Modelling water, nutrients, and organic carbon in forested catchments: a HYPE application

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Abstract:

Both monitoring and model simulation are useful for understanding and detecting changes in the environment. To understand and simulate leaching in small forested catchments, it is important to have knowledge of soil processes. Here, we describe recent development of the Hydrological Predictions for the Environment (HYPE) model for forested catchments. HYPE includes an organic carbon (OC) variable in addition to previously published nitrogen (N), phosphorus (P), and water flow models. The aspects addressed in the current study included P concentrations under low-flow conditions and high concentrations of inorganic N. HYPE was further developed based on nine small forested catchments (0.5–200 ha) in Sweden, which were calibrated separately using local data. The model (excluding the OC variable) was tested on a larger set of forest catchments from the operational HYPE model of Sweden (S-HYPE). We observed the following: (1) dissolved organic P could make a significant contribution to the total P concentration in a stream during low-flow periods, (2) the inorganic N concentration simulated in a stream improved when part of the atmospheric N was retained in the soil, (3) the soil flow path formulation was critical for simulating concentration dynamics, and (4) evaluating an additional variable (OC) further elucidated the soil runoff processes in the model. Copyright © 2016 Swedish Meteorological and Hydrological Institute. Hydrological Processes published by John Wiley & Sons, Ltd.

KEY WORDS catchment; nutrients; organic carbon; HYPE; multi-basin calibration; soil processes

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INTRODUCTION

Monitoring of forest leaching is essential to understand and detect changes in the environment, and this is particularly important in Sweden where coniferous forests dominate the landscape. Organic substances constitute an integrated part of surface water chemistry and ecology in forestland, where relationships between organic carbon (OC) and both flow and acidification have been observed (Erlandsson et al., 2008). In boreal areas, the major contribution of OC is from wetlands and forests, whereas the relative contribution from peat and till soils is affected by season (spring flood) and groundwater levels (Laudon et al., 2011). The riparian zone in a boreal landscape is usually rich in OC and largely governs OC levels in the streams (Laudon et al., 2011). Organic nutrients are also present in forest streams, and in Sweden the organic nitrogen (ON) fraction of the total nitrogen (TN) is higher in forest soil leaching than in leaching from agricultural lands, where inorganic nitrogen (IN) is more likely to dominate (Stepanauskas et al., 2000; Sponseller et al., 2014). Organic phosphorus (OP) is less studied, although Mattsson et al. (2005) have found that concentrations of dissolved organic phosphorous (DOP) and phosphate are similar in boreal rivers in Finland, and the same research group (Mattsson et al., 2003) has also reported an association between exported phosphorus (P) and humic substances in small forest streams.

Process-based models such as ForSafe (Wallman et al., 2005) and MAGIC (Cosby et al., 2001) are used to simulate nutrients, OC, and other substances in runoff from forest stands or forested catchments. Furthermore, models such as INCA (Whitehead et al., 2004), COUP (Jansson and Karlberg, 2011), and SWAT (Arnold and Fohrer, 2005) can simulate catchments with both forest and other land cover. The Hydrological Predictions for the Environment (HYPE) model employed in this study has previously been used to simulate nutrient loads from mixed land use in Sweden (Strömqvist et al., 2012) and in other parts of Europe (Donnelly et al., 2016). Models that simulate stream water quality can be useful for monitoring the environment, for example, to assess the status of ungauged catchments (Strömqvist et al., 2012) and illustrate changes in the environment (Whitehead et al., 2004; Futter et al., 2011). Using models in environmental monitoring can also encourage communication between...
those performing the monitoring and modelling (Grimvall et al., 2014).

When HYPE was first set up to simulate nutrient loads in Sweden (Strömqvist et al., 2012), greater effort was focused on land uses and point sources with high nutrient loads than on land with low nutrient loads (e.g., forests). Therefore, in the present study, we set up the HYPE model for small forest catchments to focus on nutrient leaching from forest soils. The catchments in this model have to be small so that they will not include lakes, because lakes can have a substantial impact on nutrient concentrations, which can be difficult to separate from the influence of the forestland in the analyses. Another reason we chose to use small catchments is that HYPE is assumed to work on different scales, although it has primarily been set up on larger scales (Andersson et al., 2015). Working on a very small scale entails greater variability in chemistry and hydrology and can therefore provide new insights into the functioning of the process formulations of the model. Also, OC is common in forest streams, and hence it was included for the first time in the version of HYPE developed in our study.

It is necessary to understand various processes in the soil in order to explain and simulate forest leakage from small catchments. Factors known to influence the nutrient budget in soil include atmospheric deposition, plant residues, vegetation uptake, denitrification of nitrogen (N) (Yanai et al., 2013), and adsorption/desorption and weathering of P (Vincent et al., 2012), and these are possibly complemented by other processes such as gaseous losses (volatilization) and percolation to deeper soil layers (Yanai et al., 2013). The main source of dissolved organic carbon (DOC) in soil is release from litter and the humus layer (Kalbitz et al., 2000), and other sources are biological production through root exudates and release during microbial processes (Neff and Asner, 2001). The DOC concentration in soil solution is highly affected by adsorption/desorption on soil surfaces and can be reduced through microbial decomposition and plant uptake (Neff and Asner, 2001). Additional processes transform nutrients in the soil between different states and species. The relative importance of sources and processes varies between catchments, and available estimates are tentative, but it is the solutes in the soil that eventually determine what ends up in soil runoff.

Consequently, formulation of soil transformation processes is important when simulating forest leakage. Soil processes that are common in catchment models include vegetation uptake (N and P), denitrification (N), decomposition/mineralization (N, P, and DOC), adsorption/desorption (P), and release from litter and/or soil (DOC). Some model descriptions incorporate other processes: SWAT includes ammonia volatilization and nitrification and immobilization of dissolved IN (Neitsch et al., 2011), whereas both COUP and INCA-N (Wade et al., 2002a) include nitrification; HYPE and SWAT include soil erosion of P; INCA-P has immobilization of OP (Wade et al., 2002b); INCA-C includes sorption/desorption of DOC (Futter et al., 2011), whereas DOC is immobilized in COUP and HYPE. A balanced selection of processes and a general process description are required to achieve a good soil model.

The model of a catchment simulates flow and concentrations in a stream, which also represents the point in the landscape where observations are often made. Soil leaching is affected on the way to and in a stream. Examples of processes that can influence concentrations of substances in the stream are soil erosion, nutrient uptake, mineralization, and denitrification (Bernhardt et al., 2005; Brookshire et al., 2005; Vincent et al., 2012). In forests, processes in the riparian zone have a marked effect on OC levels in streams (Laudon et al., 2011).

In the earlier HYPE model (which only simulated nutrients and flow), the simulation of the small forest catchments showed no P at low flow, excessively high IN concentrations (especially during winter), and fine-scale variations that were particularly irregular for organic substances. These weaknesses were not observed in the mixed landscape setups of HYPE performed on a larger scale; Strömqvist et al. (2012) and Arheimer et al. (2012) found that the main problem was related to input data and nutrient soil storage over time. Nevertheless, Strömqvist et al. (2012) stated that only the average P level was convincing, and Jiang et al. (2014) noted that better formulation of IN retention was needed in HYPE.

Still in a mixed landscape catchment, it can be essential to achieve a correct simulation of the mentioned conditions in forestland. The low flow P concentration contributes very little to the yearly transport of this element, but it can have an impact on recipients. During the summer low-flow period, inflowing P can constitute an additional source of a limited nutrient for algae growth in a lake. Overly high IN concentrations during a winter with high flows and little retention can represent a large error in the transport to the sea, where N is known to cause eutrophication (Howarth and Marino, 2006). Although it is probably more important to attain correct seasonal variation in nutrient concentrations to ensure a correct total load, flows can vary quickly and then even fine-scale variation in concentrations can affect the timing of the load.

The mentioned conditions involving poor representation of nutrients and their potential impact on stream water quality imply that forest soil processes in HYPE need to be investigated and improved to render the model more suitable for assessment of the status and future.

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changes in forest environments. Stream processes should also be taken into consideration in this context, because they can affect concentrations upstream of an observation site. The objective of the present study was to investigate the influence of soil processes on stream water quality to improve description of forest catchments in HYPE. In light of the weaknesses identified in the initial model simulations, we focused on low-flow P concentration, IN dynamics in the soil, and fine-scale (day-to-day) variability in concentrations.

Here, we first present the HYPE model developed for forests, which now includes the variable OC. Thereafter, using different input data and set-up methodologies, we evaluate the model against observations on two sets of forest catchments and then assess the simulations regarding differences between catchments and temporal variations within catchments. Last, we discuss various aspects concerning how formulation of soil processes in the model affects stream concentrations of nutrient and OC.

MATERIAL AND METHODS

The HYPE model

General description. HYPE is an open source code hydrological model (http://hype.sourceforge.net; access date 20/01/2014), which was originally developed for small- and large-scale assessment of water resources and water quality in Sweden (Lindström et al., 2010). The first model simulated daily water flow (Q) and N and P concentrations based on daily precipitation and air temperature forcing. The concentration of nutrients was simulated in separate fractions: IN, ON, soluble phosphorus (SP), and particulate phosphorus (PP). Catchments were divided into sub-catchments and further into classes according to combinations of properties such as land use, vegetation, and soil type, and the soil was divided into layers. Most model parameters were coupled to land use or soil type, or were general for the model domain. This parameter structure made the model suitable for extrapolation to ungauged catchments. The HYPE model is used operationally by the Swedish Meteorological and Hydrological Institute (SMHI) to forecast Q, N, and P for Sweden (S-HYPE, see below) and Europe (Arheimer et al., 2011; Arheimer et al., 2012; Donnelly et al., 2016).

Alterations of the HYPE model. In the new HYPE model (HYPE version 4.3.0, hereafter called HYPE43), changes were made in both land and lake model routines, but only alterations related to forestland processes are reported in this paper. Watercourse processes were not changed (cf Lindström et al., 2010). The major addition to HYPE43 was the OC variable. Soil equations, which were first presented by Lindström et al. (2010), are included in the Appendix in their revised form together with parameter definitions. OC was added to Equations 14, 22, and 23.

OC in a soil layer was modelled using three pools: immobile slow turnover OC (slowC), immobile fast turnover OC (fastC), and DOC in the soil water (Figure 1). Plant residues added to the fastC pool constituted the outside source of OC. The soil pool transformations (Appendix Equation (14)) were calculated for each soil layer. The immobile soil pools (fastC and slowC) were transformed to DOC through degradation and dissolution. OC could also be transformed from fastC to slowC and from DOC to fastC. Mineralization of OC was simulated by removing a fraction of the OC at every transformation. The concentration of OC may be reduced in percolating water (Appendix Equation (22)). For selected classes, the DOC concentration in soil runoff could be altered by a hypothetical riparian zone process before it reached the watercourse (Appendix new Equation (23)). In the stream, the same formulation of the primary production/mineralization processes were used for OC as for N and P (Lindström et al., 2010, Equation 20), but with a separate calibration parameter.

Small changes were made in snow/rain separation threshold and percolation (Appendix Equations (1) and (7)). The soil layer runoff was changed to be determined by the groundwater level in the soil instead of only by the water content of the soil layer in question (Appendix Equation (9)).

Several changes were made regarding N and P in the soil, considering both internal transformations and sources (Figure 1). The organic immobile soil pools were harmonized so that both fast and slow organic nutrient turnover pools contributed to PP and ON concentrations in soil water through dissolution of immobile organic nutrients (Appendix Equation (14)). Thus the simulated PP included DOP. Soil temperature was calculated for each soil layer separately (Appendix Equation (14)), which influenced most soil processes.

Atmospheric dry deposition was added to snow pack when the ground was snow covered, instead of directly reaching the soil. A fraction of the IN concentration in precipitation and snowmelt followed the infiltrating water, whereas the remaining fraction was transferred to the fast turnover N pool (Appendix Equation (21)). ON and PP concentrations in percolating water could be reduced (Appendix Equation (22)), and the denitrification rate depended on land use (Appendix Equation (14)). Application of plant residues could be spread over several days instead of limited to once a year; such residues constituted all organic sources applied to the soil and were added to the immobile organic pools in the soil.
Catchment sets and applications of HYPE

Two catchment sets were used in a broad evaluation of the HYPE model for forest simulation: the first consisted of well-studied catchments that were set up individually; the second consisted of catchments with national and regional data available that were part of the S-HYPE application. Catchment areas were larger in the second than in the first data set.

Separately calibrated forest catchments (SFCs). Nine well-studied small forest catchments were selected for soil
model development and evaluation of simulated flow and leaching of N, P, and OC (SEPA, 1985; Sandén and Warfvinge, 1992; Arheimer et al., 1996; Temnerud et al., 2014). The selected catchments included mostly pristine forest, were distributed throughout Sweden (Figure 2), and ranged in size from 0.5 to 200 ha (Table I). Observation time series existed for periods of 12–24 years for water flow, 14–31 years for N and P (some fractions for less time or lacking), and 4–21 years for OC. The simulation period was 1977–2009. Data on the nine catchments were published in the CLEO database available on the Internet (http://www.slu.se/cleo/data, access date 29/01/2014; Temnerud et al., 2014).

HYPE was set up with detailed catchment characteristics collected from literature, the Internet, and databases (Table II). Catchments lacking detailed information were assumed to comprise 100% coniferous forest on till soil. The soil layer division was as follows: a thin (7–8 cm) humus layer, a middle layer down to a maximum depth of 0.5 m (root zone), and a third layer for catchments with deeper soils. The actual depths of the layers were determined based on observations from the catchment and data in the literature. Forcing data were from the closest grid point in a climatological database. All atmospheric deposition of IN was assumed to be dry deposition. Each of the nine catchments was calibrated manually. The first half of the period with observations was used for calibration, and the second served as the validation period. The stream OC processes were not used in the applications described in this paper, because they were deemed to be of minor importance in the small forest catchments (Köhler et al., 2002).

Representative multi-basin calibrated forest catchments (RFCs). Forested catchments with observation time series at the catchment outlets were selected from national and regional monitoring programmes (discharge data obtained from the SMHI database, access date 27/06/2011; water chemistry data acquired from the Swedish University of Agricultural Sciences [SLU] database [headed by the Swedish Agency for Marine and Water management], http://webstar.vatten.slu.se/db.html, access date 11/11/2010). The selection criteria were >50% forest, a very small lake fraction, and no agricultural land, because our aim was to study the effects of forest on leaching. Another requirement was that the catchments should be resolved in the S-HYPE (Swedish) application (see below). Eight catchments were selected for water flow, and 14 for nutrients (Figure 2, Table III). The catchment areas were 0.9–120 km². The observation periods used were 1990–2011 for Q (6–12 years) and 1995–2010 for N and P (5–16 years), although data were lacking for some periods. For the selected catchments, results were extracted from the S-HYPE application that used HYPE43.

S-HYPE: the HYPE application for Sweden. The first version of the S-HYPE application was released in January 2010 (Strömqvist et al., 2012), and since then the model has repeatedly been set up in finer resolution and improved to correct flaws in both the application and the HYPE model. This development was driven by the requirements of users, especially the Swedish Water Authorities, which employ information from the application in their environmental assessments. The third version of the application (S-HYPE2012 1.1.0) uses HYPE43 and has a median sub-catchment size of 7 km²; databases used during the setup have been reported by Strömqvist et al. (2012). Compared with the version presented by

Figure 2. Locations of the studied catchments in Sweden. Catchment sets: A1–9, separately calibrated forest catchments (SFCs) with water flow and water chemistry observations; B1–8, representative multi-basin calibrated forest catchments (RFCs) with water flow observations; C1–14, RFCs with water chemistry observations

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### Table I. Characteristics of the nine separately calibrated forest catchments (SFCs)

| Catchment code | Name             | Area (km²) | Forest fraction (%) | Other information        |
|----------------|------------------|------------|---------------------|--------------------------|
| A1             | Ammarnäs skog    | 2.2        | 100*                | Deciduous forest         |
| A2             | Aneboda          | 0.19       | 98                  | 2% open mire             |
| A3             | Berg             | 0.93       | 100                 |                          |
| A4             | Gårdsjön F1      | 0.037      | 100                 | 11% forested mire        |
| A5             | Gårdsjön G2      | 0.0052     | 100                 | Fertilized               |
| A6             | Kindla           | 0.20       | 98                  | 2% open mire             |
| A7             | Snipjärn         | 0.4        | 100*                |                          |
| A8             | Stubbetorp       | 0.87       | 100                 | 7% forested mire         |
| A9             | Svarthog        | 0.5        | 100                 | 16% forested mire        |

*No detailed land-use information available.*

### Table II. Input data on the SFCs for HYPE application

| Data type                | Data                                    | Source                                                                 |
|--------------------------|-----------------------------------------|------------------------------------------------------------------------|
| Climatological data      | Daily precipitation and air temperature | CLEO database                                                          |
|                          | Catchment area                          | CLEO database                                                          |
|                          | Soil type, land use                     | Persson and Broberg (1985); Maxe (1995); Bishop *et al.* (1994); SEPA (1985) |
|                          | Elevation                               | CLEO database                                                          |
|                          | Runoff                                  | CLEO database                                                          |
|                          | Concentration in runoff                 | CLEO database                                                          |
| Geographical data        | Catchment area                          | CLEO database                                                          |
|                          | Soil layer depth                        | CLEO database, Sandén and Warfvinge (1992); Olsson *et al.* (2009); Rosengren and Stjernquist (2004); Persson and Broberg (1985); Nyberg (1995) |
|                          | Nutrient content                        | CLEO database, Olsson *et al.* (2009)                                  |
|                          | Water holding capacity                  | CLEO database, Nyberg (1995); Sandén and Warfvinge (1992); Bengtsson (1997) |
| Time series              |                                          | CLEO database                                                          |
| Soil data                |                                          | CLEO database                                                          |
|                          | Nutrient sources                        | CLEO database (both simulated with MATCH-model and observed)           |
|                          | Litterfall                              | CLEO database, Berggren Kleja *et al.* (2008)                           |

### Table III. Characteristics of 21 selected forested catchments (RFCs) from the S-HYPE model application for evaluation of runoff (catchment code B) and water quality (catchment code C)

| Catchment code | Name             | Area (km²) | Forest fraction (%) | Lake fraction (%) | Other information |
|----------------|------------------|------------|---------------------|-------------------|-------------------|
| B1             | Orgvätar         | 2.6        | 100                 | 0                 | 21% mire          |
| B2             | Stubbetorp       | 0.88       | 100                 | 0                 |                   |
| B3/C2          | Stormyra         | 4.0        | 91                  | 0                 |                   |
| B4             | Buskbäcken       | 1.7        | 100                 | 0                 |                   |
| B5             | Härsvattenbäcken | 7.2        | 98                  | 0                 |                   |
| B6             | Hyttningsheden   | 49         | 100                 | 0.2               |                   |
| B7             | Oppli            | 67         | 98                  | 1                 |                   |
| B8             | Grätanbäcken     | 115        | 78                  | 1.7               |                   |
|                |                  |            |                     |                   |                   |
| C1             | Sägebäcken       | 4.4        | 98                  | 2                 |                   |
| C3             | Kolhärkens Pellabäcken | 10     | 100                 | 0                 |                   |
| C4             | Långlkan,före Tvärlikan | 58    | 99                  | 0.5               |                   |
| C5             | Sörjobäcken (Lillån) | 23   | 100                 | 0.3               |                   |
| C6             | Rällan, nedre, f. Rotnen | 63    | 71                  | 0.06              | 16% mire          |
| C7             | Blalägan         | 16         | 52                  | 0                 | 31% mire          |
| C8             | Hammarbäcken     | 7.7        | 82                  | 0                 | 18% mire          |
| C9             | Ádalsån Lyckemyran (D) | 50  | 88                  | 0.6               | 12% mire          |
| C10            | Kvarnbäcken (Sävarån) | 39   | 98                  | 1.7               |                   |
| C11            | Bjurången        | 43         | 95                  | 1                 | 3% mire           |
| C12            | Kvarnbäcken (Luspsjön) | 31    | 96                  | 0                 | 4% mire           |
| C13            | Rotkällan        | 84         | 86                  | 0.2               | 14% mire          |
| C14            | Yl. Kihlankijoki | 65         | 87                  | 0                 | 13% mire          |
Strömqvist and colleagues, the third release includes the following improvements:

- Detailed information on regulated lakes and dams.
- New sources of land-use information for the lake areas (Swedish Water Archive [SVAR] at SMHI) and the agricultural crop areas (Swedish Board of Agriculture).
- More recent load figures for point sources.
- Leaching from urban land instead of storm water as point source.

A step-wise multi-basin calibration technique was used for the S-HYPE application (Strömqvist et al., 2012). Sets of representative catchments were calibrated together to obtain parameter values for the represented characteristics (land use or soil type, e.g. forestland). Thereafter, those parameter values were used for that characteristic on all catchments, which gave a basic model setup. Correction parameter values were used for that characteristic on all catchments when and when improvements could be made. The calibration period (CP) was 1999–2008, and the validation period (VP) was 1990–1998.

More information on S-HYPE can be found in the literature (Strömqvist et al., 2012; Bergstrand et al., 2014), and the current version of the application is available online (http://vattenweb.smhi.se, access date 22/01/2012).

Performance criteria

Our evaluation of HYPE performance was based on several criteria (Table IV). During the calibration of the SFCs, Nash–Sutcliffe efficiency (NSE) and relative bias (RB) were used to complement visual inspection of time series; for calibration of S-HYPE, NSE, RB, and the correlation coefficient (CC) were used in addition to visual inspection. RB and CC were used to assess the

Table IV. Performance criteria equations, where \( c \) denotes a simulated value and \( r \) an observed value, and \( \bar{c} \) and \( \bar{r} \) denote the average over a period with \( m \) values

\[
\text{NSE} = 1 - \frac{\sum_{i=1}^{m} (c - r)^2}{\sum_{i=1}^{m} (r - \bar{r})^2}
\]

\[
\text{RB} = \frac{\sum_{i=1}^{m} (c - r)}{\sum_{i=1}^{m} r} \times 100\%
\]

\[
\text{CC} = \frac{\sum_{i=1}^{m} (c - \bar{c})(r - \bar{r})}{\sqrt{\sum_{i=1}^{m} (c - \bar{c})^2 \cdot \sum_{i=1}^{m} (r - \bar{r})^2}}
\]

NSE = Nash–Sutcliffe efficiency (Nash and Sutcliffe, 1970); RB = relative bias; CC = correlation coefficient

RESULTS AND DISCUSSION

Evaluation of the HYPE simulations

HYPE was evaluated against observations for forest catchment simulation on the two catchment sets, and the range of observed solute concentrations was similar in the two sets. Concentrations were in the range 200–900 μg/l for TN and 5–23 mg/l for OC. Total phosphorus (TP) was slightly lower for SFCs than for RFCs: 4–18 and 6–38 μg/l, respectively. Spatial variation was evaluated for average concentrations and flows, and temporal variation was evaluated on a seasonal scale and on finer scales.

Water flow. The observed range of flows was smaller for the SFCs than for the RFCs (Table V), as suggested by the areas of the catchments. The flow from the forest catchments was generally flashy (example in Figure 3), except during the winter low-flow period in the northern catchments when precipitation was accumulated as snow. This was a consequence of selecting small catchments with a small percentage of lakes. The fine-scale (daily) variation was satisfactorily captured, as shown by

Table V. Flow performance indicated by mean flow (MQ, m³ s⁻¹) for observations and Nash–Sutcliffe efficiency (NSE) for the calibration period (CP) and the validation period (VP)

| Catchment | Obs MQ a | NSE CP | NSE VP |
|-----------|----------|--------|--------|
| A1        | 0.0007   | 0.66   | 0.61   |
| A2        | 0.00008  | 0.58   | 0.65   |
| A3        | 0.016    | 0.68   | 0.76   |
| A4        | 0.002    | 0.70   | 0.64   |
| A5        | 0.007    | 0.66   | 0.48   |
| A6        | 0.003    | 0.55   | 0.56   |
| A7        | 0.005    | 0.42   | 0.43   |
| A8        | 0.005    | 0.67   | 0.62   |
| A9        | 0.02     | 0.72   | 0.74   |
| B1        | 0.02     | 0.75   | 0.76   |
| B2        | 0.007    | —      | 0.33   |
| B3        | 0.04     | 0.74   | 0.76   |
| B4        | 0.02     | —      | 0.47   |
| B5        | 0.06     | —      | 0.66   |
| B6        | 0.8      | 0.78   | 0.66   |
| B7        | 0.7      | 0.75   | 0.59   |
| B8        | 1.7      | 0.77   | 0.82   |

a Represents all days with observations over the entire period.
correlation coefficients >0.65 for all periods and catchments (Figure 4) and NSE values of 0.33–0.82. NSE values for SFCs were slightly lower for the CP than for the VP (Table V), which showed that, although usually used on a larger scale, the HYPE model is adequate on a small scale and for catchments without lakes.

Figure 3. Simulated and observed water flow (Q), and concentrations of organic carbon (OC), total phosphorus (TP), and inorganic nitrogen (IN) shown for catchment A2. The NSE for Q was 0.65 over the validation period (VP) 2003–2008. The correlation coefficient (CC) was 0.8 for Q, 0.3 for OC, <0 for TP, and 0.3 for IN over the VP (for nutrients 2003–2009).

Figure 4. Correlation coefficient (CC) and relative bias (RB) for SFCs and RFCs. For each site, the values for the calibration period were plotted against the values for the validation period. RB graphs were limited to 100% (12% and 4% of points outside for the SFCs and RFCs, respectively).
Nitrogen concentration. In general, the spatial variation in N was captured by the HYPE model (Figure 5). The simulated average annual and winter TN concentrations were similar to observed concentrations, except for one catchment (A5, Figure 5); HYPE did not manage to simulate the fertilization of A5 in a satisfactory way, which resulted in over-predictions of winter concentrations of IN and TN in that catchment. Summer concentrations of TN were under-predicted for SFCs and also for one RFC with high observed concentration (C2, Figure 5). The differences between the two sets of catchments emanated from the simulation of IN (Figure 6): the average IN concentration was highly under-predicted in both seasons for the RFCs, whereas it was often under-predicted in summer for the SFCs (example in Figure 3). Thus the error in IN concentration was transferred to the TN concentration for the SFCs but not for the RFCs, because ON represented the dominant

Figure 5. Observed and simulated concentrations of total nitrogen (TN), total phosphorus (TP), and organic carbon (OC) shown for the winter period (December–February; left) and the summer period (June–August; right)
fraction of N in the RFC simulations (>96%) but not in all the SFC simulations (10–91%).

Considering IN concentrations, the simulated seasonal pattern was similar to observed values (example in Figure 7, left) even though concentrations were underpredicted, and this was also evident from the positive correlation coefficients (Table VI). Both the simulated and the observed seasonal variation in IN concentration were typical for Swedish catchments (Sponseller et al., 2014). The simulated variation originated partly from the stream: stream processes reduced the IN load by 0–26% (median 3%) and the summer concentrations by up to 66% (median 28%) for some catchments (Table VII). Although we did not know the actual influence of the streams in these catchments, the indicated removal seems reasonable, because Peterson et al. (2001) assessed headwaters and found that typically less than half of the stream input of dissolved IN was exported downstream during the biologically active season.

The range of simulated ON concentrations for the individual catchments was similar to observed values, and most catchments had positive correlation coefficients (Table VI). Seasonal variation with higher ON concentrations in summer was noted for SFCs in southern Sweden and RFCs C6 and C7 in the central part of the country. This pattern could be seen in observed data (C7 and southern SFCs), but was also apparent in catchments where it was not captured by the model (e.g. C8). For other catchments,
Table VII. Median change in simulated substance concentrations due to in-stream processes in nine SFCs and nine RFCs over a period of at least 20 years, with no lakes or upstream sub-catchments included in the calculations

| Substance            | Median change in average concentration | Median maximum decrease in monthly concentration | Median maximum increase in monthly concentration |
|----------------------|----------------------------------------|-----------------------------------------------|-----------------------------------------------|
| Inorganic nitrogen   | -3%                                    | -28%                                          | 1%                                            |
| Organic nitrogen     | 0%                                     | -4%                                           | 0%                                            |
| Total nitrogen       | 0%                                     | -8%                                           | 1%                                            |
| Soluble reactive phosphorus | 0%                                 | -4%                                           | 2%                                            |
| Particulate phosphorus | 0%                                  | -4%                                           | 0%                                            |
| Total phosphorus     | 0%                                     | -4%                                           | 1%                                            |
| Organic carbon       | 0%                                     | 0%                                            | 0%                                            |

Simulated ON concentrations peaked during high-flow periods, typically two times annually in spring and autumn (e.g. C12 in Figure 7 [left]). The SFCs showed irregular fine-scale variation in simulated ON concentrations discussed further in section headed Forest soil process formulations in HYPE. Sponseller et al. (2014) found seasonal variation in ON concentrations at many sites in Sweden and attributed this to production of organic matter in the soil during the warm period. On the other hand, Arheimer et al. (1996) concluded that low-flow ON levels being higher in summer than during the dormant season could be attributed to biological activity within or in the vicinity of the stream. We included both these processes in the HYPE model, but the seasonal variation in ON concentrations was hardly affected by stream processes (a median of 2% change summer concentration change; Table VII). The elevated concentrations related to high flow were explained by the stream flow peak in spring carrying with it the ON that had been accumulated in upper soil layers during the cold months when there was little flow, and by the high ON concentrations during autumn months that originated from the ON that had been produced in the soil and the stream during summer and was released during high flows. Arheimer et al. (1996) also found flow-related high ON concentrations in 20 Nordic forest streams and that flow explained 18% of the ON variation. They attributed this to stream bank erosion losses in peat areas and leaching of ON from soil during rainfall events. In the HYPE model, in-stream erosion is not considered to contribute to ON but to P.

Phosphorus concentration. In the HYPE model, the average P concentrations were less well simulated than the N levels, with considerable differences between catchments (Figure 5). In general, winter TP concentrations were over-predicted (Figure 5), whereas the modelled summer concentration was too low for one catchment (C2). After the changes in the model, PP concentration was simulated with a base level above zero due to the added soil leaching of OP (see section headed Forest soil process formulations in HYPE). This improved the low-flow P concentration, but at the same time the PP concentration was spiky and correlated with flow due to simulated soil erosion processes. In-stream sedimentation and re-suspension had very little impact on TP concentration (Table VII).

As noted for ON, two types of pattern were observed in measured P time series (examples shown in Figure 7 [right]). One pattern was represented by catchments C9, C12, and C14, which were dominated by high PP (and TP) concentrations at flow peaks, and were located in northern Sweden where the snowmelt flow peak predominated. The other pattern was reflected by catchments A2, A3, C1, C2, C3, and C7, which exhibited seasonal variation with the highest concentrations of TP and PP in summer/autumn, and were located in southern Sweden where summers were warmer. Most catchments could not be classified or showed characteristics of both patterns. The flow dependence of P was simulated by erosion from soil and in-stream re-suspension, and these processes were determined by surface runoff and higher stream flow compared to the previous year. Catchments with flow-corrected variation in observed PP levels, but not catchments with seasonal variation in PP, were satisfactorily simulated by the HYPE model (Figure 7 [right], Figure 3). The seasonal variation in PP might have been simulated by degradation in soil or watercourse primary production, because these processes were temperature dependent. Verheyen et al. (2015) studied three catchments, one of which was forested, and found a seasonal pattern with increased dissolved P concentrations during summer under base-flow conditions in the forest catchment, which these authors attributed to in-stream formation of P. We used stream P processes in some of the catchments we simulated, but this had only a minor effect on seasonal variation in P (maximum 8%; Table VII). It is possible that seasonal variation in DOP from soil (Qualls and Haines, 1991; Fabre et al., 1996) can contribute to variation in modelled PP in streams, but that did not occur in our simulations.
Organic carbon concentration. OC was not included in the S-HYPE application and hence was evaluated only in our SFCs. The spatial variation in OC was captured well in the winter averages (Figure 5), whereas OC levels were generally slightly under-predicted in summer.

The temporal variation in OC was best simulated in the catchments in southern and central Sweden (A2, A3, A6, and A8; CC = 0.2–0.6 for the VP; see example A2 in Figure 3). In these catchments, OC showed seasonal variation with higher concentrations in summer/autumn, and the spring flood was weaker in the south than in the north. As for ON, the catchments showed irregular fine-scale variation in OC, but HYPE nonetheless captured the seasonal variation to some extent. The northern SFCs (A1 and A9; no OC observations available for A7) had a pronounced spring flood and elevated OC concentrations around the same time, whereas the HYPE simulations showed a short dip in OC concentrations during spring flood for the northern catchments. Other high-flow events might also cause a dip in simulated concentrations (see also Forest soil process formulations in HYPE). The poor fine-scale variation resulted in low performance criteria values. Most HYPE NSE values were negative (positive only for A3 [0.3 for the VP]). It is plausible that better NSE values can be achieved with better fine-scale variation, considering that Futter et al. (2011) simulated three of the present catchments (A2, A4, and A6) and noted NSE 0.4–0.5.

Forest soil process formulations in HYPE

The first aspect investigated was the low-flow P. The P concentration in earlier HYPE simulations was zero at low flow, whereas observed levels were above zero (see example in Figure 3). Which were the sources of the P? In HYPE, the PP concentration was derived from erosion from soil and stream banks, and primary production in the watercourse. These PP sources did not yield sufficient P for the forest stream flow, particularly during low flows. Furthermore, SP was only a small fraction of the TP, so we turned our attention to other P species. A significant portion of the P in soil water might consist of DOP, primarily in the form of acids (Qualls and Haines, 1991; Fabre et al., 1996). Qualls and Haines (1991) studied a forest ecosystem and found a higher concentration of DOP than of dissolved inorganic phosphorus (DIP) in throughfall, soil, and stream water. Vähätalo et al. (2003) also observed higher levels of DOP than of DIP in a humic headwater lake surrounded by coniferous forest, and Baldwin (2013) concluded that OP might constitute a major part of the P in aquatic systems. Accordingly, we added DOP production in the soil as a new source of P transported to streams.

A simple formulation of the process of dissolution of soil OP to DOP proved to be adequate for simulating higher low-flow concentrations of TP in forest streams. In INCA, DOP is produced by both dissolution and transformation of DIP through microbial decomposition (Wade et al., 2002b). The second process might have contributed to higher TP concentrations in HYPE, but we did not test that strategy because the DOP concentrations were satisfactorily increased by the initial, simpler dissolution approach. Moreover, we did not consider any other processes that might influence DOP in HYPE, such as adsorption of DOP to soil (Vincent et al., 2012). It is also plausible that various transformations of OP can occur in a stream. Baldwin (2013) suggested that hydrolysis (enzymatic and abiotic), adsorption/desorption, and photolysis can occur in aquatic systems, but concluded that further studies were needed to determine the importance of those processes. Vähätalo et al. (2003) observed that photolysis in a humic lake transformed DOP into forms that are readily available to phyto- and bacterioplankton. Thus DOP might also be an additional source of bioavailable P during summer. In our study, adding dissolution of soil OP to the HYPE model improved the low-flow P concentration, which indicates that this process may simulate the source of the low-flow P in small forest streams. The addition of dissolution did not increase the complexity of the model, because it was equivalent to the dissolution process already used for organic nitrogen. If future studies in other environments or locations demonstrate that other processes and factors in addition to the soil phosphorus formulations play an important role in this context, we will address this issue again. However, at present we feel that adding dissolution of soil OP to HYPE was an adequate change.

The second aspect we investigated was the dynamics of inorganic nitrogen in the soil. In earlier versions of HYPE, IN concentrations simulated in streams were over-predicted in small forest catchments, both SFCs and RFCs. This deficiency was traced to the atmospheric deposition, but the fate of the atmospheric N deposited in the soil was not clear. Simulated IN concentrations were governed by atmospheric deposition, mineralization, plant uptake, and denitrification; the latter three processes were temperature dependent and had the greatest effect during the warm summer period, whereas atmospheric deposition varied with precipitation. During the winter, the temperature-dependent processes had little influence on the IN, and atmospheric deposition gave higher IN concentration in HYPE than were observed in the streams. Thus deposited N must have been retained in the soil. Watmough et al. (2005) reported that 0–70% of atmospheric N was retrieved in runoff from forest catchments in Europe and North America. In other investigations, part of the atmospheric N was accumulated in trees, denitrified, or lost through runoff (Nadelhoffer et al., 1999; Yanai et al., 2013), or stayed...
in the soil (e.g. 70% reported by Nadelhoffer et al., 1999). It seems that the actual processes responsible for retention of atmospheric IN are not yet known, although some studies have suggested gaseous losses and accumulation in mineral soil (Yanai et al., 2013), and accumulation in litter, forest floor, and mineral soil (Nadelhoffer et al., 1999). The COUP model included a process for immobilization of ammonium (Jansson and Karlberg, 2011) that might have retained part of the atmospheric deposition.

A simple approach seemed justified in our study, because our aim was to describe the general effects of atmospheric IN retention, which might be caused by several processes. Thus we introduced a land-use-dependent calibration parameter to determine the portion of the atmospheric nitrogen that was to be transferred to an immobile soil pool. The fastN pool was used for this purpose, and hence release of N from the soil was delayed, but N was not lost from the system. This change entailed complexity similar to that of the current process formulations in the model, which was advantageous because we wanted to maintain the same level of complexity throughout the model (Lindström et al., 2010). With the new process we applied, 10–90% of atmospheric IN deposition on forestland was retained in the SFCs, which indicates that this process represents a large portion of the N flow in some forest systems. Simulated IN levels in the SFCs were good in HYPE (Figure 6), and the addition of this process improved the model. HYPE43 could simulate catchments where atmospheric deposition was large and retained in the soil (i.e. not immediately leached in runoff). In S-HYPE, the new process retained 80–90% of atmospheric nitrogen in the soil, and that level might be regarded as excessive considering that the IN concentration in stream flow was underestimated for RFCs (Figure 6). This aspect could be improved in the next S-HYPE application by reconsidering this parameter for forestland in the step-wise multi-basin calibration. A median of 21% of atmospheric N was retrieved in runoff in the SFCs, whereas the corresponding figure was 41% in the RFCs, despite a higher parameter value.

The third aspect was the fine-scale variation in stream concentrations. Both the timing of flow and the origin of substances are governed by the soil flow paths in HYPE (Lindström et al., 2010). In our study, all of the small forest catchments simulated flow that was dominated by the faster flow paths components, i.e. surface runoff and runoff from the upper soil layers. The lowest soil layer constituted the base-flow component. In the HYPE model, concentrations of substances in the flow components in all classes were determined by the concentrations in the soil layer they originated from, and mixing of the flows gave the total soil leaching. The threshold-governed runoff together with large concentration differences between soil layers due to coarse soil layer division (average concentrations in soil layers were simulated) gave an abrupt change in runoff concentration when a soil layer began (or ceased) to contribute to runoff, especially in the SFCs. For low-flow periods, concentrations in runoff originating from the deepest soil layer were nearly constant (e.g. for OC in summer 2008 in Figure 3). The soil layers led to excessive fine-scale variation in concentrations of substances in HYPE, and this was most pronounced for organic variables (ON and OC) due to their dependence on the slow turnover pools in the soil, which caused slow variation in concentrations in soil water.

The changes in the HYPE43 model did not solve the problem with fine-scale variation. After altering soil runoff to be determined by the water in the entire soil column, we expected less abrupt changes in runoff and concentrations of runoff, but only one or a few time steps were affected after a threshold was reached. This problem and possible solutions should be of interest in all soil layer models. Further insight into this matter came from the use of two catchment sets with different set-up methodologies. The day-to-day variation was more marked in the SFCs than in the RFCs. One explanation for this difference was that the RFCs were larger and were therefore simulated with more spatial division: the RFCs were set up with 15 different forest classes, whereas the SFCs had a maximum of four. Moreover, the RFC forest classes had different soil types or soil depths. In addition, the soils in the RFCs had more reliable base flow, because all forest classes had three soil layers. These aspects, together with the different flow paths, led to responses that increased gradually in a manner similar to the HBV beta-function (Bergström, 1995). The total runoff was not very sensitive to each soil layer threshold when the soil layers and classes were numerous, as was the case in the RFCs. Also, the uppermost soil layer was thicker in the RFCs and thus responded less rapidly to rain or drought. Concurrently, the difference in solute concentrations between soil layers was smaller. The upper soil layer in the RFCs had a larger storage volume and hence solutes were not washed out as quickly from that layer as compared to the thinner upper soil layer in the SFCs. In conclusion, the choice of soil layer and spatial division (number and thicknesses of soil layers, and number of classes) had a pronounced effect on fine-scale variation in our forest catchments. The small-scale spatial heterogeneity should be addressed in a HYPE application through spatial division, although in the future it might be appropriate to consider making further changes in processes in the HYPE model.

Another problem with fine-scale variation was the dip in OC and ON concentrations during spring flood in the northern catchments. High OC concentrations during high...
flow have been noted in small forest catchments (Raymond and Saiers, 2010; Xu et al., 2012), although the opposite has been observed in wetlands (Buffam et al., 2007). In a study conducted by Ågren et al. (2008), high-flow episodes were often correlated with high DOC concentrations in summer/autumn, but Buffam et al. (2007) also noted such a relationship during spring flood. HYPE clearly did not simulate the increase in OC with high flow that was apparent in the observations from the northern catchments. The spring flood dip in the model was caused by dilution of solutes in the thin upper soil layer by snowmelt in combination with the rapid runoff from the upper soil layer and surface runoff. An additional factor in this context was poor representation of the impact of the riparian zone on stream OC concentrations, an effect that is known to be marked in boreal streams (Laundon et al., 2011). Buffam et al. (2007) reported that the increase in DOC they found in forest catchments during spring flood could be explained by the flow paths from mineral soil to upper riparian organic soil. The HYPE model in our study had a simple equation that altered the OC concentration between soil runoff and the stream flow, but that did not satisfactorily describe the functioning of the riparian zone.

Parameterization and calibration

Multi-basin models usually include catchments with different characteristics. We found that calibrating parameters that depend on catchment characteristics (e.g. soil type and land use) was a favourable way to extend parameter values to ungauged catchments (see also Donnelly et al., 2009). Dunn and Lilly (2001) performed similar calibration and found that three of their soil hydrological classification-dependent parameters could be transferred to another catchment and provide reasonable flow in that location. Regional methods may offer another approach for calibration of large model domains (e.g. Parajka et al., 2007; Kim and Lee, 2014).

The stepwise multi-basin calibration method used for S-HYPE (Strömqvist et al., 2012) was suitable for regional simulation of forest catchments, as shown by the two forest catchment sets (SFCs and RFCs). The SFCs that were calibrated separately had better correlation coefficients with smaller differences between the CP and the VP, and fewer negative correlation coefficients than the RFCs (Figure 4). On the other hand, the SFCs showed larger bias for the VP than for the CP, whereas the RFCs showed approximately the same level of relative bias for the two periods (Figure 4). We conclude that the bias of the SFCs was overly adjusted to the calibration period, which resulted in larger bias for the VP but had little effect on the correlation coefficients. The error in the days with observations was given too much weight in the calibration of the SFCs. The regional simulation limited the possibility to reduce this error, because several catchments had to share the parameter values. Accordingly, the representative multi-basin calibration was more stable for the VP.

Water flow and average nutrient concentrations from the forest catchments were simulated satisfactorily by the HYPE model after the modifications presented here. The parameter structure of HYPE together with the benefits of better forest simulations could be utilized in the S-HYPE model, which increased the possibility of achieving good simulation of catchments with mixed land use. In addition, each new situation we tested strengthened the credibility of the entire model. Hence performing a study focused on developing a special part of a model (in this case forest soil) proved to be a good method to improve the generality of the model and thus enable the use of new locations.

CONCLUSIONS

In this study, the HYPE model was further developed for forestland and evaluated in particular for forested catchments in Sweden. Water flow and nutrient concentrations were simulated for a set of catchments calibrated using representative multi-basin catchments. The same variables, and OC concentration (a new variable simulated by HYPE), were also evaluated on a set of separately calibrated forest catchments. The soil process formulations were discussed regarding aspects related to weaknesses found in the model.

The main conclusions from the present work are as follows:

- DOP could make a significant contribution to the TP concentration in streams during low-flow periods. DOP leaching from soil was included in the PP concentrations simulated by HYPE.
- Atmospheric deposition of N had a marked impact on IN dynamics in soil. In HYPE, when part of the atmospheric N was retained in the soil, the simulated IN concentration improved.
- The formulation of soil layer runoff was critical for correct simulation of concentration dynamics. For small catchments, the small-scale spatial heterogeneity should be taken into consideration through spatial division during model set-up. Evaluating an additional variable (OC) and using two sets of catchments with different set-up methodology better elucidated the soil runoff process in the model.
- The HYPE model satisfactorily simulated water flow and average nutrient concentrations from forest catchments, which increased the possibility of improving simulation of mixed land-use catchments.
The development of the HYPE model continues. Currently, one focus area is urban land use, and, in future work concerning forests, the representative multi-basin calibration approach will be used on the OC variable.

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APPENDIX: HYPE SOIL MODEL EQUATIONS

Soil model equations are changed for the HYPE version 4.3.0, while the equation numbers are left as in Lindström et al. (2010). Development and testing of the HYPE (Hydrological Predictions for the Environment) water quality model for different spatial scales. Hydrology Research 41: 295–319. DOI: 10.2166/nh.2010.007. Equations 21–23 are added.

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1 Snow accumulation
\[ q_{SNOW} = P \cdot \alpha_{SNOW} \]
\[ \alpha_{TTSF} = p_{TTMP} \cdot p_{PTTD} \]
\[ \alpha_{SNOW} = 1 - \frac{T_{CLASS} - (\alpha_{TTSF} - p_{PTTD})}{2 \cdot \alpha_{PTFD}} \quad \text{if} \quad \alpha_{TTSF} - p_{PTINT} < T_{CLASS} < \alpha_{TTSF} + p_{PTINT} \]
\[ \alpha_{SNOW} = 1 \quad \text{if} \quad T_{CLASS} < \alpha_{TTSF} - p_{PTINT} \]
\[ \alpha_{SNOW} = 0 \quad \text{if} \quad T_{CLASS} > \alpha_{TTSF} + p_{PTINT} \]
\[ T_{CLASS} = T_{AIR} - p_{TICALT} \cdot c_{AH} \]

2 Snowmelt
\[ q_{MELT} = \min (p_{CMLT} \cdot (T_{CLASS} - p_{TTMP}) \cdot W_{SNOW}) \]

3 Infiltration
\[ q_{INR} = (P \cdot (1 - \alpha_{SNOW}) + q_{MELT}) - q_{SR} - q_{MPOR} \]

4 Surface runoff
\[ q_{SR} = p_{RCSR} \cdot (P \cdot (1 - \alpha_{SNOW}) + q_{MELT} - p_{THQR}) \quad \text{if} \quad P \cdot (1 - \alpha_{SNOW}) + q_{MELT} > p_{THQR}, \ W_{SOIL}(u) > p_{THQR} \]

5 Macropore flow
\[ q_{MPOR} = p_{RCPMP} \cdot (P \cdot (1 - \alpha_{SNOW}) + q_{MELT} - p_{THQR}) \quad \text{if} \quad P \cdot (1 - \alpha_{SNOW}) + q_{MELT} > p_{THQR}, \ W_{SOIL}(u) > p_{THQR} \]

6 Saturated overland flow
\[ q_{SOLF} = \max (p_{RCSOF} \cdot (W_{SOIL}(u) - \alpha_{WC}(u)), 0) \]

7 Percolation
\[ q_{PERC} = \min (\max (W_{SOIL(i)} - \alpha_{FC}(i), 0), \alpha_{WC}(j) - W_{SOIL}(j), p_{MPERC}(i)), i = u, m \quad \text{and} \quad j = m, l \]

8 Evapotranspiration
\[ q_{ET}(i) = 0 \quad \text{if} \quad W_{SOIL}(i) - a_{1} < 0, \ i = u, m \]
\[ q_{ET}(i) = \min (\alpha_{EAV}(i) \cdot E_{POT}, W_{SOIL}(i) - a_{1}) \quad \text{if} \quad W_{SOIL}(i) - a_{1} > p_{LP} \cdot p_{P\theta_{3}} \cdot c_{SLAY} \cdot 10^{3}, \ i = u, m \]
\[ q_{ET}(i) = \left( \alpha_{EAV}(i) \cdot E_{POT} \cdot \frac{W_{SOIL}(i)-a_{1}}{p_{LP} \cdot p_{P\theta_{3}} \cdot c_{SLAY} \cdot 10^{3}} \right) \quad \text{if} \quad 0 < W_{SOIL}(i) - a_{1} < p_{LP} \cdot p_{P\theta_{3}} \cdot c_{SLAY} \cdot 10^{3}, \ i = u, m \]
\[ E_{POT} = p_{CEVP} \cdot (T_{CLASS} - p_{TTMP}) \cdot (1 + p_{CEAM} \cdot \sin(2 \pi \cdot \frac{\theta_{103} - \theta_{PBP}}{365})) \quad \text{if} \quad T_{CLASS} > p_{TTMP} \]
\[ \alpha_{EAV}(u) = \frac{\Theta_{SLAY} - \Theta_{SLAY}^{(m)} \cdot \Theta_{SLAY}^{(u/m)}}{\Theta_{SLAY}^{(m)}} \cdot \alpha_{EAV}(m) = 1 - \alpha_{EAV}(u) \]

9 Soil runoff
\[ q_{RUNF}(i) = a_{RC}(i) \sum_{j \in J} (W_{SOIL}(j) - a_{FC}(j)) \quad \text{if} \quad \sum_{j \in J} (W_{SOIL}(j) - a_{FC}(j)) > 0 \quad i = u, m, l \quad j \geq i \quad \text{means all soil layers above i (for soil layers above stream)} \]
\[ q_{RUNF} = a_{RC} \cdot \left( \sum_{j \in J} (W_{SOIL}(j) - a_{FC}(j)) + (W_{SOIL}(i) - a_{FC}(i)) - p_{\theta_{3}} \cdot c_{SLAY} \cdot 10^{3} \cdot (1 - c_{STRD} / c_{SLAY}) \right) \]
\[ \text{if} \quad ((W_{SOIL} - a_{FC}) - p_{\theta_{3}} \cdot c_{SLAY} \cdot 10^{3} \cdot (1 - c_{STRD} / c_{SLAY})) > 0 \quad \text{(for soil layer with stream)} \]
\[ q_{RUNF} = 0 \quad \text{(for soil layer below stream)} \]
\[ q_{RC}(u) = p_{RCU} + p_{RCSL} \cdot c_{SLAY} \]
\[ a_{RC}(m) = a_{RC}(u) \cdot e^{-Q_{RC} \cdot (c_{SLAY}(u) + c_{SLAY}(m) / 2)} \]
\[ q_{RC} = \frac{\ln(q_{RC}(u) / p_{RC})}{c_{SLAY}(u) \cdot (c_{SLAY}(u) + c_{SLAY}(m) / 2)} \]
10 Tile drainage
\[ q_{TILE} = \max \left( \min \left( p_{RCT} \frac{d_{DSN}}{c_{SLAY}} - \alpha_3, W_{SOIL} - a_{FC} \right), 0 \right) \] (for soil layer with tile)

14 Soil pool transformation processes

\[ F_{DEGN} = p_{DEGN} \cdot C_{IN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{MINN} = p_{MINN} \cdot X_{FASTP} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPS} = p_{DSPS} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPN} = p_{DSPN} \cdot X_{FASTN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ F_{DSPF} = p_{DSPF} \cdot X_{SLOWN} \cdot f(T_{SOIL}) \cdot f(\Theta) \]

\[ f(T_{SOIL}) = \begin{cases} 
\frac{2(T_{SOIL}^2 - 20)}{2(T_{SOIL} - 20)} & T_{SOIL} > 50 \\
\frac{5}{2} & 0 < T_{SOIL} \leq 50 \\
0 & T_{SOIL} \leq 0 \end{cases} \]

\[ T_{AIR} = \frac{a_{SOILMEM}(i) + C_{FROST} \cdot d_{SNOW}}{T_{SOIL}(t, i, t)} \]

\[ a_{SOILMEM}(u) = P_{SURFMEM} \cdot (\Theta_0 + C_{FROST} \cdot d_{SNOW}) \]

\[ a_{SOILMEM}(m) = P_{SURFMEM} \cdot (\Theta_0 + C_{FROST} \cdot d_{SNOW}) \]

\[ a_{SOILMEM}(l) = P_{SURFMEM} \cdot (\Theta_0 + C_{FROST} \cdot d_{SNOW}) \]

\[ a_{SOILMEM}(d) = P_{DEEPMEM} \]

\[ d_{SNOW} = P_{DEEPMEM} \cdot \max(\frac{1}{W_{SNOW}}, 0) \]

\[ a_{SNOW}(t) = P_{SNACT} \cdot W_{SNOW} \cdot \frac{1}{W_{SNOW}} \]

\[ f(\Theta) = \frac{\min \left( 1, \left( \frac{\Theta_0 - \Theta}{P_{SNACT}} \right) \cdot (1 - P_{SNACT}) \cdot \left( 1 - \frac{\Theta - \Theta_0}{P_{SNACT}} \right) c_{SNACT} \right)}{P_{SNACT}} \]

\[ f_2(\Theta) = \frac{((\Theta_0 - \Theta_0) - P_{SMEND})/(1 - P_{SMEND})}{F_{PACT}} \]

\[ f_3(\Theta) = \begin{cases} 1 & \text{if } \Theta < P_{SNACT} \\
0 & \text{else} \end{cases} \]

\[ f(C_{IN}) = \frac{1}{c_{C_{IN}}} \]

16 Phosphorus adsorption/desorption in soil

\[ F_{PADS} = P_{FRCO} \cdot \left( C_{SPRO} \cdot C_{FROST} \cdot c_{SLAY} \cdot c_{BULKED} \cdot X_{PARTP} \right) \]

17 Plant uptake

\[ F_{PUSN} = \min(\alpha_{PUSN} \cdot X_{IN}) \]

\[ F_{PUSN} = \min(\alpha_{PUSN} \cdot X_{SP}) \]

\[ \alpha_{PUSN} = \frac{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})}{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})} \cdot P_{PUSN} \cdot c_{PUSN} \cdot (\Theta_0 - \Theta) \]

\[ \alpha_{PUSN} = \frac{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})}{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})} \cdot P_{PUSN} \cdot c_{PUSN} \cdot (\Theta_0 - \Theta) \]

\[ \alpha_{PUSN} = \frac{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})}{P_{PUSN} \cdot (P_{PUSN} \cdot P_{PUSN})} \cdot P_{PUSN} \cdot c_{PUSN} \cdot (\Theta_0 - \Theta) \]

\[ f(T_{AIR}) = \begin{cases} 0 & T_{AIR} \geq P_{THR} \\
\min \left( 1, \left( \frac{1}{P_{MAX} - P_{THR}} \right) T_{AIR} - \frac{P_{THR}}{P_{MAX} - P_{THR}} \right) & T_{AIR} < P_{THR} \end{cases} \]
21 Immobilization of inorganic nitrogen during infiltration
\[ F_{\text{ININF}} = p_{\text{PONATM}} \cdot C_{\text{IN}} \cdot q_{\text{INF}} \]

22 Reduction during percolation
\[ F_{\text{ONPERC}} = p_{\text{PONRED}} \cdot C_{\text{ON}} \cdot q_{\text{PERC}} \]
\[ F_{\text{PPPERC}} = p_{\text{PPRED}} \cdot C_{\text{PP}} \cdot q_{\text{PERC}} \]
\[ F_{\text{OCPERC}} = p_{\text{OCRED}} \cdot f(T_{\text{SOIL}}) \cdot f(\theta) \cdot C_{\text{OC}} \cdot q_{\text{PERC}} \]
\[ f(T_{\text{SOIL}}) \cdot f(\theta) \text{ as in Equation 14} \]

23 Riparian zone processes
\[ F_{\text{OCRIPZ}} = p_{\text{RIPZ}} \cdot f(T_{\text{SOIL}}) / C_{1} \cdot c_{\text{H}} / 1000 \cdot f(d_{\text{GRW}}) / C_{1} \cdot f(T_{10} < T_{20}) \]
\[ f(d_{\text{GRW}}) = \exp(-p_{\text{RIPE}} \cdot d_{\text{GRW}}) \]
\[ f(T_{10}, T_{20}) = \begin{cases} P_{\text{RIP}} & T_{10} < T_{20} \\ 1 & \text{else} \end{cases} \]
\[ f(\theta) \text{ as in Equation 14 except for sinking groundwater table ($p_{\theta1} \leq \theta < \theta_{\text{SAT}}$):} \]
\[ f(\theta) = \min \left[ 1, \left( \frac{\theta_{\text{SAT}}}{\theta} \right)^{p_{\text{SMEX}}} \cdot (1 - p_{\text{SATACT}} \cdot p_{\text{SATACT}}) \right] \]

Notation

State variables
\[ C_{\text{IN}}, X_{\text{IN}} \] concentration of inorganic nitrogen (mg/l) or soil pool (kg/km²)
\[ C_{\text{OC}}, X_{\text{OC}} \] concentration of organic carbon (mg/l) or soil pool (kg/km²)
\[ C_{\text{ON}}, X_{\text{ON}} \] concentration of organic nitrogen (mg/l) or soil pool (kg/km²)
\[ C_{\text{PP}}, X_{\text{PP}} \] concentration of particulate phosphorus (mg/l) or soil pool (kg/km²)
\[ C_{\text{SP}}, X_{\text{SP}} \] concentration of inorganic phosphorus (mg/l) or soil pool (kg/km²)
\[ W_{\text{SNOW}} \] water content of snow (mm)
\[ W_{\text{SOIL}} \] soil moisture (mm)
\[ X_{\text{FASTC}} \] fast turnover C soil pool (kg/km²)
\[ X_{\text{FASTN}} \] fast turnover N soil pool (kg/km²)
\[ X_{\text{FASTP}} \] fast turnover P soil pool (kg/km²)
\[ X_{\text{PARTP}} \] mineral P soil pool (kg/km²)
\[ X_{\text{SLOWC}} \] slow turnover C soil pool (kg/km²)
\[ X_{\text{SLOWN}} \] slow turnover N soil pool (kg/km²)
\[ X_{\text{SLOWP}} \] slow turnover P soil pool (kg/km²)

Process variables
\[ F_{\text{DEGN}} \] degradation of slowN (kg/km².d)
\[ F_{\text{DEGP}} \] degradation of slowP (kg/km².d)
\[ F_{\text{DENTIT}} \] denitrification in soil (kg/km².d)
\[ F_{\text{DISN}} \] dissolution of fastN to ON (kg/km².d)
\[ F_{\text{DISP}} \] dissolution of fastP to PP (kg/km².d)
\[ F_{\text{DISSN}} \] dissolution of slowN to ON (kg/km².d)
\[ F_{\text{DISSP}} \] dissolution of slowP to PP (kg/km².d)
\[ F_{\text{FCOC}} \] transformation of OC to fastC (kg/km².d)
\[ F_{\text{FCFC}} \] transformation of fastC to slowC (kg/km².d)
\[ F_{\text{FININF}} \] immobilization of IN (kg/km².d)
\[ F_{\text{MINC}} \] mineralization of organic carbon (kg/km².d)
\[ F_{\text{MINN}} \] mineralization of fastN (kg/km².d)
\[ F_{\text{MINP}} \] mineralization of fastP (kg/km².d)
\[ F_{\text{OCFC}} \] transformation of fastC to OC (kg/km².d)
\[ F_{\text{OCCS}} \] transformation of slowC to OC (kg/km².d)
\[ F_{\text{OCPERC}} \] retention of OC in percolation (kg/km².d)
\[ F_{\text{OCRIZ}} \] riparian zone addition of OC to runoff (kg/km².d)
\[ F_{\text{ONPERC}} \] retention of ON in percolation (kg/km².d)
\[ F_{\text{PODS}} \] adsorption/desorption of SP (kg/km².d)
\[ F_{\text{PPPERC}} \] retention of PP in percolation (kg/km².d)
\[ F_{\text{PUTN}} \] plant uptake of N (kg/km².d)
$F_{\text{PUTP}}$ plant uptake of P (kg/km².d)
$q_E$ evapotranspiration (mm/d)
$q_{\text{INF}}$ infiltration (mm/d)
$q_{\text{MELT}}$ snowmelt (mm/d)
$q_{\text{MOMPOR}}$ macropore flow (mm/d)
$q_{\text{PERC}}$ percolation (mm/d)
$q_{\text{RUNF}}$ soil runoff (mm/d)
$q_{\text{SNOW}}$ snow fall (mm/d)
$q_{\text{SOFL}}$ saturated overland flow (mm/d)
$q_{\text{SR}}$ surface runoff due to excess infiltration (mm/d)
$q_{\text{TILE}}$ tile drainage runoff (mm/d)

Other variables
$a_{\text{SNOW}}$ age of snow (d)
$C_{\text{SPEC}}$ SP equilibrium concentration (mg/l)
$d$ index for deep (soil)
$d_{\text{SNOW}}$ snow depth (cm)
$d_{\text{GRW}}$ ground water level below surface (m)
$d_{\text{TILE}}$ water stage above tile depth (m)
$E_{\text{POT}}$ potential evapotranspiration (mm/d)
$i$ soil layer index (u, m or l)
$j$ soil layer index (u, m or l)
$l$ index for lowest soil layer (—)
$m$ index for second soil layer (—)
$P$ precipitation (mm/d)
$t$ time step (d)
$T_{10}$ 10-day average air temperature for subbasin (°C)
$T_{20}$ 20-day average air temperature for subbasin (°C)
$T_{\text{AIR}}$ air temperature for subbasin (°C)
$T_{\text{CLASS}}$ air temperature for class (°C)
$t_{\text{DNO}}$ day number of year (d)
$T_{\text{SOIL}}$ temperature of soil layer and deep soil (°C)
$u$ index for upper soil layer (—)
$a_1$ maximum water content not available for evapotranspiration (mm)
$a_3$ maximum water content available for runoff (mm)
$a_{\text{ERC}}$ exponential rate of runoff coefficient (1/m)
$a_{\text{EVAP}}$ fraction of evapotranspiration from soil layer (—)
$a_{\text{FC}}$ water content at threshold for runoff (mm)
$a_{\text{PUT}}$ potential plant uptake (g/m².d)
$a_{\text{PUTAUT}}$ potential plant uptake in autumn for autumn sown crop (g/m².d)
$a_{\text{RC}}$ soil runoff coefficient (1/d)
$a_{\text{SNOW}}$ snow fraction of precipitation (—)
$a_{\text{SOILMEM}}$ soil temperature memory (d)
$a_{\text{TITOF}}$ temperature threshold for rain/snow fractionation of precipitation (°C)
$a_{\text{WC}}$ maximum water content of soil (mm)
$\Theta$ water content of soil (—)
$\Theta_{\text{SAT}}$ water content at saturation (—)

Model parameters
$p_{\text{CEAM}}$ amplitude of evapotranspiration seasonal correction (general) (—)
$p_{\text{CED}}$ decrease of evapotranspiration with soil depth (general) (1/m)
$p_{\text{CEPH}}$ phase of evapotranspiration seasonal correction (general) (d)
$p_{\text{CEVP}}$ rate of potential evapotranspiration (land use) (mm/d.°C)
$p_{\text{CMLT}}$ snow melt coefficient (land use) (mm/d.°C)
$p_{\text{COH}}$ cohesion of soil (soil type) (kPa)
$p_{\text{DEEPMEM}}$ soil temperature memory for deep soil (general) (d)
$p_{\text{DEGN}}$ degradation of slowN to fastN (land use) (1/d)
**pDEGP**
degradation of slowP to fastP (land use) (1/d)

**pDENEX**
exponent in soil moisture function for denitrification (general) (—)

**pDENIT**
denitrification rate in soil (land use) (1/d)

**pDENSo**
snow density of new snow (general) (—)

**pDENSDT**
change of snow density with time (general) (1/d)

**pDESN**
transformation fastN to ON (land use) (1/d)

**pDESP**
transformation fastP to PP (land use) (1/d)

**pDENSN**
transformation slowN to ON (land use) (1/d)

**pDENSP**
transformation slowP to PP (land use) (1/d)

**pDMEM**
soil temperature memory depth coefficient (land use) (1/m)

**pFRCO**
coefficient in Freundlich equation (soil type) (1/kg)

**pFREX**
exponent in Freundlich equation (soil type) (—)

**pHSATIN**
half saturation point for IN concentration (general) (mg/l)

**pKHO**
transformation of slowC to OC (general) (—)

**pKLH**
transformation of fastC to slowC (general) (—)

**pKLO**
transformation of fastC to OC (general) (—)

**pKOF**
transformation of OC to fastC (general) (—)

**pKOFLIM**
soil moisture threshold for transformation of OC to fastC (general) (—)

**pLP**
limit for potential evapotranspiration (general) (—)

**pMINC**
fraction mineralization of organic carbon (general) (—)

**pMINN**
mineralization of fastN to IN (land use) (1/d)

**pMINP**
mineralization of fastP to SP (land use) (1/d)

**pMPERC**
maximum percolation (soil type and soil layer) (mm/d)

**pOCRED**
reduction of OC during percolation (general) (—)

**pONRED**
reduction of ON during percolation (land use) (—)

**pPADS**
adsorption/desorption rate (soil type) (1/d)

**pPNRAT**
PN ratio in plant uptake (crop type) (—)

**pPONATM**
fraction of infiltration IN immobilized (land use) (—)

**pPPRED**
reduction of PP during percolation (land use) (—)

**pPUT1**
plant uptake parameter (crop type) (g/m²)

**pPUT2**
plant uptake parameter (crop type) (g/m²)

**pPUT3**
plant uptake parameter (crop type) (1/d)

**pRCLO**
soil runoff coefficient for lowest layer (soil type) (1/d)

**pRCMP**
runoff coefficient for macropore flow (soil type) (—)

**pRCPL**
runoff coefficient dependence on slope (general) (1/d,%)

**pRCOF**
runoff coefficient for saturation overland flow (land use) (1/d)

**pCRSR**
runoff coefficient for surface runoff (soil type) (—)

**pRCT**
tile drainage runoff coefficient (soil type) (1/d)

**pRCU**
soil runoff coefficient for top layer (soil type) (1/d)

**pRIPE**
riparian zone effect on OC, groundwater level dependence (general) (—)

**pRIPS**
autumn factor of riparian zone effect on OC (general) (—)

**pRIPI**
riparian zone effect on OC (land use) (—)

**pRILOW**
lower range in soil moisture function (—), for NP (general), for OC (land-use)

**pRIUP**
upper range in soil moisture function (general) (—)

**pPSACT**
activity at saturation (—), for NP (general), for OC (land-use)

**pPSMND**
coefficient in soil moisture function for denitrification (general) (—)

**pSMEX**
exponent in soil moisture function (general) (—)

**pSMEM**
soil temperature memory for surface (land use) (d)

**pTSALG**
air temperatures elevation dependence (general) (°C/m)

**pTHRO**
flow threshold for surface runoff and macropore flow (soil type) (mm/d)

**pTHRD**
soil moisture threshold for surface runoff and macropore flow (soil type) (mm)

**pTINT**
half temperature interval for mixed snow and rain (general) (°C)

**pTMAX**
parameter in winter crop nutrient uptake calculation (general) (°C)

**pTTMP**
temperature threshold (land use) (°C)

**pTTPD**
difference in temperature threshold for snow/rain fractionation (general) (°C)

**pTTFR**
temperature threshold for plant nutrient uptake during late autumn (general) (°C)

**pΘ1**
fraction of soil layer where water is not available for evapotranspiration (soil type) (—)

**pΘ2**
fraction of soil layer where water is available for evapotranspiration but not for runoff (soil type) (—)

**pΘ3**
fraction of soil layer where water is available for runoff (soil type) (—)
Constants/input data

- $c_{BD2}$: day number of sowing date in spring (d)
- $c_{BD5}$: day number of sowing date in autumn (d)
- $c_{BULKD}$: bulk density of soil (kg/m$^3$)
- $c_H$: class’ elevation (m)
- $c_{SLAY}$: soil layer thickness (m)
- $c_{SLOPE}$: slope of subbasin (%)
- $c_{SPFROST}$: soil temperature snow dependence (10 d/cm)
- $c_{STRD}$: stream depth below soil layer upper limit (m)
- $c_{TILE}$: depth of tile and drainage pipe (m)
- $c_{WDEEP}$: deep soil temperature weight (0.001 for soil layers, 0 for deep soil temperature)
- $c_{AH}$: class’ elevation deviation from subbasin mean elevation (m)