Table 12.1 Block **A** – **Basic** Information

Record	Type	Symbol	Description
1,2			Comment lines
3	Char	*Hed*	Heading
4			Comment line
4.1.	Logical	*icheck*	**.true.** enables writing output file 'icheck.out', contains information on the inputs
4.2.	Logical	*run_inf*	**.true.** enables writing output file 'run_inf.out' contains warning messages during execution
4.3.	Logical	*t_level*	**.true.** enables writing output file 't_level.out' contains information for specified print times
4.4.	Logical	*a_level*	**.true.** enables writing output file 'a_level.out' contains information for each atmospheric time step
4.5.	Logical	*co2_inf*	**.true.** enables writing output file 'co2_inf.out', contains CO_2 fluxes and concentrations for each atmospheric time step
4.6.	Logical	*nod_inf*	**.true.** enables writing output file 'nod_inf.out', contains node-specific information for specified print times
4.7.	Logical	*balance*	**.true.** enables writing output file 'balance.out', contains water, nitrogen and CO_2 balance
4.8.	Logical	*point*	**.true.** enables writing output file 'point.out', contains information for observation nodes at all atmospheric time steps
4.9.	Logical	*nod_pool*	**.true.** enables writing output file 'nod_pool.out', contains node-specific C and N pools for atmospheric time steps
4.10.	Logical	*reduction*	**.true.** enables writing output file 'reduction.out', contains node-specific C and N turnover rate modifiers for atmospheric time steps
4.11.	Logical	*nod_prod*	**.true.** enables writing output file 'nod_prod.out', contains node-specific CO_2 production
4.12.	Logical	*matlab*	**.true.** enables writing output file 'matlab.out', contains a set of out variables for each atmospheric time step
4.13.	Logical	*invers*	**.true.** enables writing output file 'invers.out'
4.14.	Logical	*term*	**.true.** enables writing output to the screen terminal
5.1.	Char	*LUnit*	Length unit (e.g. mm, cm or m)
5.2.	Char	*TUnit*	Time unit (e.g. hour or day)
5.3.	Char	*MUnit*	Mass unit for the concentration variables (e.g. mg, g or kg)
5.4.	Integer	*MaxIt*	Maximum number of iterations allowed during any time step (usually 20)

5.5.	Real	*TolTh*	Absolute water content tolerance for nodes in the unsaturated part of the flow region [-] (its recommended value is 0.0001). *TolTh* represents the maximum desired absolute change in the value of the water content , $\theta_{w,}$ between two successive iterations during a particular time step.
5.6.	Real	*TolH*	Absolute pressure head tolerance for nodes in the saturated part of the flow region [L] (its recommended value is 0.1 cm). *TolH* represents the maximum desired absolute change in the value of the pressure head, *h*, between two successive iterations during a particular time step.
5.7.	Logical	*QuitNC*	**.true.** if program execution should be aborted in case convergence in the water flux is not given; **.false**. if the original handling of no convergence in the water flux is intended
6.1.	Logical	*Short0*	**.true.** if printing of output at each time level (time-level information) is to be suppressed and the information printed only in specified print times; **.false.** if this information is to be printed on each time level
6.2.	Logical	*lWat*	Set this logical variable equal to **.true.** if transient water flow is to be considered. Set equal to **.false.** if initial condition given in Block B (e.g. *hOld*) is to be kept constant throughout the simulation.
6.3.	Logical	*lCO2*	Set this logical variable equal to **.true.** if carbon dioxid transport is to be considered.
6.4.	Logical	*lRoot*	Set this logical variable equal to **.true.** if the root growth is to be considered.
6.5.	Logical	*lTemp*	Set this logical variable equal to **.true.** if heat transport is to be considered.
6.6.	Logical	InitWC	**.true.** if the node-specific initialization of the water flux model with water content is intended **.false.** if the original node-specific initialization of the water flux model with pressure head is intended
6.7.	Logical	*Plants*	Set this logical variable equal to **.true.** if crop growth is to be considered; 'plants.in' required
6.8.	Logical	*Nitrogen*	Set this logical variable equal to **.true.** if nitrogen transport and uptake is to be considered; input Blocks I and J and Tab. 13 to 17 in 'plants.in' required
6.9.	Logical	*Phosphorus*	Set this logical variable equal to **.true.** if Phosphorus transport and uptake is to be considered; input Blocks J and K and input in 'plants.in' required

6.10.	Logical	*Transport*	Set this logical variable equal to **.true.** if solute transport is to be considered; Block J required. Note: set equal to **.true.**, when leaching output in 'a_level.out' for nitrogen or phosphorous transport is wanted
7.1.	Logical	*TopInf*	**.true.** if time dependent boundary condition is to be imposed at the top of the profile; data are supplied via input file 'atmosph.in'. **.false.** in the case of time independent surface boundary conditions.
7.2. 7.2.	Logical	*AtmBC*	**.true.** if variable boundary conditions are supplied via the input file 'atmosph.in', **.false.** if the file 'atmosph.in' is not provided (i.e., in case of time independent boundary conditions).
7.3.	Logical	*SinkF*	Set this variable equal to **.true.** if the water extraction from the root zone occurs.
7.4.	Logical	*WLayer*	Set this variable equal to **.true.** if water can accumulate at the surface with zero surface runoff.
7.5.	Logical	*lAmpl*	**Optional**: **.true.** if time dependent amplitudes of the daily temperature for the daily amplitude concept should be read as column 12 from atmosph.in (**Note**: Only works with kProd=3) **.false.** column 12 is not read from atmosph.in Default setting is **.false.**
8.1.	Logical	*BotInF*	**.true.** if time dependent boundary condition is to be imposed at the bottom of the profile; control data are supplied via input file ATMOSPH.IN **.false.** in case of time independent bottom boundary conditions.
8.2.	Logical	*qGWLF*	Set this variable equal to **.true.** if the discharge-groundwater level relationship q_w (GWL) is applied as bottom boundary condition.
8.3.	Logical	*FreeD*	**.true.** if free drainage is to be considered as bottom boundary condition.
8.4.	Logical	*SeepF*	**.true.** if seepage face is to be considered as bottom boundary condition.
9.1.	Integer	*KodTop*	Code specifying type of boundary conditions (BC) for water flow at the surface. Code number is positive for Dirichlet BC and negative for Neumann BC. In the case of ´Atmospheric BC´ set *KotTop=**-1***.
9.2.	Integer	*KodBot*	Code specifying type of boundary condition for water flow at the bottom of the profile. Code number is positive for a Dirichlet BC and negative for a Neumann BC. In case of a seepage face or free drainage BC set

			KodBot=***-1***.In case of *KodBot*=**6** bottom boundary will be defined as open column MSO boundary.
9.3.	Real	*HTop*	**Optional:** Prescribed pressure head at the top at t=0, only relevant if the water flux is initialised with pressure heads instead of water content (initWC=.true.) **Note:** If initWC is .false. the input for HTop must be removed.
9.4.	Real	*HBottom*	**Optional:** Prescribed pressure head at the bottom at t=0, only relevant if the water flux is initialised with pressure heads instead of water content (initWC=.true.) **Note:** If initWC is .false. the input for *HBottom* must be removed.
10.1.	Real	*rTop*	Prescribed top flux [LT^{-1}] (in case of a Dirichlet BC set this variable equal to zero).
10.2.	Real	*rRoot*	Prescribed potential transpiration rate [LT^{-1}] (if no transpiration occurs or if transpiration is variable in time set this variable in time set this variable equal to zero).
10.3.	Real	*rBot*	Prescribed bottom flux [LT^{-1}] (in case of a Dirichlet BC set this variable equal to zero).
10.4.	Real	*hCritS*	Maximum allowed pressure head at the soil surface [L].
10.5.	Real	*hCritA*	Absolute value of minimum allowed pressure head at the soil surface.
11.1.	Real	*xSurf*	z-coordinate of the uppermost node (=soil surface)
11.2.	Real	*GWL0L*	Reference position of the groundwater table (e.g., the z-coordinate of the soil surface).
11.3.	Real	*Agh*	Value of the parameter A, [LT^{-1}] in the q_w(GWL)-relationship, equation (10.1); set to zero if *qGWL*=**.false.**
11.4.	Real	*Bgh*	Value of the parameter B_{qh} [L^{-1}] in q_w (GWL)-relationship, equation (10.1); set zero if *qGWL*=**.false.**

Table 12.2 Block **B** – **Nodal** Information

Record	Type	Symbol	Description
1			Comment lines.
2.1.	Integer	*NumNP*	Number of nodal points.
2.2.	Integer	*NMat*	Number of soil materials. Materials are identified by the material number, *MatNum*, specified in Block B.
2.3.	Integer	*NLay*	Number of subregions for which separate water balances are being computed. Subregions are identified by the subregions number, *LayNum*, specified in Block B.
2.4.	Integer	*NObs*	Number of observation nodes for which values of pressure head, the water content, temperature (for *lTemp*=**.true.**), and carbon dioxide (for *lCO2*=**.true.**) are printed at each time level.
2.5.	Integer	*NSolutes*	Number of solutes. If logical variable *Nitrogen* is **.true.** set *NSolutes*=3.
3	Integer	*ObsNod*	Observation points (listed starting with highest value).
4	Real	*dx*	dx-increments [L] (*NumNP*-1 items). Specify the number of increments and the spatial distance between nodes, separated by '*'
5.1.	Integer	*Node*	Nodal number
5.2.	Real	*hOld*	Initial value of the pressure head at node n [L] If *lWat*=**.false. (**Block A), then *hOld(n)* represents the pressure head which will be kept constant during simulation. Note: If *initWC* (Block A) is **.true.** the initial water content [-] has to be specified for the nodes
5.3.	Integer	*MatNum*	Index for material whose hydraulic and transport properties are assigned to node *n*.
5.4.	Integer	*LayNum*	Subregion number assigned to node *n*.
5.5.	Real	*Beta*	Value of the water uptake distribution, h(z) [L^{-1}], in the soil root zone at node *n*. Set *Beta(n)* equal to zero if note *n* lies outside in the root zone.
5.6.	Real	*Co2Conc*	Initial value of the carbon dioxide concentration at node *n* [L^3L^{-3}].
5.7.	Real	*Temp*	Initial soil temperature at node *n* [°C].
5.8.	Real	*Conc(1)*	Initial concentration of the first solute at node n [M/L^3].
5.9.	Real	*Conc(2)*	Initial concentration of the second solute at node n [M/L^3].
5.10	Real	*Conc(NSolutes)*	Initial concentration of the NSolutesth solute at node n [M/L^3].

Note: If logical variable *Nitrogen* is **.true.** *Conc(1)* is the initial concentration of Urea, *Conc(2)* is the initial concentration of liquid phase Ammonium and *Conc(3)* is the initial concentration of Nitrate.

Table 12.3 Block **C** – **Material** Information

Record	Type	Symbol	Description
1			Comment line
2.1.	Real	*hTabMin*	Absolute value of the lower limit [L] of the pressure head interval for which a table of hydraulic properties will be generated internally for each material (e.g. 1000 m). One may assign to h_b the highest (absolute) expected pressure head to be expected during a simulation. If the absolute value of the pressure head during program execution lies outside of the interval [h_a,h$_b$], then appropriate values for the hydraulic properties are computed directly from the hydraulic functions (i.e., without interpolation in the table).
2.2.	Real	*hTabMax*	Absolute value of the upper limit [L] of the pressure head interval below which a table of hydraulic properties will be generated internally for each material (h_a must be greater than 0.0; e.g. 0.001 cm, see section 7.4.7 Unsatchem.pdf).
2.3.	Integer	*NPar*	Number of parameters specified for each material in records 4.1. to 4.13 (θ_s, θ_r, α, n, Ks, tau = Bpar) (i.e., 9 in case of the modified van Genuchten`s model (hysteresis) or 13 in case of Durner's bimodal model).
2.4	Integer	*iModel*	1 = Mualem van Genuchten with 10 parameters (θ_s, θ_r, α, n, Ks, tau or lambda= Bpar) (see 2.3) 2= Durner Model (dual porosity) additional 3 parameters (w2, α2, n2)
2.5	Integer	*NTab*	Number of entries for the internal interpolation table for θ(h) and K(h). If not defined NTab will be set to 100
4.1.	Real	*Par(1,M)*	Parameter θ_r for material M [-]
4.2.	Real	*Par(2,M)*	Parameter θ_s for material M [-]
4.3.	Real	*Par(3,M)*	Parameter θ_a for material M [-]
4.4.	Real	*Par(4,M)*	Parameter θ_m for material M [-]
4.5.	Real	*Par(5,M)*	Parameter α for material M [L^{-1}]
4.6.	Real	*Par(6,M)*	Parameter n for material M [-]
4.7.	Real	*Par(7,M)*	Parameter K_s for material M [LT^{-1}]
4.8.	Real	*Par(8,M)*	Parameter K_k for material M [LT^{-1}]
4.9.	Real	*Par(9,M)*	Parameter θ_k for material M [-]
4.10.	Real	*Par(10,M)*	Parameter λ (tortuosity) for material M [-]
4.11	Real	*Par(11,M)*	Parameter w2 (weighting factor Durner model) for material M [-]

4.12	Real	*Par(12,M)*	Parameter α2 (alpha for macropore domain Durner model) for material M [-]
4.13	Real	*Par(13,M)*	Parameter n2 (n for macropore domain Durner model) for material M [-]

Table 12.4 Block **D** – **Time** Information

Record	Type	Symbol	Description
1			Comment line
2.1.		*dtInit*	Initial time increment Δt [T]. Initial time step should be estimated based on the problem being solved. For problems with high pressure gradients (e.g. infiltration into an initially dry soil), Δt should be relatively small.
2.2.	Real	*dtMin*	Minimum permitted time increment, Δt_{min} [T].
2.3.	Real	*dtMax*	Maximum permitted time increment, Δt_{max} [T].
2.4.	Real	*DtMul*	If the number of required iterations at a particular time step is less than or equal to 3, then Δt for the next time step is multiplied by a dimensionless number *dMul* ≥.0 (it is recommended that this value not exceed 1.3).
2.5.	Real	*DtMul2*	If the number of required iterations at a particular time step is greater than or equal to 7, then At for the next time step is multiplied by *dMul2* ≤ 1.0 8e.g. 0,33).
2.6.	Integer	*NumOfPrints*	Number of specified print-times at which detailed information about the pressure head, water content, flux, temperature, CO_2, solute concentrations, water, CO_2,and solute balances will be printed.
3.1.	Real	*TPrint (1)*	First specified print-time [T].
3.2.	Real	*TPrint (2)*	Second specified print-time [T].
3.3.	Real	*TPrint (MPL)*	Last specified print-time [T]. All print-time have to be within one line.

Table 12.5 Block **G** – **Heat** Transport Information

Record	Type	Symbol	Description
1			Comment line
2.1.	Real	*Ampl*	Temperature amplitude at the soil surface [K].
2.3.	Real	*tPeriod*	Time interval for completion of one temperature cycle (usually 1 day) [T].
3.1.	Integer	*kTopT*	Code which specifies the type of upper boundary condition =1: Dirichlet boundary condition, =-1: Cauchy boundary condition.
3.2.	Real	*tTop*	Temperature of the upper boundary, or temperature of the incoming fluid [°C].
3.3.	Integer	*kBotT*	Code which specifies the type of lower boundary condition =1: Dirichlet boundary condition, =0: continuous temperature profile, zero gradient, =-1: Cauchy boundary condition.
3.4.	Real	*tBot*	Temperature of lower boundary, or temperature of the incoming fluid [°C].
4.1.	Real	*Beta*	Longitudinal thermal dispersivity of material *M*, λ_L [L].
4.2.	Real	*θn*	Volumetric solid phase fraction of material M, *θn* [-].
4.3.	Real	*θo*	Volumetric organic matter fraction of material M, *θo* [-].
4.4.	Real	*B1*	Coefficient b_1 in the thermal conductivity function [$MLT^{-3}K^{-1}$] (e.g. $Wm^{-1}\ K^{-1}$) (see equation (4.6)).
4.5.	Real	*B2*	Coefficient b_2 in the thermal conductivity function [$MLT^{-3}K^{-1}$] (e.g. $Wm^{-1}\ K^{-1}$) (see equation (4.6)).
4.6.	Real	*B3*	Coefficient b_3 in the thermal conductivity function [$MLT^{-3}K^{-1}$] (e.g. $Wm^{-1}\ K^{-1}$) (see equation (4.6)).
4.7.	Real	*Cn*	Volumetric heat capacity of solid phase of material M, *Cn* [$ML^{-1}\ T^{-2}\ K^{-1}$] (e.g. $Jm^{-3}\ K^{-1}$).
4.8.	Real	*Co*	Volumetric heat capacity of organic matter of material M, *Co* [$ML^{-1}\ T^{-2}\ K^{-1}$] (e.g. $Jm^{-3}\ K^{-1}$).
4.9.	Real	*Cw*	Volumetric heat capacity of liquid phase of material M, *Cw* [$ML^{-1}\ T^{-2}\ K^{-1}$] (e.g. $Jm^{-3}\ K^{-1}$).

Table 12.6 Block **H** – **Carbon Dioxide** Transport and Production Information

Record	Type	Symbol	Description
1			Comment line
2.1	Logical	*lStagn*	Set this variable equal to **.true.** if the gas phase is to be considered stagnant, e.i., there is no gas convention. Otherwise the simplified gas convection expression is considered (see section 5.1.).
2.2	Integer	*iGasDiff*	**Optional**: Code specifying the estimation of the effective diffusion coefficient **=1**: Millington & Quirk (1963) (original soilco2) **=2**: Moldrup et al. (2000) **=3**: Moldrup, Olesen et al. (2000), (Parameters *Eps100* and *Campb* required) **=4**: double linear function according to Weihermüller er al. (2008) **=5**: Kristensen et al. (2010), parameters *Eps*, *H* and *Xm* required (**Note**: If iGasDiff is not specified the default of 1 (Millington & Quirk 1963) is applied)
2.3	Real	*CO2dtmin*	**Optional**: In case a value >0 is given, this value is used as the minimum time step in the routine that controls the time step according to the CO2 flux. For negative values the default time stepping according to the water flux is enabled. (**Note**: Could only be used if iGasDiff is given as previous record)
3.1.	Integer	*kTopCO*	Code specifying type of boundary condition (BC) for the CO_2 transport at the soil surface. Code number is positive for Dirichlet BC and negative for stagnant boundary layer at the soil surface.
3.2.	Real	*CO2Top*	Value of the time independent BC at the surface [L^3L^{-3}]. For *kTopCO*<0 *CO2Top* represents the thickniss of the stagnant boundary layer [L].
3.3.	Integer	*kBotCO*	Code specifying type of boundary condition at the bottom of the profile. Code number is positive for Dirichlet and negative for Cauchy BC. In the case of `Free drainage´ set *kBotCO*=0.
3.4.	Real	*CO2Bot*	Value of the time independent BC at the bottom of the soil profile [L^3L^{-3}]. In case of `Free drainage´ set *CO2Bot*=0.
4.1.	Real	*DispA*	Molecular diffusion coefficient of CO_2 in air at 20°C, D_a [L^2T^{-1}].
4.2.	Real	*DispW*	Molecular diffusion coefficient of CO_2, in water at 20°C, D_w [L^2T^{-1}].

4.3.	Real	*Disper*	Longitudinal dispersivity of CO_2 of material M, D_L [L]. The same record as above must be provided for each material *M* (specified *NMat*).
4.4.	Real	*Eps100/Eps*	**Optional:** Parameter *Eps100* (iGasDiff=3) or fracture porosity *Eps* [-] for iGasdiff=5
4.5.	Real	*Campb/H*	**Optional:** Parameter *Campb* (iGasDiff=3) or fracture tortuosity factor *H* [-] for iGasdiff=5
4.6	Real	*Xm*	**Optional:** Matrix tortuosity factor *Xm* [-] for iGasdiff=5
5.1.	Real	*gamSO*	Optimal CO_2 production by soil microorganisms for the whole soil profile at 20°C under optimal water, solute, and CO_2 concentration condition, γ_{s0} [$L^3L^{-2}T^{-1}$].
5.2.	Real	*gamRO*	Optimal CO_2 production by plant roots for the whole soil profile at 20°C under optimal water, solute, and CO_2 concentration conditions γ_{r0} [$L^3L^{-2}T^{-1}$].
5.3.	Real	*PDDMax*	The cumulative value of temperature when the CO_2 production reaches the maximum value. Set equal to zero if degree day concept is not used to calculate the time reduction coefficient for plant CO_2 production. In that case the time reduction coefficient is equal to one during the whole season.
5.4.	Integer	*kProd*	Code specifying the type of spatial distribution function for CO_2 production by soil microorganisms. =0: Exponential function. =1: van Genuchten`s distribution function. =3: Carbon pools (RothC)
6	Real	*xR*	Maximum depth of the CO_2 soil production (only if *kProd*=1) [L].
7.1.	Real	*B1*	Activation energy of the CO_2 production by soil microorganisms E [$ML^2T^{-2}M^{-1}$], divided by universal gas constant R [$ML^2T^{-2}K^{-1}M^{-1}$]; $B_1=E_1/R$ [K].
7.2.	Real	*B2*	Activation energy of the CO_2 production by plant roots E_2 [$ML^2T^{-2}M^{-1}$], divided by universal gas constant R [$ML^2T^{-2}K^{-1}M^{-1}$]; $B_2=E_2/R$ [K].
7.3.	Real	*cM1*	Michaelis` constant of CO_2 production by plant roots [L^3L^{-3}]. It is equal to the CO_2 concentration at which the CO_2 production is reduced by half from the optimal value γ_{r0}.
7.4.	Real	*cM2*	Michaelis` constant of CO_2 production by plant roots [L^3L^{-3}]. It is equal to the CO_2 concentration at which the CO_2 production is reduced by half from the optimal value γ_{s0}.

7.5.	Real	*HB1*	Value of pressure head at which the CO_2 production by soil micro-organisms is at the optimal level [L].
7.6.	Real	*HB2*	Value of the pressure head below which the CO_2 production by soil micro-organisms ceases [L].
7.7.	Real	*fS6*	additional scaling factor for the rate constants
7.8.	Real	*Patm*	**Optional**: atmospheric pressure; **Note**: in case 7.8. to 7.10. are not specified the default values of SoilCO2/RothC are used.
7.9.	Real	*gasconst*	**Optional**: Gas constant
7.10.	Real	*MolCO2*	**Optional**: Molecular weight of CO_2
8.1.	Real	*kDPM*	Decomposition rate constant of DPM pool [1/T].
8.2.	Real	*kRPM*	Decomposition rate constant of RPM pool [1/T].
8.3.	Real	*kBIO*	Decomposition rate constant of BIO pool [1/T].
8.4.	Real	*kHUM*	Decomposition rate constant of HUM pool [1/T].
8.5.	Real	*Pdepth*	Depth to which fresh plant is incorporated [L].
8.6.	Real	*CO2alf*	Choose initial pool distribution over depth **=-1.0** one input value for each node (order is node n to 1) **=0.0** one input value for each material (order is 1 to n materials) **>0.0** one input value for each pool, exponential distribution of initial concentration on the nodes. Could only be used when a single material was specified for the entire soil profile. CO2alf is the scaling factor in an exponential approach to distribute the pool over depth (defines the slope of the exponential function).
9.1.	Integer	*iredW*	Choose moisture reduction function =0 SOILCO2 (Simunek and Suarez 1993) =1 SOILCO2 (Simunek et al. 1996) =2 DAISY, original version =3 CANDY =4 PATCIS =5 CENTURY, hCentury (9.6.) is required =6 ROTHC =7 no reduction =8 DAISY, without reduction function according to soil aeration =10 reduction factors for n water content intervals =11 stepwise linear function.
9.2.	Integer	*iredT*	Choose temperature reduction function =1 SOILCO2 (Simunek and Suarez 1993)

			=2 DAISY =3 CANDY =4 PATCIS =5 CENTURY =6 ROTHC =7 no reduction =8 SOILCO2 with pool dependent activation energy =9 SOILCO2 for four temperature intervals =10 reduction factors for n temperature intervals =11 Kirschbaum et al. 2000 =12 Parton et al. 1987 =13 O'Connel et al. 1990.
9.3.	Integer	*iredCO2 (1;2)*	Choose CO_2 reduction function =0 SOILCO2 =1 SOILCO2 modified by M. Herbst 21/02/06 =3 no reduction ($f(CO_2)=1.0$).
9.4.	Integer	*iReftemp*	Choose reference temperature of input or model =0 input reference temperature (Reftemp) =1 reference temperature of SOILCO2 =2 reference temperature of DAISY =3 reference temperature of CANDY =4 reference temperature of PATCIS =5 reference temperature of CENTURY =6 reference temperature of ROTHC.
9.5.	Real	*Reftemp*	Reference temperature [°C].
9.6.	Real	*hCentury*	**Optional**: Pressure head for the Century approach (Must only be specified for iredw=5).
9.7.	Real	*B1dpm*	Optional: Activation energy for the DPM pool, required only in case iredT=8. (**Note**: To specify the four pool-specific activation energies (record 9.7. to 9.10) hCentury has to be specified as the previous record, even if iredw is not set to 5.)
9.8.	Real	*B1rpm*	**Optional**: Activation energy for the RPM pool, required only in case iredT=8.
9.9.	Real	*B1bio*	**Optional**: Activation energy for the BIO pool, required only in case iredT=8.
9.10.	Real	*B1hum*	**Optional**: Activation energy for the HUM pool, required only in case iredT=8.
			Optional: Input block of 6 lines in case iredW=10 or/and iredT=10. This allows specifying intervals for temperature and water content and respective reduction factors. A number of n intervals could be specified by n-1 thresholds and n reduction factors (Interval 1 (i_1) is defined by <threshold 1 (t_1) for

			reduction factor 1 (f_1), i_2 is defined as $>t_1$ and $<t_2$ for f_2 and so on. The last interval i_n is defined as $>t_{n-1}$ for factor f_n): 1 comment line 2 number of intervals Numlnt 3 comment line 4 Numlnt-1 threshold temperatures defining the Numlnt intervals 5 comment line 6 reduction factor for each of the Numlnt intervals (**Note**: In case water content is specified too, lines 3 to 6 must be given twice. The block for water content should be given first, followed by temperature.)
10	Real		Clay content [M/M]. Required for 1 to NMat.
11.1.	Real	*iDPM*	Initial concentration of the decomposable plant material (DPM) pool [M/L^3]. **Note:** In case the initial pools are defined node-specifically the input is read from n to 1. If the initial pools are defined for each material they are read from 1 to n. That also holds for iRPM, iBIO, iHUM and iIOM
11.2.	Real	*iRPM*	Initial concentration of the resistant plant material (RPM) pool [M/ L^3]. Note: specified for each node, material or each pool, see record 8.6 (*CO2alf),* defining the initial pool distribution over depth
11.3.	Real	*iBIO*	Initial concentration of the biomass (BIO) pool [M/L^3]. Note: specified for each node, material or each pool, see record 8.6 (*CO2alf),* defining the initial pool distribution over depth
11.4.	Real	*iHUM*	Initial concentration of the humus (HUM) pool [M/L^3]. Note: specified for each node, material or each pool, see record 8.6 (*CO2alf),* defining the initial pool distribution over depth
11.5.	Real	*IOM*	Initial concentration of the inert organic matter (IOM) pool [M/L^3]. Note: specified for each node, material or each pool, see record 8.6 (*CO2alf),* defining the initial pool distribution over depth

Table 12.7 Block **I** – **Nitrogen** Mineralisation, Transformation and Uptake Information

Record	Type	Symbol	Description
1			Comment line
2.1.	Logical	*1Npools*	Set this variable equal to **.true.** to enable mineralistion/immobilisation of organic nitrogen
2.2.	Logical	*NrootUpt*	Set this variable equal to **.true.** to enable diffusive and convective root uptake of nitrogen
2.3.	Logical	*Lnfixat*	Set this variable equal to **.true.** to enable nitrogen fixation
2.4.	Real	*Rkfixopt*	Nitrogen fixation rate constant [M L^{-2} T^{-1}]
2.5.	Real	*Denthresh*	Threshold that defines effective saturation denitrification starts. [-] Default value (according to Aulakh et al., 1992) is 0.8. A negative number indicates the use of the denitrification to effective saturation response suggested by DelGrossso et al. 2000.
3			Comment line
4.1.	Real	*Ro*	C/N ratio of the biomass [-]
5.1.	Real	*Fh*	Humification coefficient; WAVE default = 0.4, negative value indicates the use of the RothC value = 0.54 [-]
6			Comment line
7.1.	Real	*Rknitri*	Nitrification rate constant [T^{-1}], liquid phase NH_4 to NO_3
8.1.	Real	*Rkdenit*	Denitrification rate constant [T^{-1}]
9.1.	Real	*Rhyd*	Urea hydrolysis constant [T^{-1}], CH_4N_2O to liquid phase NH_4
10.1.	Real	*Rkvol*	Ammonia volatilization rate constant [T^{-1}], liquid phase NH_4 to NH_3
11.1.	Real	*w0_dens*	Root length density at top [L L^{-3}]
12.1.	Real	*rorad*	Mean root radius [L]
13.1.	Real	*rdo*	Travel distance resistance between bulk soil and root [L^{-1}]
14			Comment line
15.1.	Real	*C2Nfact*	factor of N from C (=N/C), used to calculate initial N pools from initial C pools (defined in block H of selector.in) and to estimate input to N_{lit} and N_{man} pool for organic fertilization [-]
16			Comment line
17.1.	Integer	*nNtimes*	Number of mineral nitrogen fertilizer events [-]
18			Comment line
19.1.	Real	*Ntime(1)*	Timestep of first mineral nitrogen fertilizer application [T]
19.2.	Real	*Ntopurea(1)*	Amount of N applied as Urea [M L^{-2}] at first mineral nitrogen fertilizer application

19.3.	Real	*Ntopnh4(1)*	Amount of N applied as Ammonium [M L^{-2}] at first mineral nitrogen fertilizer application
19.4.	Real	*Ntopno3(1)*	Amount of N applied as Nitrate [M L^{-2}] at first mineral nitrogen fertilizer application. Note: Fertilizer application time step and amount of nitrogen for the three species have to be within one line. Provide as many lines as *nNtimes*.
20			Comment line
21.1.	Real	*iNitLit*	Initial concentration of the decomposable plant material (DPM) nitrogen pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth
21.2.	Real	*iNitMan*	Initial concentration of the resistant plant material (RPM) nitrogen pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth
21.3.	Real	*iNitHum*	Initial concentration of the humus (HUM) nitrogen pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth

Block I need not supplied if logical variable *Nitrogen* (Block A) was set equal to **.false.**.
Note: In order to simulate Nitrogen, logical variable *Transport* can be set to **.false.**, however the input block K for solute transport information is required. This block K contains the solute transport parameters for three species, where solute 1 is Urea, solute 2 is Ammonium and solute 3 is Nitrate.

OUTPUTS
a_level.out – contains leaching of Urea, Ammonium and Nitrate (set logical variable *a_level* to .true.) for every atmospheric time step. Note that logical variable *transport* (rec 6.10, Block A) also has to be .true.
mass.out – contains sums of liquid phase and adsorbed Urea, Ammonium, Nitrate concentrations, Ammonia production over the entire profile, and masses of total mineral and total organic N
nod_inf.out – contains liquid phase and adsorbed Urea, Ammonium, Nitrate concentrations at every node for print times
nod_pool.out – contains organic nitrogen pools at every node for every atmospheric time step (set logical variable *nod_pool* to .true.)
conc.out - contains liquid phase and adsorbed Urea, Ammonium, Nitrate concentrations at every node for every atmospheric time step. Note: This file is written only when logical variable *nod_pool* is .true.
nitrogen.out – contains root uptake and sink term of Ammonium and Nitrate and rates of Urea hydrolysis, nitrification, denitrification and ammonia volatilization

plantupt.out – contains plant organ-specific N demand, total root N uptake rate, convective and diffusive root N uptake rates, organ-specific N masses, growth reduction factor due to N limitation and organ-specific N concentrations

Table 12.8 Block **J** – **Phosphorus** Mineralisation, Transformation and Uptake Information

Record	Type	Symbol	Description
1			Comment line
2.1.	Logical	*1Ppools*	Set this variable equal to **.true.** to enable mineralistion/immobilisation of organic Phosphorus
2.2.	Logical	*ProotUpt*	Set this variable equal to **.true.** to enable diffusive and convective root uptake of Phosphorus
2.3.	Integer	*SoilGen*	Soil genetic classification: 0=calcareous,1=slighlty weathered, 2=moderately weathered, 3=highly weathered
2.4.	Logical	*lPmin*	Set this variable equal to **.true.** to enable sorption of mineral Phosphorus in the P_{ACTIVE} and in the P_{STABLE} pool
3			Comment line
4.1.	Real	*PSP*	Phosphorus sorption parameter PSP [-] defines the fraction of P that remains labile and does not move to P_{ACTIVE}, internally limited to: 0.05<PSP<0.75. Note: records 4.1 to 4.4 are specified for each material.
4.2.	Real	*stab_act_rat*	P_{STABLE} to P_{ACTIVE} ratio [-], should always be >1. Default value suggested by Jones et al. (1984) is 4.0.
4.3.	Real	*rev_rate_mod*	Reverse rate modifier [-], reverse fluxes (P_{STABLE} to P_{ACTIVE} and P_{ACTIVE} to P_{LABILE}) are slowed down by this rate modifier. Default value suggested by Jones et al. (1984) is 0.1.
4.4.	Real	*bo*	P flux coefficient b_o[-] affecting the P_{ACTIVE} to P_{STABLE} flux rate. According to Jones et al. (1984) expressed as =exp(-1.77*PSP-7.05) for non-calcareous soils. For calcareous soils set to 0.0076.
5			Comment line
6.1.	Real	*PhosRo*	C/P ratio of soil biomass [-]
7.1.	Real	*PhosFh*	Organic Phosphorus humification coefficient; WAVE default = 0.4, negative value indicates the use of the RothC value = 0.54 [-]
8			Comment line
9.1.	Real	*RkCMPi*	Humus P mineralization rate constant [T^{-1}], negative value indicates the use of the RothC humus pool rate constant kHUM (Block H, record 8.4.)
10.1.	Real	*Pho_rdo*	Phosphorus travel distance resistance between bulk soil and root [L^{-1}]

11.1.	Real	*P_conv_diff_factor*	Maximum convective to total phosphorus uptake ratio [-]
12			Comment line
13.1.	Real	*P_Fert_lab*	fraction of labile (soluble) Phosphorus in organic fertilizer [-], EPIC default=0.2
14.1.	Real	*P_Fert_C*	Fraction of P from C [-], required to calculate the amount of Phosphorus in organic fertilizer
15			Comment line
16.1.	Integer	*P_Fert_num*	Number of mineral Phosphorus fertilization events [-]
17			Comment line
18.1.	Real	*PTopTime*	Timestep of mineral Phosphorus fertilizer application [T], provide as many lines as *P_Fert_num*.
18.2.	Real	*PTopMass*	Amount of P applied [M L^{-2}] at respective mineral Phosphorus fertilizer application, provide as many lines as *P_Fert_num*.
19			Comment line
20.1.	Real	*P_init_Lit*	Initial concentration of the decomposable plant material (DPM) Phosphorus pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth
20.2.	Real	*P_init_Man*	Initial concentration of the resistant plant material (RPM) Phosphorus pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth
20.3.	Real	*P_init_Hum*	Initial concentration of the humus (HUM) Phosphorus pool [M L^{-3}] Note: specified for each node, material or each pool, see Block H, record 8.6 (*CO2alf),* defining the initial pool distribution over depth

Block J need not supplied if logical variable *Phosphorus* (Block A) was set equal to **.false.**. **Note**: In order to simulate Phosphorus transport, logical variable *Transport* can be set to **.false.**, however the input block K for solute transport information is required. This block K contains the solute transport parameters for Phosphorus. Note: Simulation of Phosphorus transport and uptake is only possible, when nitrogen transport and uptake is also considered. In Block K the fourth solute is P.

OUTPUTS
a_level.out – contains leaching of phosphorus (set logical variable *a_level* to .true.) for every atmospheric time step
mass.out – contains sums of mineral and organic P, as well as total P
nod_inf.out – contains liquid phase and adsorbed P at every node for print times
nod_pool.out – contains organic phosphorus pools at every node for every atmospheric time step (set logical variable *nod_pool* to .true.)

conc.out - contains liquid phase and adsorbed phosphorus concentrations at every node for every atmospheric time step. Note: This file is written only when logical variable *nod_pool* is .true.
phosphorus.out – contains, flux rates from P_{labile} to P_{active} and from P_{active} to P_{stable}, P fraction remaining in the labile pool, crop development stage, temperature sum, P demand of the entire plant, total plant weight, sink term of labile P, actual P content of the entire plant, actual convective root P uptake, total P uptake demand, actual diffusive P uptake, total mass of P in plant, growth reduction factor due to P limitation, source/sink term of labile P concentration (as a consequence of P mineralization/immobilization and cycling of mineral P pools), root uptake sink term of labile P concentration

Table 12.9 Block **K**– **Solute** Transport Information

Record	Type	Symbol	Description
1			Comment line
2.1.	Real	*Epsi*	Temporal weighing coefficient. =0.0 for an explicit scheme, =0.5 for a Crank-Nicholson implicit scheme. =1.0 for a fully implicit scheme.[-]
2.2.	Logical	*lUpW*	**.true.** if upstream weighing formulation is to be used **.false.** if the original Galerkin formulation is to be used.
2.3.	Logical	*lArtD*	**.true.** if artificial dispersion is to be added in order to fulfill the *PeCr* stability criterion
2.4.	Logical	*LTDep*	**.true.** if at least one transport or reaction coefficient (*ChPar*) is temperature dependent. Otherwise, if *lTDep*=**.true.**, then all values of *ChPar*(*i,M*) should be specified at a reference temperature *Tr*=20°C. For nitrogen transport only, set to **.false.**
2.5.	Real	*cTolA*	Absolute concentration tolerance [M L^{-3}], the value is dependent on the units used (set equal to zero if nonlinear adsorption is not considered)
2.6.	Real	*cTolR*	Relative concentration tolerance [-] (set equal to zero if nonlinear adsorption is not considered).
2.7.	Integer	*MaxItC*	Maximum number of iterations allowed during any time step for solute transport - usually 20
2.8.	Real	*PeCr*	Peclet/Courant Stability criterion Set equal to zero when *lUpW* is equal to **.true.** – usually 2
2.9.	Logical	*lTort*	**.true.** if the tortuosity factor [Millington and Quirk, 1961] is to be used. .**false.** if the tortuosity factor is assumed to be equal to one.
3			Comment line
4.1.	Real	*ChPar(1,M)*	Bulk density of material *M*, ρ [M L^{-3}], specified for 1 to NMat
4.2.	Real	*ChPar(2,M)*	Longitudinal dispersivity for material type M, D_L [L], specified for 1 to NMat
4.3.	Real	*ChPar(3,M)*	Dimensionless fraction of the adsorption sites classified as type-1, i.e., sites with instantaneous sorption, when the **chemical nonequilibrium** option is considered. Set equal to 1 if equilibrium transport is to be considered. Dimensionless fraction of the adsorption sites in contact with mobile water when the **physical nonequilibrium** option is considered. Set equal to 1 if all sorption sites

			are in contact with the mobile water, specified for 1 to NMat
4.4	Real	*ChPar(4,M)*	Immobile water content. Set equal to 0 when the **physical nonequilibrium** option is not considered., specified for 1 to NMat
5			Comment line
6			Comment line
7.1.	Real	*ChPar(5,M)*	Ionic or molecular diffusion coefficient in free water, D_w [L^2 T^{-1}]
7.2.	Real	*ChPar(6,M)*	Ionic or molecular diffusion coefficient in gas, D_g [L^2 T^{-1}]
8			Comment line
9.1	Real	*ChPar(7,M)*	Linear adsorption isotherm coefficient, k_s, for material type *M* [L^3 M^{-1}]. Set equal to zero if no adsorption is to be considered, specified for 1 to NMat. For linear sorption only record 9.1 has to be specified, records 9.2 and 9.3 can be skipped.
9.2	Real	*ChPar(8,M)*	Langmuir η parameter [L^3 M^{-1}] of the non-linear Langmuir adsorption isotherm for material type *M*. Specified for 1 to NMat. Set record 9.3 (Freundlich n) to 1 for Langmuir sorption.
9.3	Real	*ChPar(9,M)*	Freundlich n parameter [-] of the non-linear Freundlich adsorption isotherm for material type *M*. Specified for 1 to NMat. Set record 9.2 (Langmuir η) to zero for Freundlich sorption. Note that records 9.2 and 9.3 have to be given for Freundlich or Langmuir sorption.
10			comment
11.1.	Integer	*kTopCh*	Code which specifies the type of upper boundary condition =1: Dirichlet boundary condition, =-1: Cauchy boundary condition. =-2: a special type of boundary condition for volatile solutes
11.2.	Real	*cTop(1)*	Concentration of the upper boundary, or concentration of the incoming fluid, for the first solute [M L^{-3}]
11.3.	Real	*cTop(2)*	Concentration of the upper boundary, or concentration of the incoming fluid, for the second solute [M L^{-3}] (not specified if *NS* < 2).
11.4.	Real	*cTop(NS)*	Concentration of the upper boundary, or concentration of the incoming fluid, for the *NS*th solute [M L^{-3}]
12			comment
13.1.	Integer	*kbotCh*	Code which specifies the type of lower boundary condition =1: Dirichlet boundary condition,

			=0: continuous concentration profile, =-1: Cauchy boundary condition
13.2.	Real	*cBot(1)*	Concentration of the lower boundary, or concentration of the incoming fluid, for the first solute [M L^{-3}]
13.3.	Real	*cBot(2)*	Concentration of the lower boundary, or concentration of the incoming fluid, for the second solute [M L^{-3}] (not specified if *NS* < 2).
13.4.	Real	*cBot(NS)*	Concentration of the lower boundary, or concentration of the incoming fluid, for the *NS*th solute [M L^{-3}]
14			Comment
15.1.	Real	*cRootMax(1)*	Maximum allowed concentration in the root solute uptake term for the first solute [M L^{-3}]. When the nodal concentration is lower than *cRootMax*, all solute is taken up. When the nodal concentration is higher than *cRootMax*, additional solute stays behind.
15.2.	Real	*cRootMax(2)*	Maximum allowed concentration in the root solute uptake term for the second solute [M L^{-3}].
15.3.	Real	*cRootMax(NS)*	Maximum allowed concentration in the root solute uptake term for the NSth solute [M L^{-3}].
16			Comment line
17.1.	Real	*tPulse*	Time duration of the concentration pulse [T]
18			comment
19			comment
20.1.	Real	*Ctime*	Timestep(s) for solute application on top and bottom. All time steps have to be within one line
21			comment
21.1	Real	*Ctop*	Solute concentration [M L^{-3}] applied at top of the profile for timesteps 1 to n, all concentrations have to be within one line
22			Comment
22.1	Real	*Cbot*	Solute concentration [M L^{-3}] applied at bottom of the profile for timesteps 1 to n, , all concentrations have to be within one line

Records 6 to 9 need to be specified for each solute,
Block K need not supplied if logical variable *Transport* (Block A) was set equal to **.false.**. In order to simulate Nitrogen, input block K for solute transport information is required. This block K then contains the solute transport parameters for at least three species, where solute 1 is Urea, solute 2 is Ammonium and solute 3 is Nitrate. In case of simulation of Phosphorus transport and uptake P is solute 4. Records 18 – 22 must only be specified when Nitrogen is not simulated.