Fundamentals of HERMES2GO

Version 1.03, February 2021

Content

1. Introduction:

There are many models to simulate processes in agroecosystems which differ in their complexity depending on their purpose, their scale of application and their potential end users. Of course, models for testing scientific hypotheses on processes are more complex and mechanistic compared to others which are designed to be used operationally for practical agricultural applications in agriculture, like irrigation or fertilization or those which should give answers for large areas with limited or generalized data availability. Regarding their potential errors more complex and simpler models have their advantages and disadvantages. While the numerous parameters of complex models and the interaction of processes increase the risk of error propagation, which can be summarized as parameter error, the negligence of important processes can lead to an increasing structural error when models are simplified (Grunwald 1997).

The HERMES model has been primarily developed for its application in agricultural practice where detailed information on management is usually available but knowledge about soil properties at the field scale is often limited to a few basic properties like texture and soil organic matter content. This makes the model also suitable to operate on a catchment or regional scale, where soil information from soil maps is provided in an aggregated and generalized way. The objective of this document is to describe the main characteristics of the present version of HERMES, while its data structure and requirements and examples are provided in a separate manual.

2. Characteristic of HERMES

The HERMES model was initially developed in the mid 1980's from a simple model to estimate soil mineral nitrogen on arable soils in early spring (Nuske 1983) as a base for fertilizer recommendations. Based on a simple model approach from Richter et al. (1978) describing nitrate transport assuming quasi stationary flux conditions during winter and experimental work on nitrogen mineralization of Richter et al. (1982) a preliminary model was developed by Nuske (1983) to simulate nitrogen dynamics in loess soils over the winter period. The aim was to create a tool which allowed the calculation of soil mineral nitrogen content in early spring which is usually determined by soil sampling as a basis for fertilizer recommendation (Wehrmann and Scharpf, 1986). Combining this concept with a complete water balance submodel for transient water flux and a module for the dynamic simulation of crop growth for winter wheat a new model (HERMES) was built by Kersebaum (1989) which was able to simulate nitrogen dynamics in the soil-crop system for the whole growing season. The simulated deficiency between nitrogen supply from soil and the demand of the growing crop was used to calculate recommendations for nitrogen fertilizer applications for the whole growing season. In the following years the model was modified for other crops than winter wheat and a module for denitrification was added (Kersebaum, 1995). Recently a soil temperature module was added to account for soil temperature effects on crop germination and temperature dependent soil process such as mineralisation and denitrification. In its present version the model is able to simulate crop rotations using a generic approach for crop growth which can be extended by the user for other crops by creating their individual crop parameter files.

Thus, HERMES (Kersebaum, 1995, 2007) is a process-oriented functional model designed to simulate crop growth, water and nitrogen dynamics for arable land. The model has been used under Central European conditions to calculate nitrogen fertilization recommendations at the field and sub-field scale (Kersebaum and Beblik, 2001; Kersebaum et al., 2003a) and for regional calculations of nitrogen pollution under different management options (Kersebaum, 2000, Kersebaum et al., 2003b). It was adopted for applications in other regions like Canada (Kersebaum et al. 2008), India, China (Michalczyk et al. 2014, 2020), and Africa (Falconnier et al. 2020). The model has been compared in several international model comparisons studies providing data sets to different modellers and showed its capability to simulate water and nitrogen dynamics in arable fields (de Willigen, 1991, Diekkrüger et al. 1995, Kersebaum et al. 2007) and climate effects on crop growth (e.g., Asseng et al. 2013, 2015; Bassu et al. 2014, Kollas et al. 2015; Falconnier et al. 2020.

The model is comprised of submodules for the water balance, soil temperature, N transport and transformations, crop development and growth, including N uptake. The main algorithms were described previously in detail by Kersebaum and Richter (1991), Kersebaum (1995) and Kersebaum and Beblik (2001), and therefore only a brief description is presented here.

Recently the original HERMES model has been transferred to a new program language. It is now programmed in GO, which makes it suitable to run on Windows and LINUX platforms in a parallel mode, which enhances the computation speed significantly especially when using the model for a large number of fields/polygons in regional applications.

2.1 Water balance

Soil water is simulated by a simple capacity-based approach. The capacity parameters required by the model are attached to the model by external data files which are consistent with the German soil texture classification and their capacity parameters (Ad-hoc-AG Boden, 2005). An example for some soils is given in table 1. The basic values are modified by soil organic matter content, bulk density. In case of water logging water holding capacity of single horizons can be raised by a hydromorphic factor. For shallow groundwater sites capillary rise is calculated dependent on soil texture and the distance to the groundwater using tabulated values of Ad-hoc-AG Boden (2005). These fluxes are defined for a water content of 70% of crop available water and are used by the model as a steady state flux up to the deepest soil layer with less than 70% of available water capacity. An example for different soils is given in table 1. Because soil information is often very limited under practical conditions the chosen capacity approach seemed to be appropriate to be used on a field as well as on a regional scale because parameters are more robust and can easily be derived from rough basic soil information (Addiscott and Wagenet, 1985). Functional approaches of this kind have been shown to perform as well as mechanistic water models based on the potential concept under field conditions (de Willigen, 1991; Diekkrüger et al., 1995; Kersebaum et al., 2007b).

Table 1: Selected texture classes (10 out of 34) from Ad-hoc AG Boden (2005) with their particle size distribution, capacity parameters depending on soil texture class and daily capillary rise rates

Texture class:	SG†	SM†	SF†	SL2	LS2	LT2	UT3	UT4	TU3	TU2
	% (w/w)									
Sand	>85	>85	>85	67–85	25–43	15–45	<23	<18	<20	<25
Silt	<10	<10	<10	10–25	40–50	30–50	65–88	65–83	50–65	30–55
Clay	<5	<5	<5	5–8	17–25	25–35	12–17	17–25	30–45	45–65

Bulk density class‡:	Capacity parameters								
	Field capacity			Wilting point			Total pore space		
	1–2	3	4–5	1–2	3	4–5	1–2	3	4–5
	% (v/v)								
Texture class									
SG† (coarse sand)	12	8	6	4	3	2	46	41	35
SM† (middle sand)	14	10	8	5	4	3	50	42	34
SF† (fine sand)	16	14	12	6	5	4	50	45	35
SL2 (loamy sand)	28	25	23	8	7	6	51	43	36
LS2 (sandy loam)	40	34	31	19	18	17	53	43	37
LT2 (clay loam)	42	36	32	24	22	21	53	43	37
UT3 (loamy silt)	39	37	35	13	12	12	50	43	38
UT4 (clay silt)	39	37	35	16	16	16	51	44	38
TU3 (silty clay)	45	38	35	28	25	25	53	44	38
TU2 (slight silty clay)	47	42	36	31	30	26	52	46	39

	Daily rates of capillary rise									
Groundwater distance (cm) line 1 line 2	10 110	20 120	30 130	40 140	50 150	60 160	70 170	80 180	90 190	100 200
	mm d^{-1}									
Texture class										
SG† 0.1–1 m	5.5	5.0	1.5	0.9	0.4	0.2	0	0	0	0
1.1–2 m	0	0	0	0	0	0	0	0	0	0
SM†	5.5	5.3	5.1	3.0	1.0	0.5	0.3	0.2	0.1	0
	0	0	0	0	0	0	0	0	0	0
SF†	5.5	5.3	5.2	5.1	3.5	1.9	0.8	0.4	0.3	0.2
	0.1	0	0	0	0	0	0	0	0	0
SL2	5.5	5.3	5.1	3.1	1.7	1.0	0.6	0.4	0.3	0.2
	0.1	0.1	0	0	0	0	0	0	0	0
LS2	5.5	5.3	5.1	2.6	1.6	1.3	1.0	0.7	0.4	0.2
	0.1	0	0	0	0	0	0	0	0	0
LT2	5.2	5.0	2.3	1.2	0.7	0.4	0.3	0.2	0.1	0.1
	0	0	0	0	0	0	0	0	0	0
UT3	5.5	5.5	5.5	5.5	5.4	5.3	5.2	5.1	5.0	4.2
	3.4	2.9	2.4	2.0	1.5	1.2	1.2	1.1	1.0	0.8
UT4	5.5	5.4	5.3	5.2	5.1	5.0	4.2	3.3	2.6	2.1
	1.7	1.4	1.2	1.0	0.8	0.7	0.6	0.5	0.45	0.4
TU3	5.2	5.0	3.1	2.4	1.8	0.7	0.4	0.3	0.2	0.2
	0.1	0	0	0	0	0	0	0	0	0
TU2	5.0	3.2	1.3	0.7	0.5	0.3	0.2	0.2	0.1	0.1
	0	0	0	0	0	0	0	0	0	0

† Name modified for model use.

‡ Bulk density classes: 1–2 = <1.4 g cm^{-3}, 3 = 1.4–1.6 g cm^{-3}, 4–5 = >1.6 g cm^{-3}.

There is an option to correct the daily precipitation data for the systematic error of Hellmann measurements at 1m height compared to soil surface precipitation. For Germany the model uses an external table according to Richter (1995) with monthly correction factors which have to be modified when the model is used in other regions. However, the correction can be switched off to use the original data. A crop specific potential evapotranspiration (PET) is calculated from daily weather data. Presently, four options of evapotranspiration formula are included in the model:

- Calculation of PET with the empirical HAUDE formula (Haude, 1955) using crop specific monthly coefficients of Heger (1978) and the daily vapour pressure deficit at 2 p.m.,
- Calculation of a reference evapotranspiration for grass with the TURC-WENDLING formula (Wendling et al., 1991). The formula requires the diurnal average temperature and global radiation sum.
- Calculation of grass reference evapotranspiration using the Penman Monteith approach (Allen et al., 1998) which requires additionally the daily average wind speed and average relative humidity.
- Calculation of grass reference evapotranspiration according to Priestley-Taylor (Priestley and Taylor, 1972) which requires daily minimum and maximum temperature and global radiation only.
- Reading pre-calculated reference evapotranspiration directly from the weather file.

For the latter three formulas the model uses crop coefficients (kc) describing the relation between crop and reference grass evapotranspiration to calculate potential evapotranspiration specific to the crop growth stage and soil coverage. The relative factors can be defined for bare soil and within the crop parameter file for the end points of development stages. Within the end points of development stages there is a linear interpolation for kc values. Sunshine duration can be used instead of global radiation using the Ångström formula (Ångström, 1924). As an additional option a grass reference evapotranspiration from any other externally calculated formula can be given in the weather data file. Recent versions of HERMES (Kersebaum and Nendel, 2014) allow to consider the effect of changing CO_2 concentrations of the atmosphere on crop transpiration using an approach of Yu et al. (2001) to modify the stomatal conductance within the Penman Monteith calculation procedure:

$$r_s = \frac{C_s\left(1+\frac{D}{D_0}\right)}{a \cdot A_g} \quad \textbf{(1)}$$

where *a* is a constant, A_g denotes the gross photosynthesis rate, D/D_0 describes the air water vapour deficit and C_s is the ambient CO_2 concentration at leaf level, which was set equal to C_a in this case. D_0 and *a* were used for parameter calibration using the data of the German FACE experiment (Weigel and Dämmgen, 2000).

Partitioning between evaporation and transpiration is a function of leaf area index (LAI), estimated by the crop growth model. The calculation of actual evaporation and transpiration considers the soil water status and vertical root distribution of specific crops, using an empirical function (Gerwitz and Page, 1974) to distribute the dry matter allocated to the roots over depth. Maximum rooting depth can be defined for soil profiles as a default for wheat and modified if crop specific rooting depth is different from cereals.

2.2 Soil temperature simulation

The vertical temperature distribution in the soil profile (Ts_i) is calculated with a spatial resolution of 10 cm for each layer i with:

$$Ts_{i,t+\Delta t} = Ts_{i,t} \cdot \alpha_{i,t} \cdot (Ts_{i+1,t} - 2 \cdot Ts_{i,t} + Ts_{i-1,t}) \cdot \Delta t/\Delta z^2 \quad \textbf{(2)}$$

with

$$\alpha i,t = \lambda i,t \,/\, cwi,t \quad \textbf{(3)}$$

which uses the layer specific heat conductivity $\lambda_{i,t}$ and the heat capacity $cw_{i,t}$ at time t. The heat capacity $cw_{i,t}$ is calculated for each time step from the constant heat capacity of the dry soil considering the organic matter content and the time variable air and water content of each soil layer. Heat conductivity $\lambda_{i,t}$ considers soil bulk density, organic matter content and the simulated water content.

2.3 Nitrogen dynamics

The N mineralisation sub-module follows the concept of net-mineralisation, simulating mineral N release from two pools of potentially decomposable organic matter according to first-order kinetic reactions:

$$N_{\min}(t) = N_{slow} * (1 - e^{-k_{slow}(T,\Theta)*t}) + N_{fast} * (1 - e^{-k_{fast}(T,\Theta)*t}) \qquad \textbf{(4)}$$

Pools are conceptually derived from incubation experiments, and mathematically separating N release into two pools with different reaction coefficients (Richter et al., 1982). The basic size of the slow mineralisable pool was derived from soil organic matter nitrogen using a standard percentage of 13% according to Nuske (1983). However, this percentage has to be adjusted depending on site conditions and history. Another possibility is to run the model for a longer period of about 20 years in advance with the typical weather and management to let the pools equilibrate to the conditions.

Resistant compounds from crops are added to this slow decomposing pool at harvest time. A smaller, much faster mineralising pool is fed by easily decomposable compounds of different crop residues and manure. Nitrogen in crop residues recycled to the soil is calculated automatically using the simulated N uptake and a crop specific relation of the N export with the yield allowing simulation of complete rotations. Daily mineralisation coefficients are calculated based on the mean soil temperature using two Arrhenius functions from Nuske (1983) and Nordmeyer and Richter (1985):

$$k_{slow} = 4.0 * 10^{9} * e^{-8400/(T+273)} \qquad \textbf{(5)}$$

$$k_{fast} = 5.6 * 10^{12} * e^{-9800/(T+273)} \qquad \textbf{(6)}$$

Soil moisture effects on N mineralisation are implemented according to Myers et al. (1982). Daily denitrification N_{den} (kg N ha^{-1}) is simulated for the top soil (0–30 cm depth) using Michaelis–Menten kinetics, modified by reduction functions dependent on water-filled pore space (Θr) and temperature (T) (Richter and Söndgerath, unpublished, cited in Schneider, 1991):

$$N_{den} = \frac{V_{\max} * (NO_3)^2}{(NO_3)^2 + K_{NO3}} * f(\Theta_r) * f(T) \quad \textbf{(7)}$$

with a maximum denitrification rate Vmax (1.274 kg N ha^{-1} day^{-1}), the soil nitrate content NO_3 (kg NO_3-N ha^{-1}) in 0-30 cm and the Michaelis–Menten coefficient for nitrate K_{NO3} (74 kg NO_3-N ha^{-1}) and functions for water content and temperature:

$$f(\Theta_r) = 1 - e^{-(\frac{\Theta_r}{\Theta_{crit}})^6} \quad \textbf{(8)}$$

$$f(T) = 1 - e^{-(\frac{T}{T_{crit}})^{4.6}} \quad \textbf{(9)}$$

Critical values T_{crit} for air temperature and Θ_{crit} for water-filled pore space are set to 15.5 °C and 0.766 cm^3 cm^{-3} pore space, respectively.

2.4 Plant growth

The sub-model for crop growth represents a generic approach, which is able to simulate different crops using external crop parameter files. The sub-model was built on the basis of the SUCROS model (Van Keulen et al., 1982). Driven by global radiation and temperature, the daily net dry matter production by photosynthesis and respiration is simulated.

Three different algorithms to consider the response of photosynthesis to [CO_2] were taken from the literature and tested in the framework of the HERMES model:

I) The Mitchell approach (Mitchell et al. 1995) used a set of algorithms based on the ideas of Farquhar and von Caemmerer (1982) and Long (1991), calculating the maximum photosynthesis rate

$$A_{\max} = \frac{(C_i - \Gamma^*) \cdot V_{c\max}}{C_i + K_c \cdot \left(1 + \frac{O_i}{K_o}\right)} \quad \textbf{(10)}$$

where C_i and O_i are the intercellular CO_2 resp. O_2 concentrations, Γ^* is the CO_2 compensation point of photosynthesis in absence of dark respiration, V_{cmax} is the maximum Rubisco saturated rate of carboxylation, and K_C and K_O are Michaelis-Menten constants for CO_2 and O_2. The calculation of the latter four parameters is carried out according to Long (1991). Some modifications were applied to simplify the algorithms for suboptimal light conditions and light use efficiency.

II) The Nonhebel approach is a much simpler approach extracted from the SUCROS87 model (Nonhebel 1996). Here, the initial light use efficiency (*EFF*) is directly affected by CO_2 as

$$EFF = \left(\frac{C_a - \Gamma}{C_a + 2\Gamma}\right) \cdot E_0 \quad \textbf{(11)}$$

where C_a denotes [CO_2] and E_0 the quantum use efficiency. Additionally, the maximum photosynthesis rate at light saturation is influenced by CO_2 using

$$A_{\max(CO_2)} = \frac{C_a - \Gamma}{350 - \Gamma} \cdot A_{\max(350)} \quad \textbf{(12)}$$

III) The Hoffmann approach (Hoffmann 1995) was similar to Nonhebel (1996) and is based on his own work with sugar beet and tree species and on data previously obtained by Gaastra (1959). He adjusted A_{max} by the factor

$$K_{CO_2} = \frac{\dfrac{C_a - \Gamma^*}{k_1 + C_a - \Gamma^*}}{\dfrac{C_{a0} - \Gamma^*}{k_1 + C_{a0} - \Gamma^*}} \quad \textbf{(13)}$$

where C_{a0} denotes the ambient [CO_2] and C_a the elevated [CO_2]. Furthermore, k_1 = 220 + 0.158 · I_g and Γ^* = 80 – 0.0036 · I_g, with I_g being the global radiation.

Dry matter production is partitioned depending on crop development stage, which is calculated from a thermal sum or degree days (°C days), modified for each stage by day length and vernalisation if applicable for a specific crop. Up to five different crop organs and ten development stages can be defined in the parameter file for partitioning (Table 2 and 3). Root dry matter is distributed over depth according to Gerwitz and Page (1974), with the rooting depth increasing exponentially with the above-mentioned modified thermal sum until a crop and soil specific maximum is reached. Grain yield is estimated at harvest from the weight of the storage organ.

Table 2: Basic crop parameters (head of crop parameter file) of HERMES (name of crop compartment can be defined by the user.

Crop: winter wheat	
Crop no./abbreviation..	1 WW
AMAX: Max. CO_2 assimilation rate (kg CO_2/ha leave/h)............................	52
Type of temperature dependency (C3 = 1/C4 = 2)....................................	1
Minimum temperature crop growth (degree Celsius)..............................	4
Maximum effective rooting depth (dm)..	12
Root distribution function no. (only 1 available)......................................	1
Crop N-content function no. (critical and max. N-contents).....................	1
Aboveground organs (numbers of compartiments increasing order)........	234
Start concentration N in ab. gr. biomass (% i. d.m.)..................................	2.0
Start concentration N in roots (% i. d.m.)...	2.0
Number of crop compartiments...	4
Compartments.. **1**root **2**leave **3**stem **4**ears	**5** –
Initial weight kg d.m./ha......................... 00053.. 00053.. 00000.. 00000..	00000
Maintenance rates of organs...................... 0.010.. 0.030.. 0.015.. 0.010..	0.000
Initial k_c factor for evapotranspiration..	0.5
Number of development phases..	6

Nitrogen recycling through crop residues is calculated automatically from the simulated crop nitrogen uptake minus the nitrogen exported at harvest with yield and removed side-products (straw, leaves, etc.). The distribution of nitrogen in the residues to the pools is set in an external parameter file for residues.

Table 3: Specific crop parameters required for each development stage (number of stages are defined by the user in the header (see table 2). Example for winter wheat.

Development phase 1: sowing to emergence					
Development phase 1 temperature sum					140
Base temperature in phase 1					1
Vernalization requirements (days)					0
Daylength requirements (hours)					0
Base day length in phase 1(hours)					0
Drought stress below AET/PET-quotient of					1
Critical air content in topsoil (cm^3 cm^{-3})					0.08
Specific leave area (area per d.m. mass) (m^2 kg^{-1})					0.002
N-content root end of 1. phase					0.02
Compartments	1root	2leave	3stem	4ears	5 –
Partitioning at emergence	0.500	0.500	0.000	0.000	0.000
Death rate at end of phase 1	0.000	0.000	0.000	0.000	0.000
k_c factor for evapotranspiration at end of phase 1					0.65
Development phase 2: emergence to double ridge					
Development phase 2 temperature sum					284
Base temperature 2					1
Verbalization requirements (days)					50
Daylength requirements (hours)					20
Base day length in phase 2 (hours)					0
Drought stress below AET/PET-quotient of					0.8
Critical air content in topsoil (cm^3 cm^{-3})					0.08
Specific leave area (area per d.m. mass) (m^2 kg^{-1})					0.002
N-content root end of 2. phase					0.02
Compartments	1root	2leave	3stem	4ears	5 –
Partitioning at end of phase 2	0.200	0.600	0.200	0.000	0.000
Death rate at end of phase 2	0.000	0.000	0.000	0.000	0.000
k_c factor for evapotranspiration at end of phase 2					1.1
Development phase 3: double ridge to ear emergence					
-					
-					
Development phase 4: ear emergence to flowering					
-					
-					
Development phase 5: grain filling					
-					
-					
Development phase 6: senescence					
development phase 6 temperature sum					25
Base temperature 6					9
Verbalization requirements (days)					0
day length requirements (hours)					0
Base day length in phase 6(hours)					0
drought stress below AET/PET-quotient of					0.6
critical air content in topsoil(cm^3 cm^{-3})					0.08
specific leave area (area per d.m. mass) (m^2 kg^{-1})					0.002
N-content root end of 6. phase					0.010
Compartments	1root	2leave	3stem	4ears	5 –
Partitioning at end of phase 6	0.000	0.000	0.000	0.000	0.000
death rate at end of phase 6	0.000	0.050	0.000	0.000	0.000
k_c factor for evapotranspiration at end of phase 6					0.25

Crop growth is limited by water and nitrogen stress. Drought stress is indicated by the ratio of actual to potential transpiration. Sensitivity of the crop to this ratio can be adjusted for each development stage in the parameter file (Table 3). Temporary limitation of soil air by water logging is considered through reducing transpiration and photosynthesis according to Supit et al. (1994). For this, a critical percentage of air filled pores has to be defined in the crop parameter file. Water and nitrogen uptake are calculated from potential transpiration and crop nitrogen status, depending on the simulated root distribution and water and nitrogen availability in different soil layers (Kersebaum 1995). The concept of critical N concentration in plants as a function of crop developmental stage (Kersebaum and Beblik 2001) or as a function of crop biomass (Greenwood et al., 1990) is applied to assess the impact of N shortage. First attempts have been made using the latter type of relation to consider nitrogen shortage for potatoes and sugar beets from literature (Kabat et al. 1995, Greenwood & Draycott, 1995, IIRB, 2003). Duval et al. (2003) found a strong similarity between the critical N dilution curve of sugar beets and potatoes. Leviel et al. (2003) used the generalized curve of Greenwood et al. (1990) to consider nitrogen stress in a CERES approach for sugar beets. This generalized function was also used for HERMES as a first attempt for potatoes and sugar beets.

3. Model limitations

The model is focussed on the most relevant processes in the soil-crop system under central European conditions. Therefore, several processes which might be important under different climatic and soil conditions are not sufficiently covered or have not yet been sufficiently tested. Therefore, some information about the main limitations and current constructions of the model should be given here. For example the soil temperature module so far uses an average parameter for solid soil and does not yet consider the differences between clay, silt and sand material. At some specific sites the model requires additional testing, e.g., the simulation of nitrogen dynamics in organic soils. A clear gap is that the model presently does not cover surface runoff and erosion processes. Actually the capacity approach does not allow for water logging at surface or in the profile. A modified approach using retardation factors is currently under construction which will also contribute to close the surface runoff gap. Although the model includes a simplified procedure to consider capillary rise from shallow groundwater, the consideration of fluctuating groundwater level is still problematic. Finally, nitrogen dynamics are not linked to carbon dynamics with the consequence that short term immobilization is not considered.

4. References

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