors five different pools of nitrogen in the soil. Two pools are inorganic forms of nitrogen, $NH4^{+}$ and $NO3^{-}$, while the other three pools are organic forms of nitrogen. Fresh organic N is associated with crop residue and microbial biomass while the active and stable organic N pools are associated with the soil humus. The organic nitrogen associated with humus is partitioned into two pools to account for the variation in availability of humic substances to mineralization.

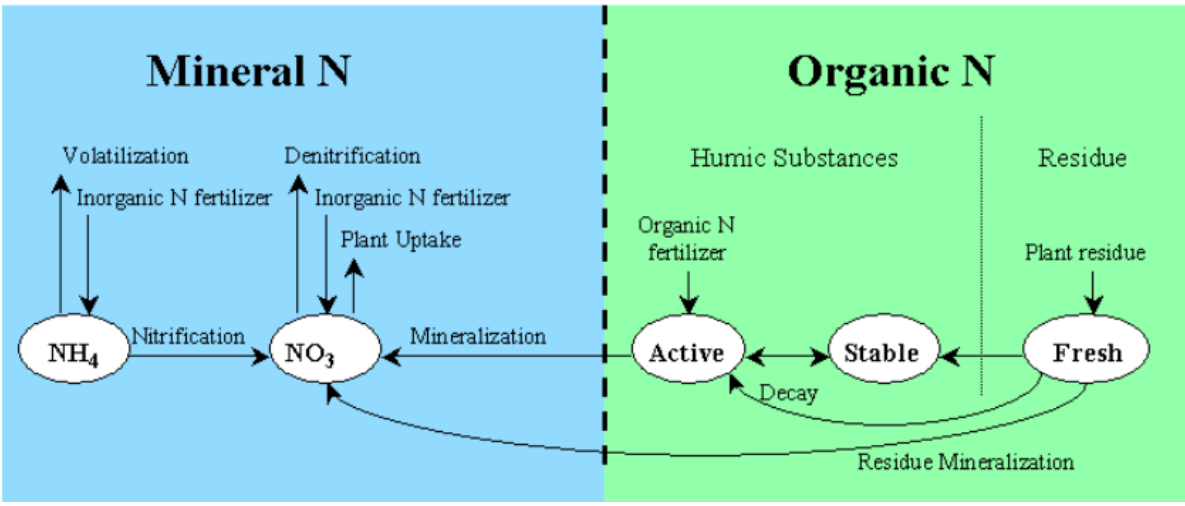


Figure 7: Soil Nitrogen pools as used and modelled by SIM model (adapted from SWAT model, Neitsh et al., 2005)

1.4.1.1 Initialization of soil Nitrogen level

By default, organic nitrogen levels are assigned assuming that the C:N ratio for humic materials is 14:1. The concentration of humic organic nitrogen is calculated as:

$$OrgN_{hum} = 10^4 \left(\frac{OrgC}{14}\right) \tag{32}$$

Where orgNhum is the concentration of humic organic nitrogen in the root zone layer (mg/kg), and orgC is the amount of organic carbon (%). The humic organic N is partitioned between the active and stable pools using the following equations:

$$OrgN_{act} = OrgN_{hum} \,.\, fr_{actN} \tag{33}$$

$$OrgN_{sta} = OrgN_{hum} \,.(1 - fr_{actN}) \tag{34}$$

Where $OrgN_{act}$ is the concentration of nitrogen in the active organic pool (kg/ha), $OrgN_{hum}$ is the concentration of humic organic nitrogen in the layer (kg/ha), fr_{actN} is the fraction of humic nitrogen in the active pool, and $OrgN_{sta}$ is the concentration of nitrogen in the stable organic pool (kg/ha). By default, the fraction of humic nitrogen in the active pool, fr_{actN}, is set to 0.02.

Nitrogen in the fresh organic pool is set to zero in all layers except the top 10 mm of soil. In the top 10 mm, the fresh organic nitrogen pool is set to 0.15% of the initial amount of residue on the soil surface.

$$OrgN_{frsh} = 0.0015.\ rsd_{surf} \tag{35}$$

Where $OrgN_{frsh}$ is the nitrogen in the fresh organic pool in the top 10 mm (kg N/ha), and rsd_{surf} is material in the residue pool for the top 10 mm of soil (kg/ha).

1.4.1.2 Mineralization/Decomposition/Immobilization

Mineralization is the microbial conversion of organic, plant- unavailable nitrogen to inorganic, plant-available nitrogen. Decomposition is the breakdown of fresh organic residue into simpler organic components. Immobilization is the microbial conversion of plant-available inorganic soil nitrogen to plant- unavailable organic nitrogen.

Bacteria decompose organic material to obtain energy for growth processes. Plant residue is broken down into glucose which is then converted to energy. If the residue from which the glucose is obtained contains enough nitrogen, the bacteria will use nitrogen from the organic material to meet the demand for protein synthesis. If the nitrogen content of the residue is too low to meet the bacterial demand for nitrogen, the bacteria will use $NH4^+$ and $NO3^-$ from the soil solution to meet its needs. If the nitrogen content of the residue exceeds the bacterial demand for nitrogen, the bacterial will release the excess nitrogen into soil solution as $NH4^+$.

A general relationship between C:N ratio and mineralization/immobilization is:

C:N > 30:1 immobilization occurs, a net decrease in soil $NH4^+$ and $NO3^-$

20:1 ≤ C:N ≤ 30:1 expect no net change; immobilization and mineralization are at equilibrium

C:N < 20:1 mineralization occurs, a net gain in soil $NH4^+$ and $NO3^-$

Two sources are considered for mineralization: the fresh organic N pool associated with crop residue and microbial biomass and the active organic N pool associated with soil humus. Mineralization and decomposition are allowed to occur only if soil temperature is above 0°C. Mineralization and decomposition are dependent on water availability and soil temperature (T_{soil}). Two factors are used in the mineralization and decomposition equations to account for the impact of temperature and water on these processes. The nutrient cycling temperature factor γ_{tmp} is calculated:

$$\gamma_{tmp} = 0.9.\frac{T_{soil}}{T_{soil} + exp(9.93 - 0.312.T_{soil})} + 0.1 \tag{36}$$

While nutrient cycling water factor γ_{SW} is calculated:

$$\gamma_{SW} = \frac{SW}{FC} \tag{37}$$

Where SW is the soil water content on a given day, and FC is the water content at field capacity.

1.4.1.3 Humus mineralization

Nitrogen is allowed to move between the active and stable organic pools in the humus fraction. The amount of nitrogen transferred from one pool to the other is calculated:

$$N_{trns} = \beta_{trns}.OrgN_{act}.\left(\frac{1}{fr_{actN}} - 1\right).OrgN_{sta} \tag{38}$$

N_{trns} is the amount of nitrogen transferred between the active and stable organic pools (kg N/ha), β_{trns} is the rate constant (1×10^{-5}), $OrgN_{act}$ is the amount of nitrogen in the active organic pool (kg N/ha), fr_{actN} is the fraction of humic nitrogen in the active pool (0.02), and $OrgN_{sta}$ is the amount of nitrogen in the stable organic pool (kg N/ha). When N_{trns} is positive, nitrogen is moving from the active organic pool to the stable organic pool. When N_{trns} is negative, nitrogen is moving from the stable organic pool to the active organic pool.

Mineralization from the humus active organic N pool is calculated:

$$N_{mina} = \beta_{min}.\left(\gamma_{tmp}.\gamma_{SW}\right)^{0.5}.OrgN_{act} \tag{39}$$

where N_{mina} is the nitrogen mineralized from the humus active organic N pool (kg N/ha), β_{min} is the rate coefficient for mineralization of the humus active organic nutrients, γ_{tmp} is the nutrient cycling temperature factor, γ_{SW} is the nutrient cycling water factor, $OrgN_{act}$ is the amount of nitrogen in the active organic pool (kg N/ha). Nitrogen mineralized from the humus active organic pool is added to the nitrate pool in the layer.

1.4.1.4 Residue decomposition and mineralization

Decomposition and mineralization of the fresh organic nitrogen pool is allowed only in the top soil layer. Decomposition and mineralization are controlled by a decay rate constant that is updated daily. The decay rate constant is calculated as a function of the C:N ratio and C:P ratio of the residue, temperature and soil water content.

The C:N ratio of the residue $\varepsilon_{C:N}$ is calculated:

$$\varepsilon_{C:N} = \frac{0.58.rsd}{OrgN_{frsh}+NO3} \tag{40}$$

where rsd is the residue in the top soil layer (kg/ha), 0.58 is the fraction of residue that is carbon, orgNfrsh is the nitrogen in the fresh organic pool (kg N/ha), and NO3 is the amount of nitrate in the soil (kg N/ha).

The C:P ratio of the residue $\varepsilon_{C:P}$ is calculated:

$$\varepsilon_{C:P} = \frac{0.58.rsd}{OrgP_{frsh}+P_{solution}} \quad (41)$$

Where $OrgP_{frsh}$ is the phosphorus in the fresh organic pool (kg P/ha), and Psolution is the amount of phosphorus in soil solution (kg P/ha). The decay rate constant δ_{ntr} defines the fraction of residue that is decomposed and is calculated:

$$\delta_{ntr} = \beta_{rsd}.\gamma_{ntr}.\left(\gamma_{tmp}.\gamma_{SW}\right)^{0.5} \quad (42)$$

Where $\beta_{rsd}$is the rate coefficient for mineralization of the residue fresh organic nutrients, γ_{ntr} is the nutrient cycling residue composition factor, γ_{tmp} is the nutrient cycling temperature factor, γ_{SW} is the nutrient cycling water factor.

The nutrient cycling residue composition factor γ_{ntr} is calculated:

$$\gamma_{ntr} = min\begin{Bmatrix} exp\left[-0.693.\left(\frac{\varepsilon_{C:N}-25}{25}\right)\right] \\ exp\left[-0.693.\left(\frac{\varepsilon_{C:P}-200}{200}\right)\right] \\ 1.0 \end{Bmatrix} \quad (43)$$

The nitrogen mineralized (mineralization) from the fresh organic N pool (kg N/ha).l is then calculated:

$$N_{minf} = 0.8.\ \delta_{ntr} \cdot OrgN_{frsh} \quad (44)$$

The nitrogen decomposed (decomposition) from the fresh organic N pool (kg N/ha)is calculated:

$$N_{dec} = 0.2.\ \delta_{ntr} \cdot OrgN_{frsh} \quad (45)$$

1.4.1.5 Nitrification and ammonia volatilization

Nitrification is the two-step bacterial oxidation of $NH4^+$ to $NO3^-$ while ammonia volatilization is the gaseous loss of ammonium, $NH4^+$ in the form of NH_3. The total amount of nitrification and ammonia volatilization is calculated in SIM and then partitioned between the two processes. Nitrification is a function of soil temperature and soil water content while ammonia volatilization is a function of soil temperature, depth and cation exchange capacity.

Four coefficients are used in the nitrification/volatilization algorithms to account for the impact of these parameters. Nitrification/volatilization occurs only when soil temperature T_{soil} exceeds 5°C. The nitrification/volatilization temperature factor η_{tmp} is calculated:

$$\eta_{tmp} = 0.41.\frac{(T_{soil}-5)}{10} \quad (46)$$

The nitrification soil water factor η_{sw} is calculated:

$$\eta_{sw} = \frac{(SW-WP)}{0.25.(FC-WP)} \quad \text{if} \quad SW<0.25.FC-0.75.WP \quad (47)$$

$$\eta_{sw} = 1 \qquad \text{if} \qquad SW \geq 0.25.FC - 0.75.WP \tag{48}$$

where SW is the soil water content on a given day (mm), WP is the amount of water at wilting point water content (mm), and FC is the amount of water at field capacity water content (mm).

The volatilization depth factor η_{midZ} is calculated:

$$\eta_{midZ} = 1 - \frac{Z_{mid}}{Z_{mid} + \exp(4.706 - 0.0305.Z_{mid})} \tag{49}$$

Where Z_{mid} is the depth from the soil surface to the middle of the layer (mm). SIM does not require the user to provide information about soil cation exchange capacity. The volatilization cation exchange factor η_{CEC} is set to a constant value 0.15.

The impact of environmental factors on nitrification and ammonia volatilization is defined by the nitrification regulator η_{nit} and volatilization η_{vol} regulator calculated as following:

$$\eta_{nit} = \eta_{tmp}.\eta_{sw} \tag{50}$$

$$\eta_{vol} = \eta_{tmp}.\eta_{midZ}.\eta_{CEC} \tag{51}$$

The total amount of ammonium lost to nitrification and volatilization is calculated using a first-order kinetic rate equation (Reddy et al., 1979):

$$N_{nit/vol} = NH4.(1 - exp[-\eta_{nit} - \eta_{vol}] \tag{52}$$

where Nnit/vol is the amount of ammonium converted via nitrification and volatilization (kg N/ha), NH4 is the amount of ammonium in soil layer (kg N/ha),η_{nit} is the nitrification regulator, and η_{vol} is the volatilization regulator.

To partition Nnit/vol between nitrification and volatilization, the estimated fraction of nitrogen lost by nitrification fr_{nit} and by volatilization fr_{vol} are calculated as following:

$$fr_{nit} = 1 - \exp(-\eta_{nit}) \tag{53}$$

$$fr_{vol} = 1 - \exp(-\eta_{vol}) \tag{53}$$

The amount of nitrogen removed from the ammonium pool by nitrification N_{nit} is then calculated:

$$N_{nit} = \frac{fr_{nit}}{(fr_{nit} + fr_{vol})}.N_{nit/vol} \tag{54}$$

and the amount of nitrogen removed from the ammonium pool by volatilization is:

$$N_{vol} = \frac{fr_{vol}}{(fr_{nit}+fr_{vol})} . N_{nit/vol} \tag{55}$$

Hence N_{nit} is the amount of nitrogen converted from $NH4^+$ to $NO3^-$ (kg N/ha), N_{vol} is the amount of nitrogen converted from $NH4^+$ to NH3 (kgN/ha), fr_{nit} is the estimated fraction of nitrogen lost by nitrification, fr_{vol} is the estimated fraction of nitrogen lost by volatilization, and $N_{nit/vol}$ is the amount of ammonium converted via nitrification and volatilization (kg N/ha).

1.4.1.6 Denitrification

Denitrification is the bacterial reduction of nitrate, $NO3^-$ to N2 or N2O gases under anaerobic (reduced) conditions. Denitrification is a function of water content, temperature, presence of a carbon source and nitrate. In general, when the water-filled porosity is greater than 60% denitrification will be observed in a soil. SIM determines the amount of nitrate lost to denitrification N_{denit} with the following equation:

$$N_{denit} = NO3.(1 - exp[-\beta_{denit} . \gamma_{tmp}. OrgC] \quad \text{if} \quad \gamma_{SW} \geq \gamma_{SW,th} \tag{56}$$

$$N_{denit} = 0.0 \quad \text{if} \quad \gamma_{SW} < \gamma_{SW,th} \tag{57}$$

Where NO3 is the amount of nitrate in the soil (kg N/ha), β_{denit} is the rate coefficient for denitrification, orgC is the amount of organic carbon in the soil layer (%), and $\gamma_{sw,thr}$ is the threshold value of nutrient cycling water factor for denitrification to occur.

1.4.1.7 Leaching and plant uptake

Because retention of nitrate by soils is minimal, nitrate is very susceptible to leaching. The quantity of nitrate leached in SIM is directly proportional to the volume of water lost by deep percolation and to the nitrate concentration in the soil layer. Nutrient uptake instead was directly related to the volume of water transpired by the plant and the NO3 concentration in the soil layer.

1.4.2 Phosphorous cycle

SIM monitors six different pools of phosphorus in the soil (Figure 8). Three pools are inorganic forms of phosphorus while the other three pools are organic forms of phosphorus. Fresh organic P is associated with crop residue and microbial biomass while the active and stable organic P pools are associated with the soil humus. The organic phosphorus associated with humus is partitioned into two pools to account for the variation in availability of humic substances to mineralization. Soil inorganic

P is divided into solution, active, and stable pools. The solution pool is in rapid equilibrium (several days or weeks) with the active pool. The active pool is in slow equilibrium with the stable pool.

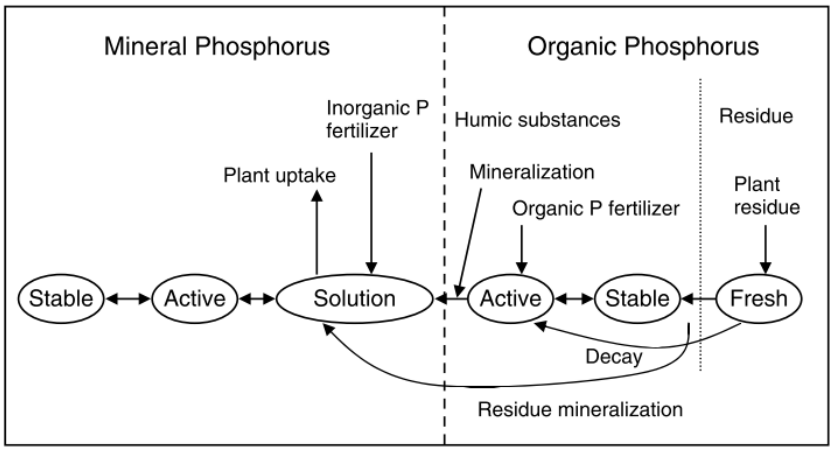


Figure 8: Soil phosphorous pools as used and modelled by SIM model (adapted from SWAT model, Neitsh et al., 2005)

1.4.2.1 Initialization of soil phosphorous level

Users must define the amount of soluble P ($P_{solution}$) at the beginning of the simulation. Accordingly, the concentration of phosphorus in the active mineral pool ($minP_{act}$) is calculated using the phosphorous availability index (*pai*) as following (Jones et al., 1984):

$$minP_{act} = P_{solution} \cdot \frac{1-pai}{pai} \tag{58}$$

The concentration of phosphorus in the stable mineral pool (*minPsta*) is initialized to (Jones et al., 1984):

$$minP_{sta} = 4.\, minP_{act} \tag{59}$$

By default, the organic phosphorus levels are assigned assuming that the N:P ratio for humic materials is 8:1. The concentration of humic organic phosphorus ($OrgP_{hum}$) in the soil is calculated:

$$OrgPhum = 0.125 \cdot OrgN_{hum} \tag{60}$$

where OrgNhum is the concentration of humic organic nitrogen in the soil (Kg/ha). In the top 10 mm, the fresh organic phosphorus pool ($OrgP_{frsh}$) is set to 0.03% of the initial amount of fresh residue (rsd_{surf}) on the top 10 mm soil layer.

$$OrgP_{frsh} = 0.0003.\ rsd_{surf} \tag{61}$$

1.4.2.2 Mineralization/decomposition and immobilization

The phosphorus mineralization algorithms developed by Jones et al. (1984) are similar in structure to the nitrogen mineralization algorithms. Two sources are considered for mineralization: the fresh organic P pool ($OrgP_{frsh}$) associated with crop residue and microbial biomass and the active organic P pool ($OrgP_{act}$) associated with soil humus. Mineralization and decomposition are allowed to occur only if the temperature of the soil layer is above 0°C. Mineralization and decomposition are dependent on water availability and temperature. Two factors are used in the mineralization and decomposition equations to account for the impact of temperature and water on these processes. The nutrient cycling temperature factor (γ_{tmp})and the nutrient cycling water factor (γ_{SW}) described in equation 36 and 37 respectively.

Phosphorus in the humus fraction ($OrgP_{hum}$) is partitioned between the active ($OrgP_{act}$) and stable ($OrgP_{sta}$) organic pools using the ratio of humus active organic N to stable organic N. The amount of phosphorus in the active and stable organic pools is calculated:

$$OrgP_{act} = OrgP_{hum} \cdot \frac{OrgN_{act}}{OrgN_{act} + OrgN_{sta}} \quad (62)$$

$$OrgP_{sta} = OrgP_{hum} \cdot \frac{OrgN_{sta}}{OrgN_{act} + OrgN_{sta}} \quad (63)$$

Where $OrgN_{act}$ is the amount of nitrogen in the active organic pool (kg N/ha), and $OrgN_{sta}$ is the amount of nitrogen in the stable organic pool (kg N/ha). Mineralization from the humus active organic P (P_{min}) pool is calculated:

$$P_{min} = 1.4 . \beta_{min} . \left(\gamma_{tmp} . \gamma_{SW}\right)^{0.5} . OrgP_{act} \quad (64)$$

Where $\beta_{min}$is the rate coefficient for mineralization of the humus active organic nutrients, γ_{ntr} is the nutrient cycling residue composition factor, γ_{tmp} is the nutrient cycling temperature factor, γ_{SW} is the nutrient cycling water factor and $OrgP_{act}$ is the amount of phosphorus in the active organic pool (kg P/ha). Phosphorus mineralized from the humus active organic pool is added to the solution P ($P_{solution}$) pool.

Mineralization from the residue fresh organic P pool (P_{minf}) is calculated as:

$$P_{minf,} = 0.8 . \delta ntr \cdot OrgP_{frsh} \quad (65)$$

where P_{minf} is the phosphorus mineralized from the fresh organic P pool (kg P/ha), δntr is the residue decay rate constant (equ.42) , and orgPfrsh is the phosphorus in the fresh organic pool (kg P/ha). Phosphorus mineralized from the fresh organic pool is added to the solution P pool.

Decomposition from the residue fresh organic P pool (P_{dec})is calculated:

$$P_{minf,} = 0.2 . \delta ntr \cdot OrgP_{frsh} \quad (65)$$

Phosphorus decomposed from the fresh organic pool is added to the humus organic pool.

1.4.2.3 Sorption of inorganic phosphorous

Equilibration between the solution ($P_{solution}$) and active mineral pool ($minP_{act}$) is governed by the phosphorus availability index (pai) as following:

$$P_{sol/act} = P_{solution} - minP_{act}.\left(\frac{pai}{1-pai}\right) \quad \text{if} \quad P_{solution} > minP_{act}.\left(\frac{pai}{1-pai}\right) \tag{66}$$

$$P_{sol/act} = 0.1.\left(P_{solution} - minP_{act}.\left(\frac{pai}{1-pai}\right)\right) \quad \text{if} \quad P_{solution} < minP_{act}.\left(\frac{pai}{1-pai}\right) \tag{67}$$

where $P_{sol/act}$ is the amount of phosphorus transferred between the soluble and active mineral pool (kg P/ha). When $P_{sol/act}$ is positive, phosphorus is being transferred from solution to the active mineral pool. When $P_{sol/act}$ is negative, phosphorus is being transferred from the active mineral pool to solution. At equilibrium, SIM assumes that the stable mineral pool is 4 times the size of the active mineral pool. When not in equilibrium, the movement of phosphorus between the active ($minP_{act}$) and stable mineral ($minP_{sta}$) pools is governed by the equations:

$$P_{act/sta} = \beta_{eqP}.(4.minP_{act} - minP_{sta}) \quad \text{if} \quad minP_{sta} < 4.minP_{act} \tag{68}$$

$$P_{act/sta} = 0.1.\beta_{eqP}.(4.minP_{act} - minP_{sta}) \quad \text{if} \quad minP_{sta} > 4.minP_{act} \tag{69}$$

where $P_{act/sta}$ is the amount of phosphorus transferred between the active and stable mineral pools (kg P/ha) and β_{eqP} is the slow equilibration rate constant (0.0006d^{-1}). When $P_{act/sta}$ is positive, phosphorus is being transferred from the active mineral pool to the stable mineral pool. When $P_{act/sta}$ is negative, phosphorus is being transferred from the stable mineral pool to the active mineral pool.

2 Software requirements

SIM was developed in VB.net to operate on windows 64 bit machines. Microsoft office must also be installed on the machine since climate and results data can be imported / exported only in excel .xlsx spreadsheet format. Also, crop, soil and irrigation management files are all stored in a Microsoft access database **.mdb**.

Note that SIM is designed to operate with **.** and **,** as decimal and thousand separators respectively.

In latin languages operating systems (i.e. French, Italian…)/ office packages, the **,** is used by default as decimal separator. In such case 2,3 used by the user for example will be read by SIM as 2300 and not 2.3. To avoid such error, ensure that the number format settings in both your PC and your excel files have **.** as decimal separator.

3 Installation

To install SIM:

1. Select **Run** from the Windows Start menu
2. Enter the full path and name of the "**SetupSIM.exe**" file or click the browse button to locate it on your computer
3. Click the **OK** button to begin the setup process.

The setup program will ask you to choose a folder where SIM software will be placed. The default folder is ***C:\ SIM***. Once the installation of SIM is successful, a new item named ***SIM*** will be added to your windows ***Start Menu*** and a shortcut with SIM logo will also be placed on your desktop. To launch SIM you can select ***SIM*** from the ***Start Menu*** or by simply clicking the SIM shortcut on your desktop.

Should you wish to remove SIM from your computer?

1. Go to **Control Panel**
2. Select **Programs and Features**
3. Double-click on the **Add/Remove** Programs item.
4. Select **SIM** from the list of programs that appears.

Click the **Add/Remove** button.

4 Get Started

Launch SIM from the Start Menu or simply click the SIM shortcut on your desktop. The main window will show 7 tab pages (**Errore. L'origine riferimento non è stata trovata.**):

- ***Climate*** tab where user must import/create his weather parameters needed to run the model
- ***Crop*** tab is the interface between the user and the crop database
- ***Soil*** tab is the interface between the user and the soil database
- ***Irrigation management*** tab is necessary to identify for the four growing stages of the plant , the adopted irrigation management
- ***Settings tab*** allows the user to assign the initial soil and water quality conditions and to select the models to be used (automatic or assigned irrigation, salinity and/or nutrient and/or biological contamination management),
- ***Results tab***
- ***QMRA (Quantitative Microbial Risk Assessment)*** tab where the daily risk assessment for different pathogens is performed

4.1 Climate

In SIM, climate data must be imported from Microsoft Excel® file (.xlsx). On an Excel spreasdsheet, use the first row for the column name (i.e. day, month, year, rain, Tmin...) and ensure that the historical climate data covers the entire length of the growing season. Note that this version of SIM model do not perform multi-year analysis.

Before you import your climate file select from the dropdown list the method you want to calculate the reference evapotranspiration (ETo) (Figure 9). Users have three options to select from:

- ✓ ETo calculated with the empirical formula of Hargreaves Samani (1985) (Equ. 14)
- ✓ ETo calculated with Penman-Monteith equation (Allen et al., 1998) (Equ.15)
- ✓ ETo imported directly from the .xlsx climate file

For the first two options (ETo to be calculated by SIM), users must assign also the field latitude (i.e. 35.6) in the appropriate box. Depending on the ETo option previously selected, the scroll bars of the required parameters will be activated. Tmin and Tmax are the only two parameters required for Hargreaves-Samani (equ.14). Penman-Monteith equation (equ.15) instead requires in addition to Hargreaves-Samani parameters land elevation (m.a.s.l.), relative humidity (%), sunshine hours (h) and wind speed (m/s).

Use the active scroll bars (Figure 9) and assign for each parameter the column number as in your .xlsx climate file. For example if you assign number 4 using the scroll bar of Tmax, you are telling SIM that the fourth coulmn on your xlsx file correspond to the Tmax value. Date in the excel file must be separated in three columns (day, month and year). The month must be written in a numerical format (i.e. 9 for July).

Once the ETo method is selected and all the required parameters are allocated based on their column number, click on the add file button and browse to your .xlsx climate file to be imported (Figure 9). Once the file is imported, the table under ***Climate*** tab will be populated and users can add new records using the add row button or can remove an existing record by clicking on the remove row button. User can also edit any record directly from the table. By clicking on the calculate ETo button , the ETo column will be populated depending on the ETo method previously selected from the dropdown list. User can also export back the modified table into a new .xlsx climate file using the save button .

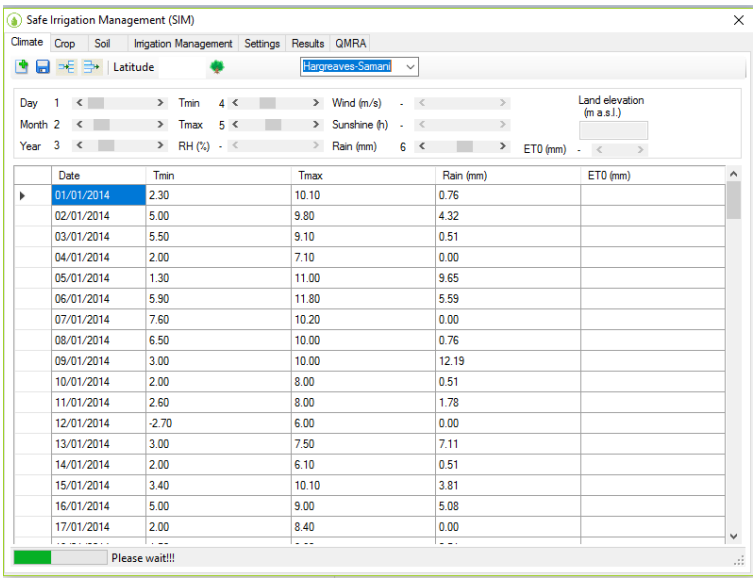


Figure 9: Climate tab used to import/export or edit climate parameters

4.2 Crop

To delete or edit an existing crop type, select the crop type from the drop down list and click on the appropriate button (Figure 10). Such operation will remove or modify the record from SIM crop database.

To add a new record, select any crop from your drop down list and modify all the parameters using the slide bars. Click on the "New" button and a new box will open asking to assign a new name for that record. By clicking OK your new record will be added to the SIM database available as .mdb in your SIM installation folder. Users have also to define the ***Ky*** parameter or the sensitivity of the crop to water stress (equ.16).

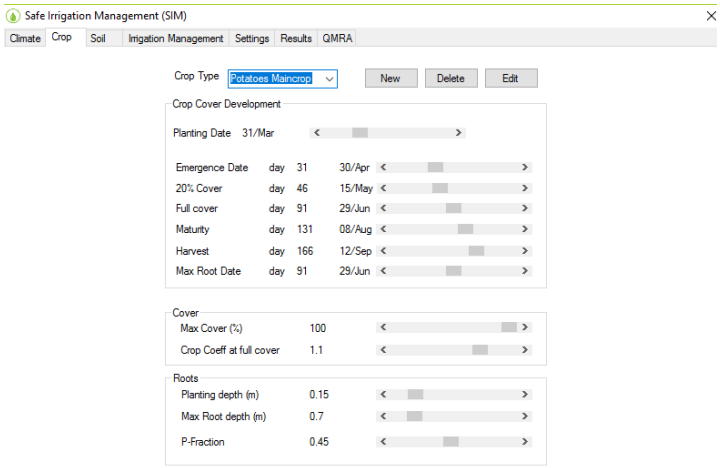


Figure 10 Crop parameters used in SIM model

4.3 Soil

Same as for crop parameters, to delete or edit an existing soil type, select the soil type from the drop down list and click on the appropriate button (**Figure 11**). Such operation will remove or modify the record from the wasim.mdb database. To add a new record, select any soil record and modify all the parameters using the appropriate slide bars. Click on the "New" button and a new box will open asking to assign a new name for that record. . By clicking OK your new record will be added to the SIM database available as .mdb in the SIM installation folder.

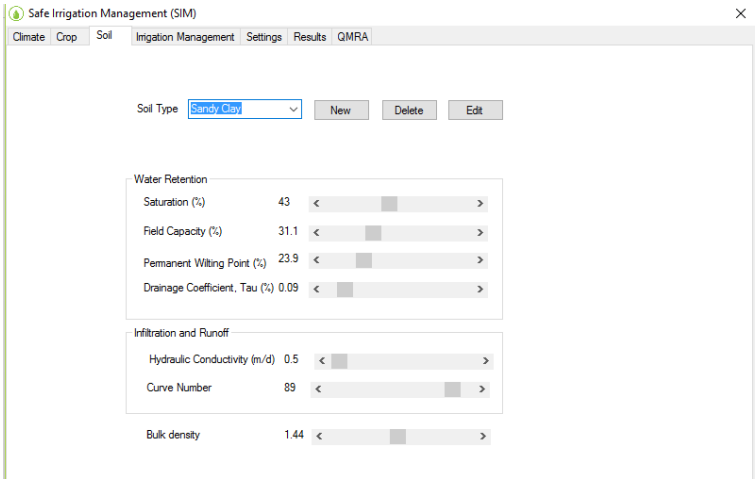


Figure 11 Soil parameters used in SIM model

4.4 Irrigation management

To create your new irrigation scheduling programme, the ***Irrigation management*** tab (**Figure 12**) will allow you to define irrigation scheduling for each of the four crop development stages (Initial, Crop development, Maturity and Late season). Irrigation programme is defined by ***Timing*** and by the ***Amount*** of water to apply, both can be selected from the appropriate dropdown lists (**Figure 12**).

Timing represents the condition by which irrigation application is triggered:

- ✓ ***Fixed interval***: fixed number of days between two consecutive irrigation events
- ✓ ***Fixed deficit (mm):*** Irrigation occurs when soil moisture deficit exceeds a given threshold expressed in mm.
- ✓ ***Fixed depletion (% AWC):*** Irrigation occurs when soil moisture deficit reaches a given percentage of the total available water content.
- ✓ ***No irrigation***: rain-fed crop

For the amount of water to be applied, user has three options:

- ✓ ***Fixed amount***: Always irrigate the same amount expressed in mm
- ✓ ***Return to fixed deficit (mm):*** Irrigate until soil moisture deficit reaches certain level expressed in mm

- ✓ ***Return to fixed depletion (%):*** Irrigate until soil moisture deficit reaches given proportion (%) of the total available water content

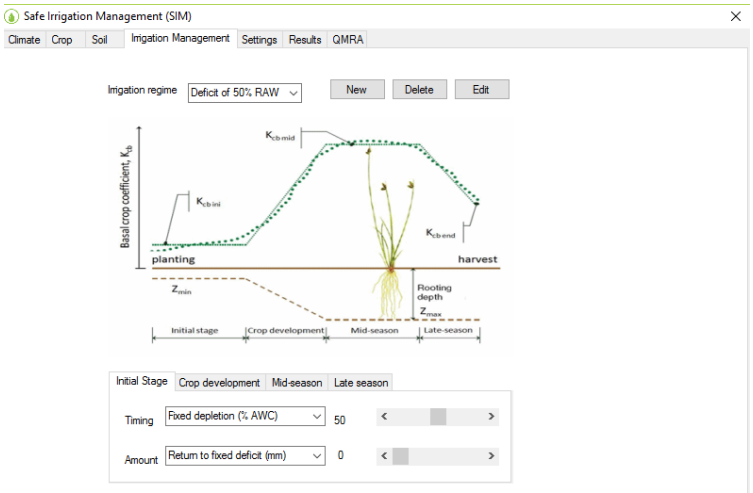


Figure 12 Irrigation management window in SIM model

5 Settings

By ticking the appropriate box (***Ecoli***, ***Nutrients***, ***Salinity*** and ***Irrigation***) under the ***Settings*** tab, users can activate the type of simulations required as shown in Figure 13. Also depending on the box ticked, parameters for the initial conditions and for the module selected are enabled or disabled.

- ✓ Under the ***Initial conditions,*** users have to define the conditions of the soil prior simulations. These include soil temperature, soil water content (expressed as % of field capacity), electrical conductivity of the soil extract (dS/m), CFU (Colony Forming Unit) content in the root zone, organic carbon (%), residual organic materials (kg/ha), nitrate, ammonia and phosphorous content.

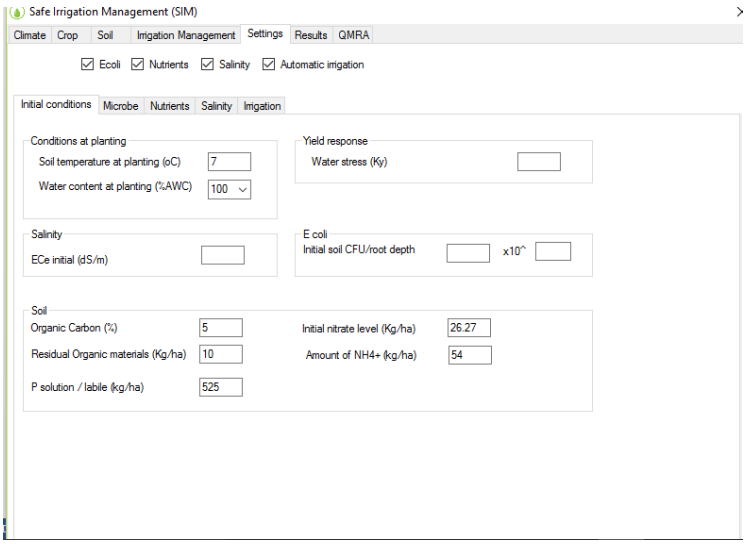


Figure 13 Simulation settings for the 4 modules of SIM model

- ✓ To run the Bacterial die-off movement module, user must tick the ***E. coli*** checkbox and assign the initial CFU (Colony Forming Unit) content in the soil (***Initial soil CFU/root depth***) under the ***Initial conditions*** tab and in the irrigation water (***irrigation water (CFU/100ml)***) under the ***Microbe*** tab. Users has three options to select from to simulate E.coli leaching (Figure 13). The first (***No leaching***) assumes that all the *E. coli* applied remain in the root zone. The second option (default) assumes that the *E. coli* leached is proportional to the volume of drainage water (***Proportional to leached water volume***) and the third option is based on maximum bacterial retention capacity (***Threshold retention capacity***) defined by the *lambda* factor and expressed as log CFU per meter of soil depth (Pang, 2009). SIM has also the capability to keep the *E. coli* level below a given threshold by mixing treated wastewater with fresh water. User can tick the ***fresh water mixture*** and assign the CFU threshold level in the appropriate box.
- ✓ By ticking the ***Salinity*** box, the salinity module in SIM is activated (Figure 13). Several parameters are needed for the salinity module such as the initial salinity conditions of the soil ($EC_{initial}$) under ***Initial conditions*** tab , water salinity (EC_{water}) and the minimum and maximum salt tolerance level of the crop under analysis (EC_{min} and EC_{max}).
- ✓ Under the ***Nutrients*** tab, users can define the nutrient content expressed in g/m^3 within the irrigation water. These include the organic and mineral nitrogen and phosphorous (Figure 14). Nitrogen and phosphorous balance models use several parameters that have default value. However, users can modify those parameters by ticking the Edit default parameters (Figure 14).

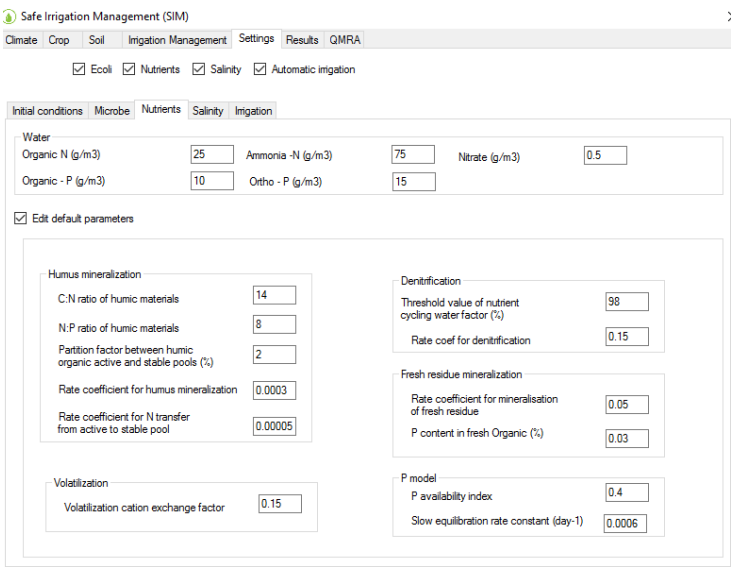


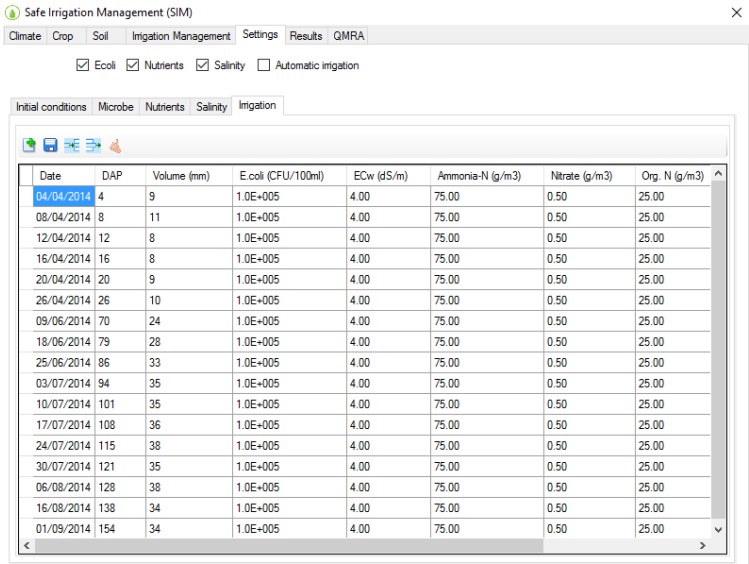
Figure 14: Nutrient management parameters tab

- ✓ Optimal irrigation scheduling and soil moisture content are the main output of SIM water balance model. When ***Automatic irrigation*** checkbox (Figure 13) is checked, SIM will automatically irrigate using the irrigation programme defined by the user (Figure 12).

  The quality of the treated wastewater might change with time. Irrigation practices in reality are not necessarily identical to the optimal theoretical ones defined by the model. For that reason, users might need the flexibility to assign at any time the volume of water actually applied as well as the changes in the salinity level, *E. coli* and nutrient content with each irrigation.

  To do so, uncheck the automatic irrigation and manually populate the new table with the new values for water, nutrients, salt and E.coli (Figure 15). Note that SIM must be first run under automatic irrigation and Use the add row button or remove an existing record by clicking on the remove row button. In each row, you have to add i) the irrigation timing expressed in day after planting (DAP), ii) irrigation volume (mm), iii) CFU content of the irrigation water (CFU/100ml) if E.coli simulation is selected, iv) electrical conductivity of the irrigation water (dS/m) if salinity simulation is selected and v) water nutrients content if nutrients options is selected. Note the thumb up button allows you to check the exact date from the inserted DAP value. To avoid confusion with the date format, users can modify only the DAP and not the date column.

  You can save the irrigation and water quality table as Excel spreadsheet using the save button or import an existing file using the add button (Figure 15).



Date	DAP	Volume (mm)	E.coli (CFU/100ml)	ECw (dS/m)	Ammonia-N (g/m3)	Nitrate (g/m3)	Org. N (g/m3)
04/04/2014	4	9	1.0E+005	4.00	75.00	0.50	25.00
08/04/2014	8	11	1.0E+005	4.00	75.00	0.50	25.00
12/04/2014	12	8	1.0E+005	4.00	75.00	0.50	25.00
16/04/2014	16	8	1.0E+005	4.00	75.00	0.50	25.00
20/04/2014	20	9	1.0E+005	4.00	75.00	0.50	25.00
26/04/2014	26	10	1.0E+005	4.00	75.00	0.50	25.00
09/06/2014	70	24	1.0E+005	4.00	75.00	0.50	25.00
18/06/2014	79	28	1.0E+005	4.00	75.00	0.50	25.00
25/06/2014	86	33	1.0E+005	4.00	75.00	0.50	25.00
03/07/2014	94	35	1.0E+005	4.00	75.00	0.50	25.00
10/07/2014	101	35	1.0E+005	4.00	75.00	0.50	25.00
17/07/2014	108	36	1.0E+005	4.00	75.00	0.50	25.00
24/07/2014	115	38	1.0E+005	4.00	75.00	0.50	25.00
30/07/2014	121	35	1.0E+005	4.00	75.00	0.50	25.00
06/08/2014	128	38	1.0E+005	4.00	75.00	0.50	25.00
16/08/2014	138	34	1.0E+005	4.00	75.00	0.50	25.00
01/09/2014	154	34	1.0E+005	4.00	75.00	0.50	25.00

Figure 15: Manual assignment for irrigation scheduling and water quality within SIM model

6 Run the model

Once all the input parameters are inserted, click on model run button under the Results tab. This will populate all the results tables and will draw a graph showing the Soil Moisture Deficit (SMD in mm), Yield Threshold Deficit (YTD in mm), Permanent Wilting Point (PWP in mm), Canopy Cover (CC %) and Irrigation Need (mm) (Figure 16).

The results of SIM model are summarized for the entire growing season or detailed (daily changes) under the ***Summary*** (Figure 16), ***plant, soil water content, water balance, Microbial quality*** (Figure 17) and ***Nutrients*** tabs (Figure 18). Salinity and CFU changes in the root zone with each irrigation are also presented graphically under ***Microbial quality / Trend*** tab (Figure 17) or numerically under the ***Microbial quality / Table*** tab.

Figure 16 Irrigation water requirement and results window of SIM model

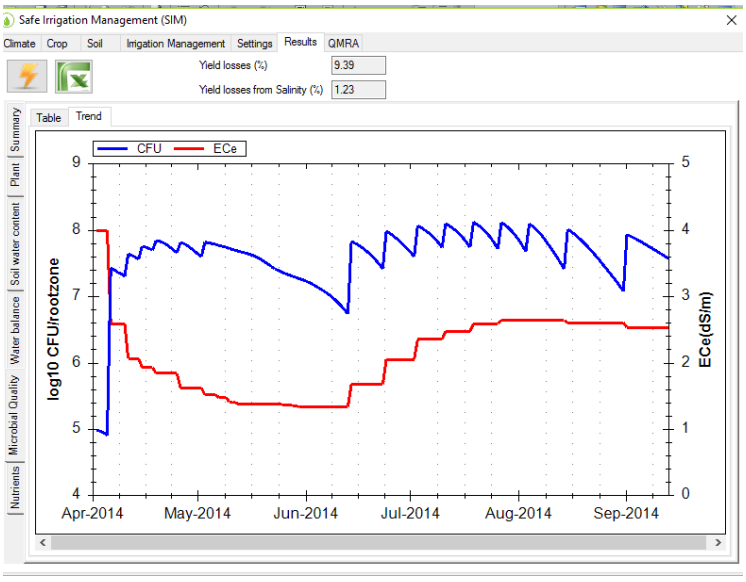


Figure 17 Salinity build-up and *E. coli* (CFU) movement in the root zone as simulated by SIM

Results of the phosphorous and nitrogen movement in the soil and between different pools are presented under the ***Nutrients*** tabs (Figure 18). The total Nitrogen and phosphorous uptake are also presented as well as their daily absorption under the ***Nutrients/Nutrient uptake*** tab (Figure 18).

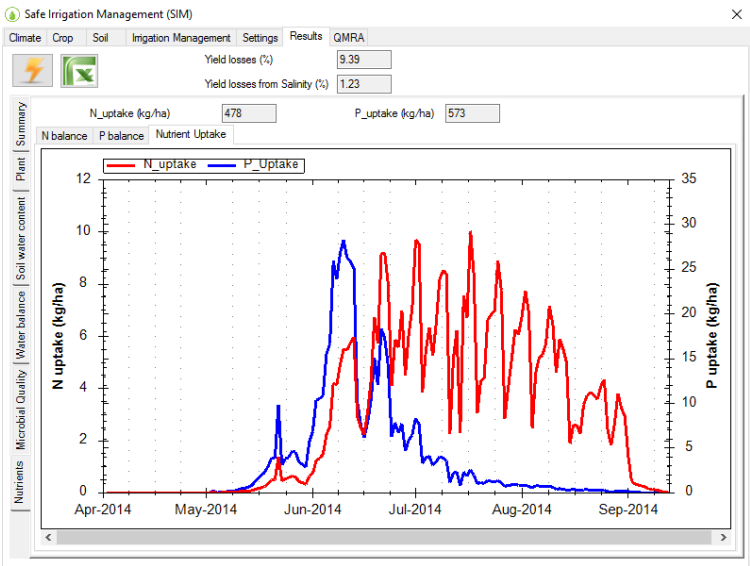


Figure 18: Nutrient uptake as simulated by SIM model

Note that all results can be easily exported into an excel spreadsheet using the export to excel button under the ***Results*** Tab.

7 Quantitative Microbial Risk Assessment (QMRA)

The user can determine the quantity of ingested soil S_i (Figure 19) and therefore decide the level of advancement of the agricultural practices, where smaller values correspond to mechanized agriculture and therefore industrialized countries and greater values correspond to developing countries or labor-intensive agriculture.

The QMRA model reads daily *E. coli* data from the '*E. coli* die-off/movement' module and generates a daily infection risk that actually indicates whether the exposed individual is above, below or at the tolerable infection risk for each of the pathogens included in the model. Therefore, and differently from the assumption made by Mara et al., (2007), the QMRA takes into account the die-off of the indicator as die-off of the pathogen when reading N_1.

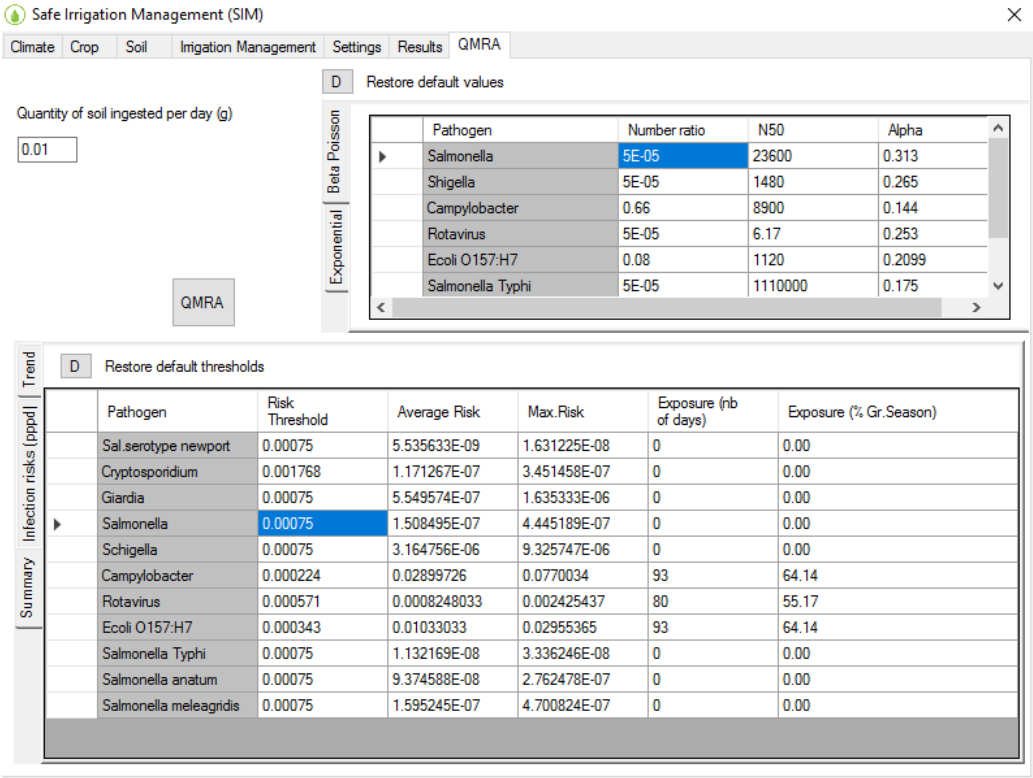


Figure 19 QMRA tab page used in SIM model

QMRA module is activated once the water balance model is performed and all the results are presented under the *Results* tab. The first input of QMRA is the quantity of daily ingested soil (g). Depending on the analyzed pathogen, the dose-response models can be beta-Poisson or exponential model (Table 2). SIM uses for each pathogen and each model default values that can be obtained by clicking on the *D* for default values button (Figure 19). Users can modify any parameter of beta-Poisson (number ratio, N50, alpha) or exponential model (number ratio, infectivity) directly from the table (Figure 19). Users can also modify the risk threshold (Table 3) for each pathogen if needed.

Click on the QMRA button and observe for each pathogen under the ***Summary*** tab page the average and maximum infection risks throughout the season as well as the pathogen exposure expressed in total number of days or percentage of growing season. The infection risks (pppd) will also be presented for each day and for each pathogen numerically under the ***infection risks (pppd)*** tab and graphically under the ***trend*** tabpage. For each cell in the ***infection risks (pppd)*** table, the font is coloured in light blue if the infection risk is lower than the assigned threshold and in red when it exceeds this threshold.

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