Ch. 1:
System and modelling concepts

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1 System and modelling concepts

1.1 Introduction

This chapter outlines the basic structure of the Daisy model system, mainly based on Hansen et al. (2012). The aim of the chapter is to provide an overview with references to the more detailed descriptions of specific processes given in other chapters and appendices.

1.2 The model

Daisy can be characterized as an explanatory, mechanistic, or physically based model. The typical scale of application is the field (a management unit). Simulations can be performed in one or two dimensions. The 2-D model is developed primarily for simulating fields with subsurface tile drains or subsoil irrigation (see Appendix 1.1[1]). Figure 1.1 provides an overview of Daisy. Daisy is driven by weather and management data provided by the user. The management data describe the agricultural practices (see Chapter 11 for more information).

Weather data

A simulation requires detailed weather data (e.g., precipitation, air temperature, air humidity, wind speed, solar radiation, diffuse short-wave radiation, and long-wave incoming radiation) with high temporal resolution (daily, hourly or finer resolution). Diffuse short-wave radiation and long-wave incoming radiation can be

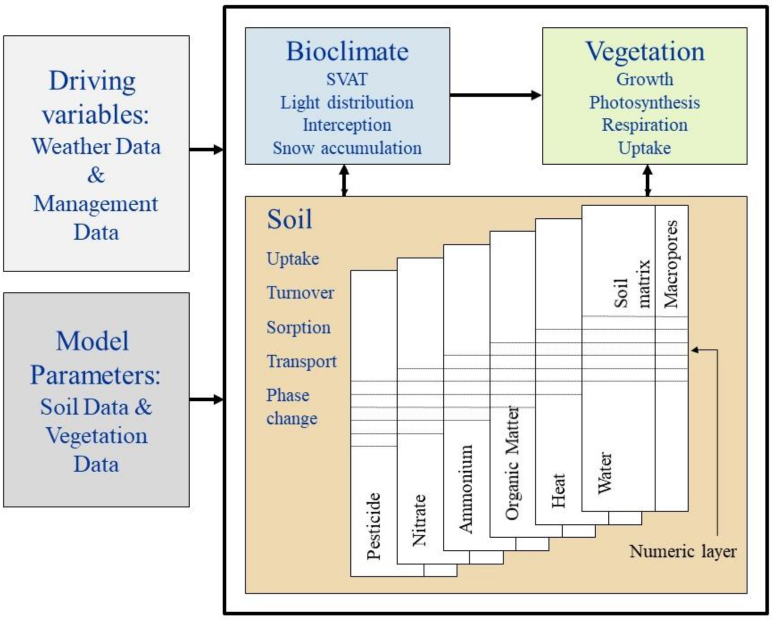

Figure 1.1. Schematic overview of the Daisy model. The main modules of the model are the bioclimate, vegetation and soil modules. The biocclimate module simulates surface processes, exchange with the atmosphere and the aerial environment of the plant. The vegetation module simulates plant-related procese, while the soil module simulates soil related processes. From Hansen et al. (2012).

[1] Appendix 1.1 is not available yet. Information is available in https://daisy.ku.dk/about-daisy/projects/safir/D3_2.pdf and https://daisy.ku.dk/pdfs/Num2D-v2.pdf.

estimated from other weather data (de Pury and Farquhar, 1997; Kjaersgaard et al., 2007). A less detailed simulation only requires limited weather data with low temporal resolution (daily values at a minimum). The minimum weather dataset comprises daily values of precipitation, air temperature, and solar radiation. Technical details and options are further treated in Chapter 2 as well as Appendix 2.1, 2.2 and 2.3.

1.2.1 Water

Surface processes

In this document, surface processes are defined as processes taking place in the space above the soil surface. On the surface, water and solutes added through rain, deposition, surface irrigation, or spraying may be stored in or continue past a number of layers, namely a snowpack, the canopy, a litter layer or surface ponding (if relevant). From the soil surface, water may infiltrate or run off. Water may evaporate from each of these compartments, and solutes may be sorbed or break down. A schematic overview of water related surface processes implemented in Daisy is provided in Figure 1.2 and these processes are further described in Chapter 3, together with the associated solute transport and transformation processes.

Water flow in soils

When water infiltrates into the soil, it can enter the soil matrix or the soil macropores (Figure 1.3). In the matrix regime, the soil water dynamics are described by the numerical solution of the Richards equation (in 1-D or 2-D) (Richards, 1931). Soil water fluxes are calculated by Darcy's law (Hansen *et al.*, 1990; Mollerup *et al.*, 2014). If continuous fractures (typically invisible in moist soil, i.e., with apertures smaller than 0.1 mm) are present, then part of the hydraulic conductivity can be assigned to the fractures and the hydraulic conductivity of the soil matrix is adjusted accordingly. Flow in macropores (typically large biopores with apertures larger than about 0.5 to 1.0 mm) depends on the rate at which the surface and/or the surrounding soil can feed the

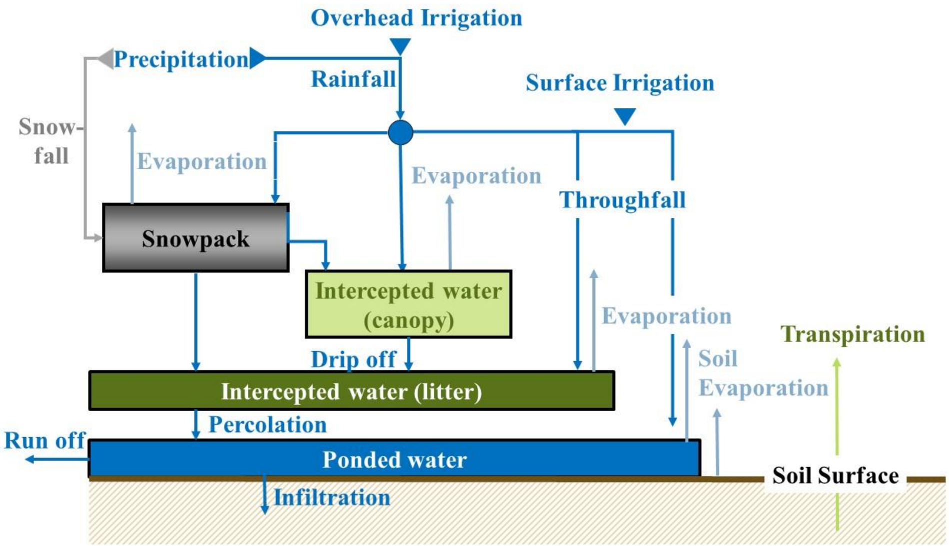

Figure 1.2. Schematic view of the water-related surface processes in Daisy (Modified from Hansen et al. (2012a).

macropores (Tofteng et al., 2002; Gjettermann et al., 2004; Holbak et al., 2021). The emptying rate of the macropores depends on the rate at which the surrounding soil can receive water, except when the macropore is directly connected to a subsurface drain. In this case, it is assumed that emptying is instantaneous.

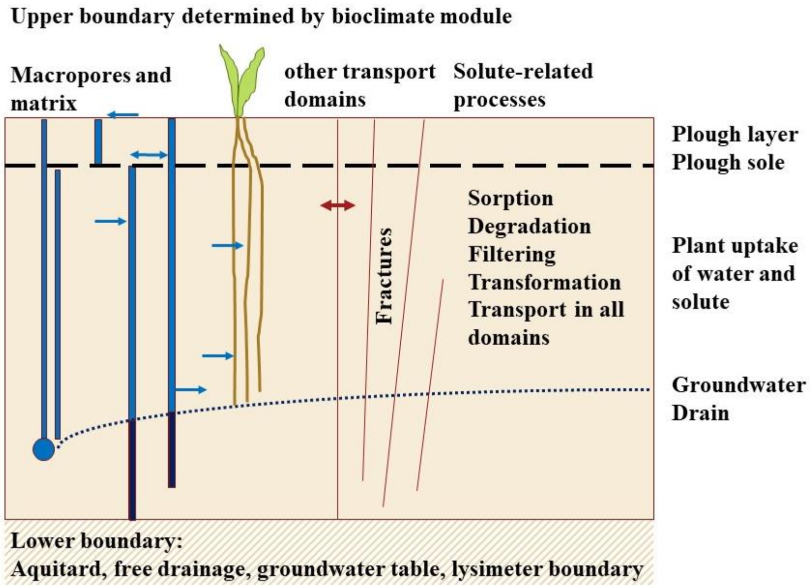

Figure 1.3. Overview of the domains used for water flow and solute transport, as well as solute-related processes. The soil matrix is domain 1, fractures domain 2 and macropores domain 3.

In the 1-D version, the modelling of tile flow is based on the Hooghoudts equation (Mollerup et al., 2014). In the 2-D version, the tile flow is based on the general flow solution (Mollerup et al., 2014). The lower boundary can be defined by a free drainage condition (deep groundwater), a groundwater table, (fixed or fluctuating), or an aquitard condition (Mollerup et al., 2014). The description of flow in matrix and macropores as well as boundary conditions are described in Chapter 4.

Uptake of water by roots

"The uptake of water by vegetation is simulated by a root water uptake model, which is based on the single root concept (Gardner, 1960), i.e., it is assumed that the uptake can be equated to the flow towards the root surface (microscopic approach). Water flow from the matrix to the root tips is driven by a gradient in soil water pressure potential between the root surface and the bulk soil. The soil water pressure potential at the root surface depends on the so-called crown potential in the xylem of the vegetation at the transition between the stem and the root and is a function of depth. The water extraction model also depends on root density and root length. The maximum water uptake is limited by potential transpiration Overview of the implemented model in Daisy is given by Hansen and Abrahamsen (2009).

Evapotranspiration

Modelling of evapotranspiration is based on the energy balance of the surface. It is assumed that evaporation from the different sources (storages) takes place in the following prioritized sequence: (1) water in the snowpack, (2) water intercepted in the canopy, (3) water intercepted in the litter layer, (4) water stored at the surface. Finally (5), evapotranspiration of water stored in the soil may take place. The distribution between the two depends on the soil cover fraction which is controlled by the leaf area index (LAI). Soil evaporation is also influenced by presence of litter. The user may choose between the following evapotranspiration models (soil-vegetation-atmosphere transfer models or SVAT models), which are implemented in Daisy:

1. A model in which the surface water balance and the surface energy and radiation balances are decoupled, which is the most commonly used version and described in Chapter 2. Here, the upper boundary is defined by the rate at which water reaches the surface or by the rate of soil evapotranspiration (Hansen et al., 1990)
2. A model in which the surface water balance and the surface energy and radiation balances are coupled, and evapotranspiration takes place from soil and canopy. This two-source model (soil and canopy) includes the stomata conductance stress function described by (van der Keur et al., 2001) which is influenced by solar radiation, temperature, vapour pressure, and soil moisture.
3. A model in which the surface water balance and the surface energy and radiation balances are coupled, and evapotranspiration takes place from soil as well as from shaded and sunlit leaves. This model includes a Ball-Berry type stomata conductance model (Ball et al., 1987; Plauborg et al., 2010), which is very detailed and requires information on leaf photosynthesis, and it takes into account chemical signalling (at present ABA) in the plant (Ahmadi et al., 2009). Leaf temperature, CO_2 pressure, and vapour pressure at leaf surfaces are state variables in this model. This module is referred to as the Sun-shade-open canopy (SSOC) module and is further described in Appendix 1.2.

In all three approaches, it is assumed that the transpiration is equal to the extraction of soil water by roots, meaning that the transpiration is coupled to the soil water through the crown water potential.

The two coupled approaches are SVAT models that are based on resistance/ conductance theory, and they require high-resolution weather data, while for the decoupled approach daily values may be sufficient. The decoupled approach is a traditional evapotranspiration model that is built on the concepts of reference evapotranspiration and potential evapotranspiration. Here, potential evapotranspiration is the maximum evapotranspiration for given vegetation. The potential evapotranspiration is related to the reference evapotranspiration by a simple crop coefficient (Hansen, 2002; Kjaersgaard et al., 2008). Depending on the available information, the reference evapotranspiration can be estimated by a number of methods, see Chapter 2 and Appendix 2.3.

1.2.2 Soil Heat

The soil temperature model is based on the 1-D or 2-D heat flow equation, which accounts for heat flow due to conduction and convection. The 1-D model is originally described by Hansen et al. (1990) and updated in Chapter 5; the 2-D version is an extension of the 1-D model into two dimensions.

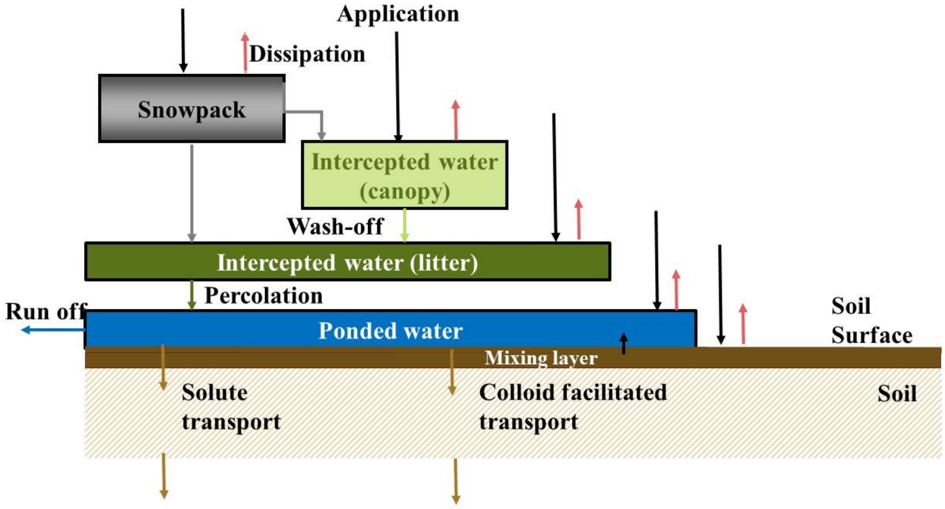

Figure 1.4. Schematic overview of solute transport processes at the surface. The solute related processes in the soil are shown in Figure 1.3 and described in table Table 1.1.

1.2.3 Solute transport

Solute transport, surface

The main components of the solute (e.g., pesticides, tracers) model are presented in Figure 1.3 and Figure 1.4. Relevant surface solute processes and solute transport in the soil are presented in Chapter 3 and Chapter 6, respectively. For nitrogen, additional transformation processes are included, see below as well as Chapter 7 and 9, while special issues related to pesticides are described in Chapter 8.

A chemical applied to the field may be intercepted by a snow layer, a canopy, a litter layer, ponded water or end up at the soil surface. Wash-off from canopy and litter depends on the "stickiness" of the chemical (e.g., the formulation of the pesticide). Dissipation takes place from the interception storages and the soil surface storage and is simulated by first-order kinetics. At the soil surface, a chemical in solution may enter the soil with the infiltrating water. A chemical may also adsorb to particles, and these may subsequently be mobilized, resulting in colloid-facilitated transport. During transport, colloids (and adsorbed chemicals) may be retained**.** Interaction between surface water and the soil takes place in a mixing layer on the soil surface.

Solute transport, soil

In the soil system, chemicals are subject to degradation, transformation and sorption. Degradation is described by first order kinetics, and the degradation rate constant may depend on soil temperature, soil moisture (expressed as soil water pressure potential or volumetric water content), soil depth, and biological activity in the soil (expressed by CO_2 evolution). Transformation describes the process when a degradation product is a new molecule with its own transport properties

Table 1.1.Flow and transport modelling in soil (Hansen et al., 2012a).

	Domain 1 (Matrix)	Domain 2(Fractures)[a]	Domain 3 (Large Biopores)[b]
Water	Richards equation[c]		By-pass[d]
Solutes	Convection-dispersion equation	Convection	By-pass
Colloids + sorbed chemicals	Convection-dispersion (very efficient filtration)	Convection (some filtration	By-pass (no filtration)

[a] The boundary between the matrix and fracture domains is defined by a boundary potential or by the corresponding effective aperture of the fracture system. The pore system of the domain comprises fractures of the effective aperture and pores of equivalent diameters larger than the equivalent aperture.

[b] The large biopores are defined separately and are superimposed on the matrix and fracture domains.

[c] Fractures are represented by a modification of the hydraulic conductivity. The contribution from continuous fractures can be superimposed on the matrix hydraulic conductivity. Water flow in the matrix and fracture domains is based on the total flow, which is partitioned according to a key defined by the ratio between the actual hydraulic conductivity and the hydraulic conductivity at the boundary potential.

[d] The by-pass is defined as a mass balance approach and it is considered as a very fast transport relative to lateral solute equilibration.

(for example transformation of parent to daughter pesticide). Sorption can be described by linear, Freundlich, and Langmuir isotherms, with support for optional kinetics.

The solute transport component of Daisy comprises of models considering one, two, or three transport domains (Table 1.1 and Figure 1.3). Domain 1 (the soil matrix) is always activated and is described by the Advection-Dispersion equation(Bear, 1972), while activation of domains 2 (fractures) and 3 (biopores) is optional. Domain 2 represents transport of solutes in fractures or big pores and it is described by a non-equilibrium transport model (Genuchten and Wierenga, 1976). Domain 3 represents transport through biopores and transport is only due to advection. Normally, domain 1 or domain 1 in combination with domain 3 are used in modeling nitrate leaching. Colloid transport is described by the same equations as general solute transport, but with additional process descriptions regarding generations of colloids (Jarvis et al., 1999; Morgan et al., 1998; Styczen and Høgh-Schmidt, 1998) and removal of colloids by filtration (Jarvis et al., 1999). Colloids that facilitate the transport of sorbing chemicals are treated as a special class of colloids. For further details, see Hansen et al. (2012b).

1.2.4 Carbon

Carbon is assumed to be present in plants, litter, organic fertilizers, and soil organic matter. In plants, litter, and organic fertilizers, carbon content is assumed to be proportional to dry matter content. Soil organic carbon can also be expressed as humus.

Plant Growth

A generic plant growth model is included in Daisy. The original version is described by Hansen et al. (1990) and Petersen et al. (1995) and generalized by Hansen and Abrahamsen (2009). An overview of the carbon flow and important processes in the new model is shown in Figure 1.5. In this figure, the solid lines represent flow of carbon, and the dashed lines represent information flows. The crop model is described in detail in Chapter 10.

The photosynthesis process is described by a simple light response curve, as described by Hansen (2002) or by a physiologically based model (Pury and Farquhar, 1997). The latter interacts with the three-source SVAT model (soil and shaded and sunlit leaves) that includes a Ball-Berry type stomata conductance model (Plauborg et al., 2010). Photosynthesis is affected by nitrogen and water stress as well as senescence. Effects of stress on other parts of the system are not considered in the model.

The canopy structure is defined by a predefined leaf density distribution that varies with height, which depends on development stage and LAI. LAI depends on leaf mass and development stage. In the case of intercropping, a composite canopy is simulated, and light interception is distributed among the crops based on individual leaf density distributions. Partitioning, leaf and root death, senescence, and nitrogen stress (stress factors) are all influenced by development stage. Maintenance respiration depends on dry mass of the plant components and on temperature. Conversion depends on the end-product formed. At conversion, CO_2-C is lost as growth respiration.

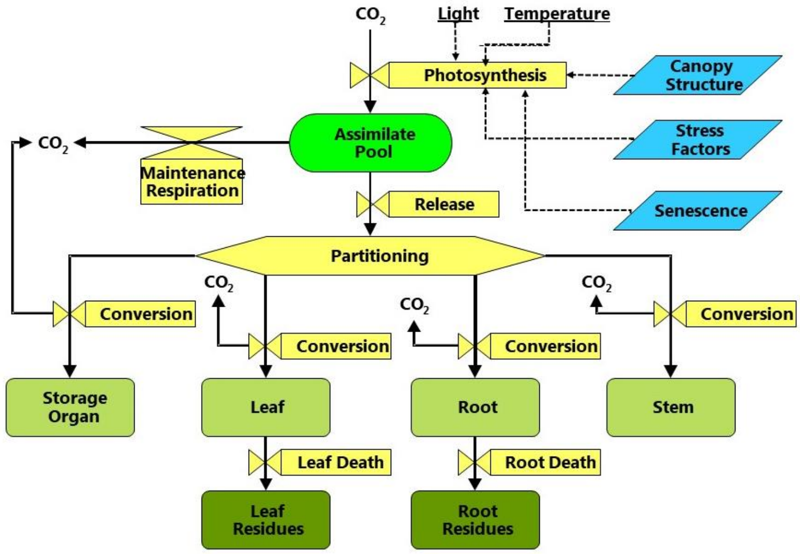

Figure 1.5. Schematic overview of the crop model included in Daisy. Soil lines represent flows of matter and dashed lines represent flows of information. Modified from (Hansen et al., 2012a).

Rooting depth depends on soil temperature and soil type. Root density distribution depends on root mass and rooting depth. The default root density distribution is based on Gerwitz and Page (1974); user-defined distributions are also supported. In the case of intercropping, the competition for water and nitrogen is based on the demand for water and nitrogen and the root distribution of the individual crops.

Litter and Organic Fertilizer

Litter is plant residue left in the field. Litter is transferred to the soil organic matter turnover model by tillage operations and by bio-incorporation. During bioincorporation, CO_2-C is lost as respiration. Organic fertilizer is transferred to the soil organic matter turnover model by tillage operations.

Soil Organic Matter

Soil organic matter consists of various products, ranging from intact plant and animal tissues and organisms that live in the soil to black organic material, designated humus, that is without traces of the anatomical structures of the organisms from which it was derived. In order to mimic the spectrum of decomposability of soil organic matter, the soil organic matter is divided into a number of pools (Figure 1.6).

Daisy distinguishes between three main types of organic matter:

1. soil organic matter (SOM), which is the humus-like substances;
2. soil microbial biomass (SMB), which is responsible for the turnover process; and

3. added organic matter (AOM), which may be plant residues, organic fertilizers, compost, etc.

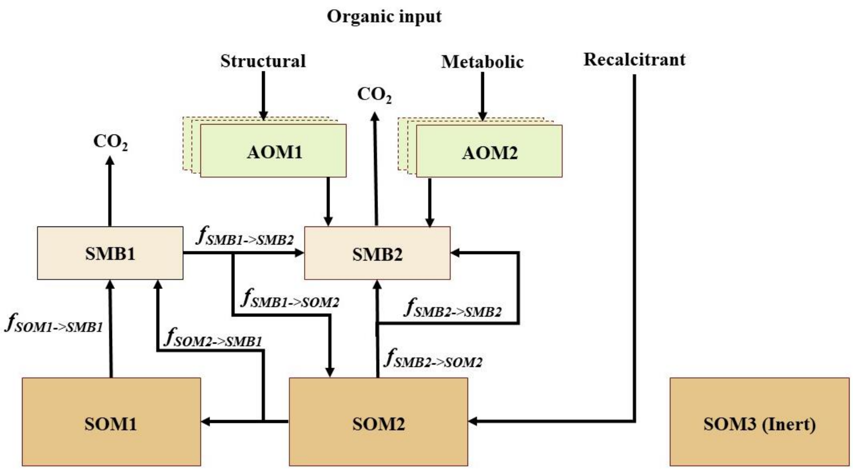

Figure 1.6. Schematic overview of the soil organic matter model included in the Daisy model. AOM= added organic matter, SMB=soil microbial biomass, and SOM=native organic matter, f_x*= partitioning coefficient. The inert SOM3 pool does not interact with the rest of the system. From Hansen et al. (2012a).*

Daisy assumes three main types of organic matter which are further divided into pools. These pools are characterized by carbon (and nitrogen) content and first-order decomposition rate coefficients. SOM1 is a pool with a relative slow decomposition rate, SOM2 is a pool with a relative fast decomposition rate, and SOM3 is considered an inert pool (Figure 1.6). SMB is divided into two pools: a slow pool (SMB1) and a fast pool (SMB2). Similarly, AOM is subdivided into a slowly decomposing pool (AOM1) and a fast decomposing pool (AOM2). If AOM contains organic material that already is partly decomposed, this part may be directly transferred to the SOM2 pool. Whenever AOM is added to the soil, a new set of AOM pools is created.

SMB utilizes organic substances to build new biomass. This process is characterized by substrate utilization efficiency. A consequence of this process is that part of the carbon is lost as CO_2. Maintenance respiration is another source of CO_2 loss. Decomposition rate coefficients and maintenance rate coefficients depend on soil temperature and soil moisture content (expressed by pF). It is assumed that the rate coefficients pertaining to SOM1, SOM2, and SMB1 depend on the clay content of the soil, mimicking physical protection against decomposition of the organic matter. The substrate utilization efficiencies are source specific. Finally, building new SMB requires nitrogen; if nitrogen deficiency occurs, decomposition will be regulated until the release of nitrogen meets the demand. For further details, see Jensen et al. (2001) and Chapter 9. The model can also consider transport of dissolved organic carbon (see Gjettermann et al. (2008).

1.2.5 Special issues related to nitrogen

Daisy considers organic nitrogen, ammonium, and nitrate. Organic nitrogen is assumed to be present in plants, litter, organic fertilizers, and soil organic matter. Ammonium is present in atmospheric deposition, fertilizers, and in the soil sorbed to particles and in the soil solution. Nitrate is present in atmospheric deposition, fertilizers, and in the soil solution. Figure 1.7 illustrates the nitrogen related processes in the model.

Atmospheric Deposition

Atmospheric deposition is assumed to take place as dry and wet deposition and in the form of ammonium or nitrate (Hansen et al., 1990). The wet deposition is assumed to be proportional to the precipitation.

Fertilization

Application of mineral (e.g., ammonium or nitrate) and organic fertilizers are management options (see chapter 11). The user may define a volatilization fraction for the fertilizer.

Incorporation of Residue and Organic Fertilizer

Material located at the surface (e.g., plant residues, fertilizers, etc.) is incorporated by soil tillage operations (e.g., ploughing, harrowing, rotavation), and the organic matter is transferred to AOM pools. Tillage is modelled by a combination of mixing and translocation (Hansen et al., 1990) and is described in Chapter 11. Plant material can also be incorporated by biological activity. Bio-incorporation results in a loss of carbon as CO_2 respiration, and the bio-incorporation rate can be made a function of the C/N of the residue and the temperature in the upper part of the soil. Bio-incorporation also transfers organic matter to AOM pools, which are distributed in the soil profile.

Mineralization and Immobilization

The turnover of N is associated with the turnover of soil organic matter carbon. After every time step, corresponding N pools are calculated from the actual amount of C in the pools using the C/N for the individual pools. Net N mineralization or net N immobilization is derived from the overall N balance. If the content of N in the assimilated organic substance is higher than that required by the biomass for growth, ammonium is excreted to the soil solution (N mineralization). On the other hand, if the N content of the assimilated organic substance is lower than that required by the biomass for growth, then ammonium or nitrate is assimilated from the soil solution and transformed into nitrogenous organic compounds (N immobilization). N immobilization may occur when AOM pools with a high C/N are present. For further details, see Jensen et al. (2001) and Chapter 9.

Nitrification

Nitrification depends on the ammonium concentration and is described by Michaelis-Menten kinetics. The maximum nitrification rate is assumed to depend on soil temperature and soil water pressure potential. The latter mimics the effects of oxygen concentration in the soil. Gaseous nitrogen (N_2O) is lost as a by-product of the nitrification process. The loss is assumed to be proportional to the nitrification rate.

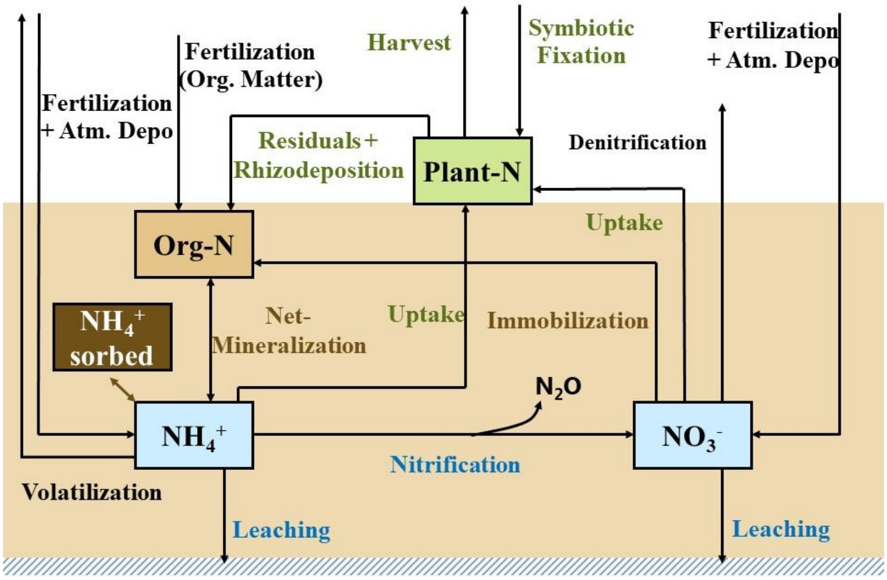

Figure 1.7. Schematic overview of the nitrogen model included in Daisy. After Hansen et al. (2012a).

Denitrification

Denitrification is simulated by means of a rather simple index-type model that works in three steps:

4. calculation of a potential denitrification rate (the rate at anoxic conditions and at ample nitrate supply), assuming that it is proportional to the CO_2-evolution simulated by the soil organic matter model;
5. calculation of an oxygen-dependent denitrification rate, taking into account the oxygen status of the soil mimicked by a function of the relative soil water content; and
6. a further reduction of oxygen-dependent denitrification rate if insufficient nitrate is present in the soil.

The availability of nitrate is assumed to be proportional to the nitrate concentration. A redox cline, below which nitrate is reduced, can be defined.

Leaching

Transport of ammonium and nitrate, and hence leaching, is simulated by the solute transport model of Daisy (see above). Ammonium is assumed to adsorb strongly to clay, so the simulated leaching is usually very small (Chapter 6 and 7 and Hansen et al. (1990).

Plant Uptake and Symbiotic Fixation

In Daisy, crop nitrogen is characterized by (1) a potential nitrogen content (when this content is exceeded, nitrogen uptake stops); (2) a critical nitrogen content (below this limit, nitrogen deficiency limits production); (3) a non-functional content (at this limit, production stops); and (4) an actual nitrogen content. The first three depend on accumulated dry matter and development stage. The potential plant uptake depends on the potential content and the actual content. Whether the potential uptake is realized or not depends on the root uptake. The root uptake is simulated by the single root concept, in which the movement of nitrogen in the soil toward the roots governs the uptake. The considered mechanisms are convection and diffusion. Ammonium is taken up in preference to nitrate. For further details, see Hansen and Abrahamsen (2009).

If the plant is a legume that can fix atmospheric nitrogen, it is assumed that the plant will take up nitrogen as described above. If the potential uptake is not fulfilled, the deficit is assumed to be supplied to the plant by symbiotic fixation.

Original text from	(Hansen et al., 1990) (Hansen et al., 2012a)	
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