Technical Report

TR-09-24

Tracey – a simulation model of trace element fluxes in soil-plant system for long-term assessment of a radioactive groundwater contamination

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October 2009

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Summary

This study provides important background information for SKB's risk assessment programme on final deposits of nuclear fuel waste in Sweden. We developed a general trace element model called *Tracey* to simulate dynamically the possible accumulation of radionuclides as a result of an eventual long-term radioactive contamination of groundwater in terrestrial ecosystems. We applied the model *Tracey* to two different forest ecosystems of Forsmark (Uppland), one mixed pine-spruce forest typical for the relatively dry elevated areas and the other one an alder forest typically for the relatively wet low land areas. The impact of various radionuclide properties and ecosystem characteristics on radionuclide accumulation was determined in a sensitivity analysis.

The overall objectives of the study are to: 1) Develop and evaluate a multi-compartmental model that dynamically simulates the transport and accumulation of a radionuclide in the soil-plant system at a time scale relevant for risk assessment of nuclear fuel waste; and 2) Asses the possible accumulation of radionuclide in terrestrial ecosystems due to an eventual long-term continuous radioactive groundwater contamination.

Specific objectives were to assess:

- The proportion of the contamination accumulated and where it is stored in the ecosystem.
- The importance of the plant uptake approach for accumulation of radionuclides.
- The most important radionuclide properties and ecosystem characteristics for accumulation and losses.
- The proportion of the contamination lost and how is it lost.
- The circumstances which stimulated export of radionuclides to other ecosystems.

A previous radionuclide model /Gärdenäs et al. 2006/ describes the transport and accumulation in the soil-plant system of a radionuclide originating from groundwater contamination. The model presented here, called *Tracey*, is a stand-alone version to allow for long simulation periods relevant for the time scale of risk assessment of nuclear waste (*i.e.* several thousand years) with time steps as short as one day. *Tracey* is a multi-compartmental model in which fluxes and storage of radionuclide are described for different plant parts (leaves, stem, roots and seeds) and for several soil layers. Each layer includes pools of slowly and quickly decomposing litter, humus, solved and absorbed trace element. The trace element fluxes are assumed to be proportional to either water or carbon fluxes, these fluxes are simulated using the dynamic model *CoupModel* for fluxes of water, carbon, nitrogen and carbon in terrestrial ecosystems.

Two different model approaches were used to describe plant uptake of radionuclides. The one called passive uptake approach is driven by water uptake and the one called active uptake approach is driven by growth. A simple approach describing adsorption to soil particles and organic matter was added. The contaminant can be added to the ecosystem by groundwater contamination or source contamination in different soil layers and leaves the ecosystem by leaching and harvest.

Tracey was applied on two types of ecosystems with contrasting hydrology: 1) A managed, mixed forest of pine-spruce (*Pinus-Picea*), which is typical for recharge (i.e. high elevation) areas in a landscape; and 2) a natural hardwood forest of European alder (*Alnus glutinosa*) which is typical for discharge areas in Forsmark, central Sweden. A number of different varieties of the two ecosystems, referred to as functional forest types, were created by varying the root depth and radiation use efficiency. Sixteen functional forest types were created for the pine-spruce forest and twelve for the alder forest. The climate was cold-temperate and based on 30-year daily weather data from Uppland in central Sweden. The assumed contamination was close to 1 mg of an unspecified trace element per m^2 and year. This load corresponds to 1 Bq per m^2 and year for ^{238}U, one of the most common long-living radionuclides in nuclear fuel waste. The assumed contamination continued during the entire simulation period, *i.e.* 10,000 years.

We assessed the sensitivity of radionuclide accumulation in an ecosystem to various radionuclide properties and ecosystem characteristics by Monte Carlo simulations. One thousand Monte Carlo-simulations were made per functional forest type and plant uptake approach (passive and active uptake). This was made possible by establishing a link between *Tracey* and the sensitivity toolbox *Eikos* /Ekström 2005, Ekström and Broed 2006/. Examples of radionuclide properties tested are adsorption coefficient and allocation pattern of radionuclide. Examples of ecosystem characteristics tested are rooting depth, radiation use efficiency and soil bulk density. Distributions of each radionuclide property and ecosystem characteristics were defined. For radionuclide properties, the distributions were based on literature data for a various radionuclides and/or micro-nutrients, and for ecosystems characteristics on literature data of several alder and pine-spruce forest research sites in Fenno-Scandinavia.

The pine-spruce ecosystems accumulated over the simulation period of 10,000 years on average 20–25% of the total load of contamination in the soil, while the alder ecosystems accumulated between 20 and 90%. The remainder of the contamination was leached, especially during episodes with high drainage flows. Trace element in the soil was predominately found adsorbed below 2 m depth in low-accumulating ecosystems (*i.e.* ecosystem where ≤ 25% of the contaminant was stored in the soil). Low-accumulating ecosystems were the alder functional forest types with passive uptake system and all pine-spruce forest types (both the ones with passive and active uptake). The adsorption coefficient (K_d) was the single most important explanatory factor for these low-accumulating systems. Adsorption was stimulated by an adsorption coefficient of ≥ 4 m^3 kg^{-1}, in combination with a soil bulk density of $\geq 1{,}000$ kg m^{-3}.

In the high-accumulating ecosystems (*i.e.* ≥ where 75% of the contaminant was stored in the soil), the trace element was predominately stored in humus in the upper soil layers. A combination of active plant uptake and deep roots stimulated accumulation of trace element in humus, particularly when the root zone was contaminated during the growing season. Of the radionuclide properties tested, a low degree of convective transport (*i.e.* high degree of dispersion) and a low adsorption coefficient further stimulated accumulation of trace elements in humus. All these factors favoured the uptake of trace elements by plants. Hence, even though accumulation of radionuclide *in* plants was low, uptake *by* plants was important for total accumulation in the ecosystems and the uptake approach used, passive or active, did matter.

Evaluation of model performance revealed that the structural complexity of the *Tracey* model was appropriate for the objectives of this study. The use of a multi-compartment soil model and the time resolution of the driving variables proved to be relevant. Accumulation was shown to be very dependent on the degree of root zone contamination in the growing season. Sources of uncertainty in the simulation results were examined. We suggest to test the ability of *Tracey* by modelling measured dynamics of trace elements, for example those of naturally occurring radionuclides in ecosystems. It was concluded that the *Tracey* model has great potential in risk assessment studies of hypothetical contaminants, as in this study, and of actual contaminants. *Tracey* can be applied to all kinds of waste deposits, from municipal waste to residual nuclear waste.

Contents

1 Introduction

Evaluation of long-term nuclear fuel waste management and soils contaminated with radionuclides requires sophisticated computer models that integrate our current understanding on flow and transport phenomena /Mallants 2006/. Several research groups are working on assessing the effects of eventual long-term contamination of soil and groundwater on possible release and accumulation of radionuclides in ecosystems /Pruess et al. 2002, Yabusaki et al. 2007/. /Avila 2006/ performed a sensitivity analysis of possible accumulation of various radionuclides in the biosphere assuming a continuous contamination of 1 Bq per m^2 and year over 10,000 years. The Avila model assumes constant annual water balance and soil moisture content. It comprises several compartments, but the soil was represented as one compartment representing the root zone with both plant roots and mineral soil and sometimes the soil layers below the root zone. Hence, the model assumes a direct input of the radionuclides to the whole unsaturated root zone. The estimations made with this model are valuable, in particular for the insight that they give concerning the importance of adsorption capacities for accumulation of various radionuclides. However, plant uptake of water and solutes takes place in the root zone, which is unsaturated most of the year, while groundwater contamination, by definition, takes place in the saturated zone. A comparison can be made with risk assessments of cadmium contamination of groundwater. /Skagg et al. 2007/ showed that Cd accumulation in soil was overestimated by a factor of two when the soil compartment was modelled as one layer instead of several layers.

Modelling a realistic root distribution and groundwater level fluctuation might thus be of great importance in reducing the uncertainties in estimations and thereby increasing their quality. *CoupModel* /Jansson and Karlberg 2004/ is such model, in which the soil is divided into several layers and the groundwater fluctuates. Equally important for our objectives is that in *CoupModel*, flows of water, heat, carbon and nitrogen in the soil-plant system are dynamically coupled in each time-step, *i.e.* carbon fluxes are affected by water, heat and nitrogen fluxes in each time step and *vice versa*. *CoupModel* is the Windows successor and integrated version of the two DOS models SOIL /Jansson and Halldin 1979/ and SOILN /Johnson et al. 1987, Eckersten et al. 1998/, which have been widely used on different ecosystems and climate regions over the past 25 years /*e.g*. Eckersten and Slapokas 1990, Gärdenäs and Jansson 1995, Beier et al. 2001, Gustafsson et al. 2004/. The model has also been applied at SKB's investigation areas Forsmark and Simpevarp /Gustafsson et al. 2006, Karlberg et al. 2007a/.

/Gärdenäs et al. 2006/ introduced into *CoupModel* a trace element sub-model to describe accumulation and transport of a radionuclide in terrestrial ecosystems after groundwater contamination. Here we present *Tracey*, an extended stand-alone version of the trace element model that allows long simulation periods at a time scale relevant for assessment of nuclear fuel waste management, *i.e*. several thousand years. The trace element model *Tracey* was written in Matlab-Simulink. Fluxes and storage of trace elements in different plant parts (leaves, stem, roots and seeds) and several soil layers (each layer includes pools of slowly and quickly decomposing litter, humus, solved and absorbed trace element) form the heart of the *Tracey* model. The trace element fluxes are assumed to be proportional to either water or carbon fluxes. The carbon and water fluxes are simulated using *CoupModel* and provided to *Tracey* as driving variables.

The uptake of radionuclides by plants is often assumed to be proportional to their water uptake and the concentration of the radionuclide in soil water, *i.e.* the *passive uptake* approach. However, it is well-known that some radionuclides can be taken up in higher concentrations than can be explained by water uptake alone /*e.g*. Greger 2004/. The *active uptake* approach assumes that uptake of radionuclides is governed by carbon assimilation.

The sensitivity of radionuclide accumulation in the terrestrial ecosystems to various properties radionuclides properties and to ecosystem characteristics was assessed. For this purpose, a link between *Tracey* and the simulation toolbox *Eikos* /Ekström 2005/ was established. Examples of radionuclide properties tested include adsorption coefficient and allocation pattern of radionuclide. Examples of ecosystem characteristics tested include rooting depth, radiation use efficiency and soil bulk density. Two types of ecosystems with contrasting hydrology were studied: 1) A mixed forest of pine-spruce (*Pinus-Picea*), typical for recharge areas i.e. high elevated areas, and 2) a natural hardwood forest of European alder (*Alnus glutinosa*) typical for discharge areas i.e. low elevated areas of the Forsmark, a region of central Sweden.

The overall objectives of the study were to:

i) Develop and evaluate a multi-compartmental model that dynamically simulates the transport and accumulation of a radionuclide in the soil-plant system at a time scale relevant for risk assessment of nuclear waste.

ii) Asses the possible accumulation of radionuclide in terrestrial ecosystems due to an eventual long-term continuous radioactive groundwater contamination.

Specific objectives were to assess:

- The proportion of the contamination accumulated and where it is stored in the ecosystem.
- The importance of the plant uptake approach for accumulation.
- The proportion of the contamination lost and how is it lost.
- The most important radionuclide properties and ecosystem characteristics for accumulation and losses.
- The circumstances which stimulate export of radionuclides to other ecosystems.

The assumed contamination was close to 1 mg of an unspecified trace element per m^2 and year. This load corresponds to 1 Bq per m^2 and year for ^{238}U, one of the most common long-living radionuclides in nuclear fuel waste. The contamination continued during the whole simulation time, *i.e.* 10,000 years.

2 Overview of model structure and links between *Tracey*, *CoupModel* and *Eikos*

The trace element model *Tracey* is a process-oriented description of trace element fluxes and pools in terrestrial ecosystems. *Tracey* is an adopted stand-alone version of a fully integrated trace element sub-model /Gärdenäs et al. 2006/ of the ecosystem process model *CoupModel* /Jansson and Karlberg 2004/. This stand-alone version was necessary to extend the simulation periods to a time scale relevant for radionuclide applications (10^3–10^5 years) and at the same time maintain the dynamical coupling between water and carbon fluxes at a daily time step. The conversion was possible since the radionuclides are considered passive tracers without any feedback on the governing water and carbon fluxes. Just as in the original model version, the fluxes of trace element in *Tracey* are assumed to be proportional to either water or carbon fluxes in the soil-plant system. These water and carbon fluxes are simulated using *CoupModel*, an ecosystem model simulating dynamically the coupling between water, heat, carbon and nitrogen in the soil-plant-atmosphere system, and are delivered to *Tracey* as driving variables (Figure 2-1).

The sensitivity of radionuclide accumulation to parameter settings of *Tracey* was investigated using *Eikos* /Ekström 2005, see Figure 2-1/, a simulation toolbox for sensitivity analysis offering different options for describing distribution of parameters, defining sampling method as well as statistical analysis of simulation results. The *Tracey* parameters included in the sensitivity analyses reflected radionuclide properties such as adsorption coefficient and also ecosystem characteristics such as soil bulk density. An extra dimension of the sensitivity analysis was obtained by including various forest functional types of carbon and water fluxes in pine-spruce and alder forests simulated with *CoupModel* in the *Tracey*-*Eikos* simulations. The flows of information between *Tracey* and *CoupModel* and *Tracey* and *Eikos* are illustrated in Figure 2-1.

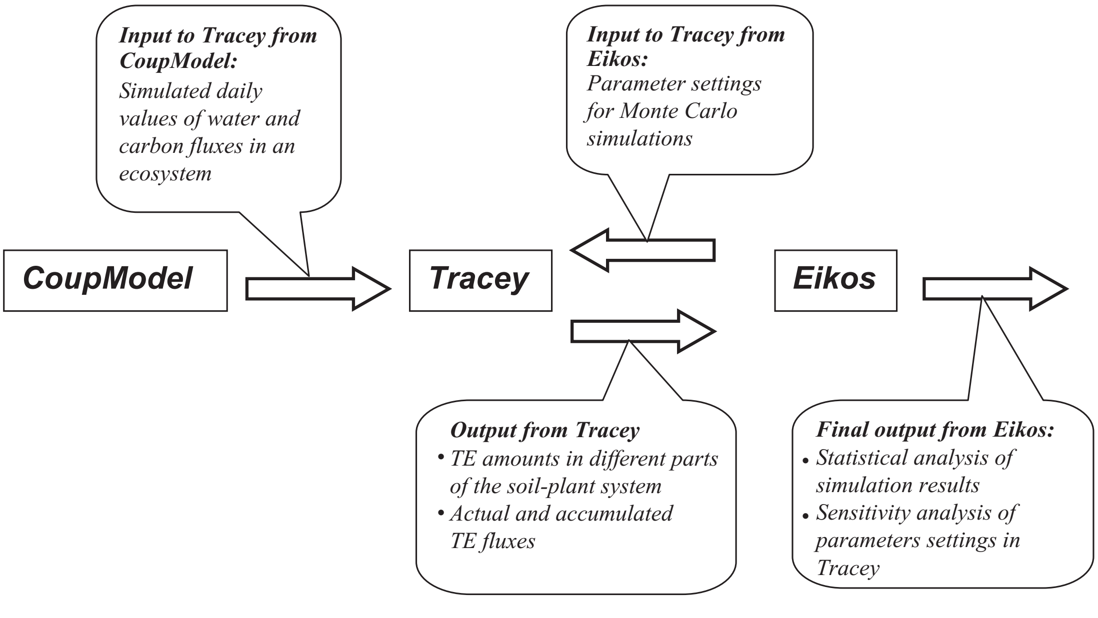


Figure 2-1. *Schematic illustration of information flows between CoupModel, Tracey and Eikos and final output of Tracey and Eikos.*

3 Trace element model *Tracey*

The cycling of a radioactive element is described as a general model of a trace element cycling in the soil-plant system. *Tracey* is written in Matlab-Simulink. The trace element is denoted by the abbreviation *TE* throughout the model description. Trace elements in different plant compartments, *i.e.* plant tissues, are represented (*e.g.* TE_{Leaf}, TE_{Stem}, TE_{Root} and TE_{Seeds} [mg *TE* m^{-2}], Figure 3-1). The sum of trace element in plant tissues grown in the current year is called trace element in young plant $TE_{YoungPlant}$, and the sum of trace element in the different plant tissues grown in previous years (*i.e.* $TE_{OldLeaf}$, $TE_{OldStem}$, and $TE_{OldRoot}$) is called trace element in old plant tissues $TE_{OldPlant}$. In the soil, trace element is found in three different soil organic matter fractions, *i.e.* $TE_{Litter1}$, $TE_{Litter2}$ and TE_{Humus}, where *Litter1* stands for the more easily decomposable material such as needles and *Litter2* for more decomposition-resistant litter such as stems and coarse branches. Trace element can also be found in the soil adsorbed to soil particles $TE_{Adsorbed}$ and solved in soil water solution TE_{Solved}. Trace element can be added to the ecosystem as a constant groundwater flux or as a constant flux in specified soil layers q_{TEin} [mg *TE* day^{-1}]. It can leave the ecosystem through percolation q_{TEperc}, leaching $q_{TEdrain}$ and harvest $q_{TEharvest}$.

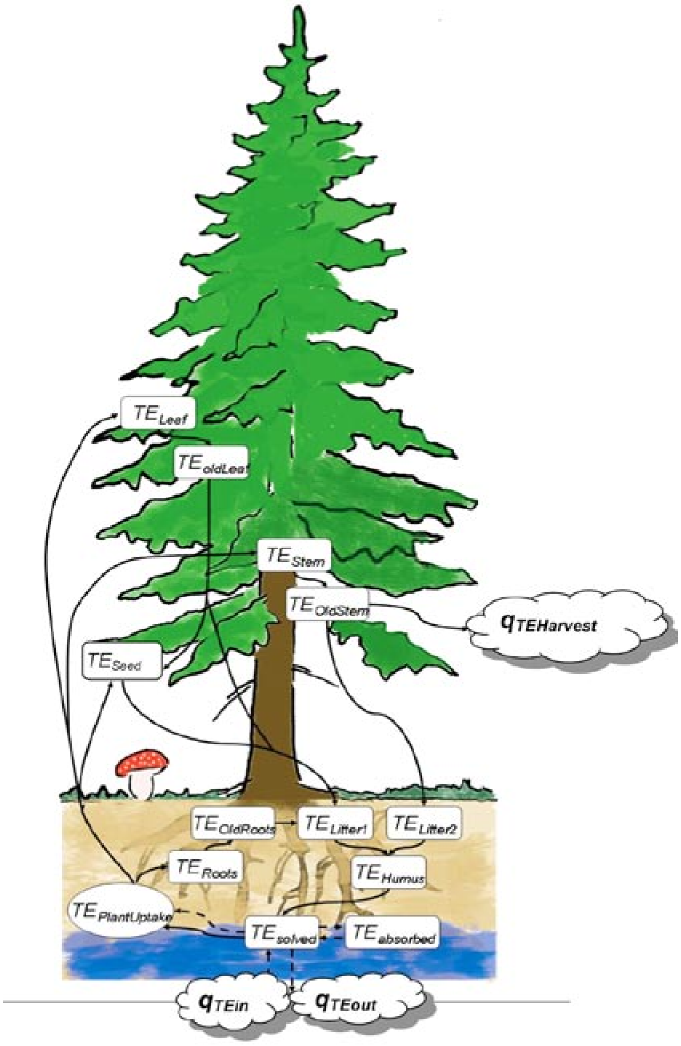


Figure 3-1. *Pools and fluxes of trace element (TE) in the model. Solid arrows represent TE fluxes that are proportional to carbon fluxes and dashed arrows represent TE fluxes that are proportional to water fluxes. Boxes represent state variables, clouds sinks or sources and circles auxiliary variables. The soil profile is divided into different layers, each of which includes all soil TE pools (adopted from /Gärdenäs et al. 2006/, original illustration by Peter Roberntz, coloured by Hans Johansson).*

The trace elements fluxes are assumed to be proportional to either water or carbon fluxes, represented by dashed and solid arrows respectively in Figure 3-1. Discrimination factors ($TE_{DProcess}$) are used to simulate reduced or enhanced trace element fluxes compared with water or carbon fluxes. The different processes governing the trace element fluxes and pools are described in detail in the following Chapters.

3.1 Contamination process

The soil profile is contaminated by a constant daily flux q_{TEIn} [mg TE m^{-2} day^{-1}], which is distributed among soil layers in proportion to the distribution of water among these layers. The daily contamination of layer i is given by the fraction of gravitational water content (*i.e.* mass of water) in that layer $m_w(z_i)$ per unit surface area [g m^{-2}] compared with that of all contaminated layers $\Sigma m_w(z_i)$ [g m^{-2}]:

$$TE_{In}(z_i) = q_{TEIN} \frac{m_w(z_i)}{\sum m_w(z_i)} \qquad ;i = i_{Sat} \text{ to } i_{Bottom} \qquad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad \text{(Eq. 3-1a)}$$

$$TE_{In}(z_i) = q_{TEIN} \frac{m_w(z_i)}{\sum m_w(z_i)} \qquad ;i = i_{Top} \text{ to } i_{Bottom} \qquad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad \text{(Eq. 3-1b)}$$

Two different contamination approaches were applied to select the soil layers to be contaminated, the *groundwater* approach (Eq. 3-1a) and the *total profile* approach (Eq. 3-1b). The groundwater approach was used for pine-spruce in the recharge areas (i.e. high elevated areas, Eq. 3-1a) and assumes that contamination only occurs in the saturated zone (*i.e.* below the groundwater level, i_{Sat}). As a consequence of this restriction, plant uptake of radionuclides is limited when roots are not in contact with groundwater. In the event of the groundwater level being below the upper end of a soil layer, the contamination of that layer was reduced proportionally.

In the total profile contamination approach, all layers from the top (i_{Top}) to the bottom (i_{Bottom}) of the soil profile are contaminated in proportion to their gravitational water content (Eq. 3-1b). This approach was used for alder in discharge areas such as downhill positions or near-stream or lake-side positions, where lateral inflow of radionuclides could be expected in the unsaturated zone in addition to groundwater contamination. The consequences of the different contamination approaches are discussed in Chapter 10 (Model response to contamination process). In both approaches, contamination is assumed to occur through the same 'channels' as outflow. This means that when the deepest soil layer has no outflow of water, that layer is not contaminated.

3.2 Plant uptake

All plant uptake of trace element is assumed to occur through roots. Two different model approaches describe plant uptake and allocation pattern, passive and active uptake respectively. Passive uptake is assumed to be driven by water uptake, and active uptake by carbon assimilation and plant demand. The active uptake approach was added to simulate high concentrations of radionuclides in certain plant tissues that could not be explained by water uptake alone and that must therefore involve other processes. Accordingly, the allocation pattern of trace element to the different plant compartments is also different for the two uptake approaches. For the passive uptake, there is constant allocation of fractions to the different plant compartments. For the active uptake, allocation is a function of the demand and growth of a plant compartment. In the model, we made the simplification that plant uptake occurs either passively *or* actively, in order to avoid making prior assumptions on the importance of passive plant uptake, as one of the aims of the study was to investigate just this factor.

Passive uptake

The passive uptake (PU) of trace element by the plant is governed by the trace element concentration in soil water within the root zone $TE_c(z_r)$ [mg TE mm^{-1} m^{-2}], the water uptake from the root zone W_{upt} rate [mm day^{-1}] and a dimensionless scaling factor representing the degree of convective plant uptake $TE_{DWUptake}$ [–]. The fraction of trace element allocated to the leaf compartment is defined by a constant allocation fraction f_{PULeaf} [–]. The passive uptake of trace element to leaf from a certain layer is described as:

$$TE_{Solved\rightarrow Leaf}(z) = TE_{DWUptake} \cdot f_{PULeaf} \cdot TE_c(z_r) \cdot W_{upt}(z) \quad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-2})$$

The scaling factor $TE_{DWUptake}$ is a discriminating factor that can be used to reduce the uptake of trace elements in relation to the water uptake. It is given in the interval between zero and one, where a value of one means that the concentration of trace element in the water taken up by roots equals the concentration of trace element in the soil water solution in that soil layer. The water uptake rate W_{upt} [mm day^{-1}] by plant roots is the driving variable simulated using *CoupModel*. By summarising, over all layers where roots are present and water uptake takes place, the total leaf uptake is estimated as:

$$TE_{Solved\rightarrow Leaf} = TE_{DWUptake} \cdot f_{PULeaf} \cdot \sum_{i=1}^{n} TE_c(z_{ri}) \cdot W_{upt}(i) \quad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-3})$$

where $i=1..n$ represents the number of layers contributing to the total uptake and allocation. Similar equations are used for allocation to seeds, root and stem using $f_{PUSeeds}$, f_{PURoot} and f_{PUStem} respectively. The sum of the plant compartment specific allocation fractions equals one:

$$1 = f_{PUSeed} + f_{PULeaf} + f_{PURoot} + f_{PUStem} \qquad [–] \qquad (\text{Eq. 3-4})$$

The total uptake for the whole plant $TE_{Solved\rightarrow Plant}$ [mg TE m^{-2} day^{-1}] is the sum of trace element allocated to the different plant compartments:

$$TE_{Solved\rightarrow Plant} = \sum_{i=1}^{n} TE_{Solved\rightarrow Leaf} + \sum_{i=1}^{n} TE_{Solved\rightarrow Seed} + \sum_{i=1}^{n} TE_{Solved\rightarrow Stem} + \sum_{i=1}^{n} TE_{Solved\rightarrow Root}$$

$$[\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-5})$$

Active plant uptake

The active uptake (*AU*) is driven by carbon allocation to each specific plant compartment $C_{a\rightarrow Leaf}$, $C_{a\rightarrow Stem}$, $C_{a\rightarrow Seeds}$ and $C_{a\rightarrow Root}$ [g C day^{-1}]. The carbon assimilation and the maximum ratio of a trace element and new carbon assimilates of a plant compartment $p_{MaxTECleaf}$[mg TE g C^{-1} m^{-2}] determine the trace element demand of a plant compartment, for instance the trace element demand of leaves is defined as:

$$TE_{DemandLeaf} = p_{MaxTECleaf} \cdot C_{a\rightarrow Leaf} \qquad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-6})$$

The trace element demand of roots, seeds and stem is estimated in a similar way, so that the total plant trace element demand equals the sum of trace element demand in different plant parts:

$$TE_{DemandPlant} = \sum_{i=Seed,\ Leaf,\ Stem,\ Root} TE_{Demand}(i) \qquad [\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-7})$$

The actual amount of trace element taken up by the plant $TE_{Solved\rightarrow Plant}$ can be less than plant demand when solved content of a trace element in the root zone $TE_{Solved}(z)_r$ [mg TE m^{-2}] and radionuclide bioavailability $TE_{BioRate}$ are limiting. The bioavailability $TE_{BioRate}$ is the fraction of the trace element the plant can take up in one day [day^{-1}]. Accordingly, the amount taken up from a root zone layer is defined as the minimum of the plant demand and available trace element:

$$TE_{Solved\rightarrow Plant}(z_r) = \min\left(TE_{DemandPlant}(z) \cdot f(z_r), TE_{solved}(z_r) \cdot TE_{BioRate}\right)$$

$$[\text{mg } TE \text{ m}^{-2} \text{ day}^{-1}] \qquad (\text{Eq. 3-8})$$

where $f(z_r)$ [–] represents the root fraction in a soil layer. The total active plant uptake is the sum of the uptake by the different plant compartments $TE_{Solved\rightarrow Plant}$ is calculated using the same equations as for passive uptake, i.e. Eq. 3-5. When plant available trace element is less than total plant demand, the amount taken up is divided over the plant compartments in proportion to their demand.

3.3 Translocation of trace elements to seeds and old plant pools

Translocation of trace elements to the seed pool from roots, leaves and stem is proportional to the carbon fluxes and the ratio of trace element to carbon content of the respective plant source pool. For example, the transfer of trace elements from leaves to seeds, $TE_{Leaf \rightarrow Seed}$, is calculated as:

$$TE_{Leaf \rightarrow Seed} = TE_{DLeaf \rightarrow Seed} \cdot C_{Leaf \rightarrow Seed} \cdot \frac{TE_{Leaf}}{C_{Leaf}} \qquad [\mathrm{mg}\ TE\ \mathrm{m}^{-2}\ \mathrm{day}^{-1}] \qquad \text{(Eq. 3- 9)}$$

where $C_{Leaf \rightarrow Seed}$ [g C m^{-2} day^{-1}] is the flux of carbon from leaves to seeds, TE_{Leaf} [mg TE m^{-2}] and C_{Leaf} [g C m^{-2}] the trace element and carbon content in the leaves respectively. $TE_{DLeaf \rightarrow Seed}$ [–] is a discriminating factor to allow for reduced or enhanced trace element flux compared with the carbon flux between the plant compartments. The translocation of trace element from roots to seeds, $TE_{Root \rightarrow Seed}$, and from stem to seed, $TE_{Stem \rightarrow Seed}$, is calculated similarly.

With every new vegetation period, *i.e.* from 1 January in the northern hemisphere, the amounts of trace element in the current year pool TE_{Leaf}, TE_{Stem} and TE_{Roots} are transferred to corresponding pools for old plant material, *i.e.* $TE_{OldLeaf}$, $TE_{OldStem}$ and $TE_{OldRoots}$.

3.4 Litterfall and soil processes

Trace element fluxes with litterfall from leaves, stem, seeds and roots to litter are calculated in the same manner as trace element fluxes to seeds, *i.e.* in proportion to carbon fluxes and the ratio of trace element to carbon content of the respective plant compartment multiplied by a discrimination factor $\mathrm{TE}_{\mathrm{DLeaf} \rightarrow \mathrm{Litter1}}$. For example, the flux of trace element with leaf litterfall is calculated as:

$$TE_{Leaf \rightarrow Litter1} = TE_{DLeaf \rightarrow Litter1} \cdot C_{Leaf \rightarrow Litter1} \cdot \frac{TE_{Leaf}}{C_{Leaf}} \qquad \text{(Eq. 3-10)}$$

Litter1 represents the more easily decomposable material, while *Litter2* represents the more decomposition-resistant material such as coarse branches and stem. The trace element fluxes follow the carbon fluxes as simulated using *CoupModel*. The belowground litter production, *i.e.* root litter, was intended to go directly to the litter compartment of the same soil layer but by mistake, litter from the old roots was transferred to the uppermost layer. However, the consequences of this mistake were of minor importance, see Chapter 13 (Sources of uncertainties).

The humified organic matter from both *Litter1* and *Litter2* ends up in the *Humus* pool:

$$TE_{Litter \rightarrow Humus} = TE_{Litter1 \rightarrow Humus} + TE_{Litter2 \rightarrow Humus} \qquad [\mathrm{mg}\ TE\ \mathrm{m}^{-2}\ \mathrm{day}^{-1}] \qquad \text{(Eq. 3-11)}$$

where

$$TE_{Litter1 \rightarrow Humus} = TE_{DLitter1 \rightarrow Humus} \cdot C_{Litter1 \rightarrow Humus} \cdot \frac{TE_{Litter1}}{C_{Litter1}}$$

[mg TE m^{-2} day^{-1}] (Eq. 3-12)

$$TE_{Litter2 \rightarrow Humus} = TE_{DLitter2 \rightarrow Humus} \cdot C_{Litter2 \rightarrow Humus} \cdot \frac{TE_{Litter2}}{C_{Litter2}}$$

Litter from all tissues except for old stem tissues, *OldStem*, is added to *Litter1*. *OldStem* litter is added to *Litter2*. During the decomposition process, part of the carbon is released as CO_2 through soil respiration. The trace element loss corresponding to the carbon content lost by soil respiration, $\mathrm{C}_{\mathrm{Litter} \rightarrow CO_2}$, is assumed to go into soil water solution:

$$TE_{Litter1 \rightarrow Solved} = TE_{DLitter1 \rightarrow Solved} \cdot C_{Litter1 \rightarrow CO_2} \cdot \frac{TE_{Litter1}}{C_{Litter1}} \qquad [\mathrm{mg}\ TE\ \mathrm{m}^{-2}\ \mathrm{day}^{-1}] \qquad \text{(Eq. 3-13a)}$$

$$TE_{Litter2 \rightarrow Solved} = TE_{DLitter2 \rightarrow Solved} \cdot C_{Litter2 \rightarrow CO_2} \cdot \frac{TE_{Litter2}}{C_{Litter2}} \qquad [\mathrm{mg}\ TE\ \mathrm{m}^{-2}\ \mathrm{day}^{-1}] \qquad \text{(Eq. 3-13b)}$$

$$TE_{Humus\rightarrow Solved} = TE_{DHumus\rightarrow Solved}\cdot C_{Humus\rightarrow CO_2}\cdot \frac{TE_{Humus}}{C_{Humus}}$$ [mg *TE* m^{-2} day^{-1}] (Eq. 3-13c)

By mistake, $C_{Litter1,2\rightarrow C02}$ was replaced by $C_{Litter1,2\rightarrow C02}-C_{Litter1,2\rightarrow Hummus}$ in the simulations, which resulted in an overestimation of trace element in litter. This mainly influenced the distribution among organic pools (see Chapter 13).

To estimate the amount of trace element in soil water solution (TE_{Solved}), the first step is to estimate the change due to contamination, fluxes from the litter and humus pools, water flows between soil layers, and drainage, not considering adsorption. This preliminary change in soil water solution is denoted $\delta TE_{SolvedNoAds}$ mg *TE* m^{-2} day^{-1}]:

$$\begin{aligned}\delta TE_{SolvedNoAds(z)} &= TE_{In(z)} + TE_{Litter\,1,2(z)\rightarrow Solved\,(z)}\\ &+ TE_{Humus\,(z)\rightarrow Solved\,(z)} + TE_{Solved\,(z-1)\rightarrow Solved\,(z)}\\ &- TE_{Solved\,(z)\rightarrow Solved\,(z+1)} - TE_{Solved\,(z)\rightarrow Drain\,(z)}\end{aligned}$$ (Eq. 3-14)

Secondly, the adsorption $TE_{Solved\rightarrow Adsorbed}$ [mg *TE* m^{-2} day^{-1}] is estimated iteratively by assuming that equilibrium should be established between the adsorbed amount and the new amount of trace element in the soil solution. The adsorption is estimated so that the ratio between the sum of adsorbed and solved *TE* on the one hand and solved *TE* on the other hand equals the sum of the volumetric soil water content θ [m^3 m^{-3}] and the product of the adsorption coefficient K_d [m^3 kg^{-1}] and the soil bulk density γ [kg m^{-3}]:

$$\frac{\left(TE_{Adsorbed}(t-1) + TE_{Solved}(t-1) + \delta TE_{SolvedNoAds}\right)}{TE_{Solved}(t-1) + \delta TE_{SolvedNoAds} - TE_{Solved\rightarrow Adsorbed}} = \left(\theta + K_d\cdot\gamma\right)$$ (Eq. 3-15)

where *(t-1)* is the previous time step.

Finally, TE_{Solved} is estimated, also taking into account the change due to adsorption:

$$TE_{Solved}(t) = \left(TE_{Solved}(t-1) + \delta TE_{SolvedNoAds} - TE_{Solved\rightarrow Adsorbed}\right)$$ [mg *TE* m^{-2}] (Eq. 3-16)

When Eq. 3-16 results in an overestimation of $TE_{Solved\rightarrow Adsorbed}$, and thus an underestimation of TE_{Solved} (Eq. 3-17), it is compensated for by an under-estimation of $TE_{Solved\rightarrow Adsorbed}$ on the following day, which results in a higher TE_{Solved}, and so on for the subsequent days. At the time scale for which this study was performed, such temporary over- or under-estimations are not important. Equations 3-14 – 3-16 are solved for each soil layer.

The flux of a trace element in water solution from one layer to the layer beneath is described as:

$$TE_{Solved(z)\rightarrow Solved(z+1)} = TE_{DWaterFlow}\cdot q_{WaterFlow\,z\rightarrow z+1}\cdot\frac{TE_{Solved}}{m_{w(z)}}$$ [mg *TE* m^{-2} day^{-1}] (Eq. 3-17)

where $TE_{DWaterFlow}$ [–] indicates how fast trace elements are transported compared with the between layer water flow ($q_{waterflow}$). For a value of 1, solute transport rate equals water flow, while a value > 1 means preferential transport of solutes and a value < 1 means dispersion.

3.5 Losses of trace elements from the ecosystem

Trace element can leave the ecosystem through leaching and plant harvest. The trace element leaching flux is the sum of transport of trace element by the water flows, drainage q_{Drain} and percolation q_{Perc}:

$$TE_{Solved(z)\rightarrow Drain(z)} = TE_{DWaterFlow}\cdot q_{Drain(z)}\cdot\frac{TE_{Solved(z)}}{m_{w(z)}}$$ [mg *TE* m^{-2} day^{-1}] (Eq. 3-18a)

$$TE_{Solved(z)\rightarrow Perc(z)} = TE_{DWaterFlow}\cdot q_{Perc(z)}\cdot\frac{TE_{Solved(z)}}{m_{w(z)}}$$ [mg *TE* m^{-2} day^{-1}] (Eq. 3-18b)

The harvest trace element flux is a function of the corresponding carbon flux, for example the harvest flux associated with harvest of old stem parts, $TE_{OldStem \rightarrow Harvest}$, is calculated as [mg TE m^{-2} day^{-1}]:

$$TE_{OldStem \rightarrow Harvest} = TE_{DOldStem \rightarrow Harvest} \cdot C_{OldStem \rightarrow Harvest} \cdot \frac{TE_{OldStem}}{C_{OldStem}} \qquad \text{(Eq. 3-19)}$$

4 Water and carbon fluxes model *CoupModel*

CoupModel /Jansson and Karlberg 2004/ simulates the flows of water, heat, carbon and nitrogen in terrestrial ecosystems taken into account their coupling in each time-step. The nitrogen and carbon balances of an ecosystem strongly depend on the water and heat balances, as processes such as growth and decomposition depend on the soil temperature and moisture content. The water and heat balances are in turn influenced by the carbon and nitrogen balances, *e.g.* water uptake varies with growth rate and nitrogen fertilisation. *CoupModel* is the Windows successor and coupled version of the two DOS models SOIL /Jansson and Halldin 1979, Jansson 1998/ and SOILN /Johnsson et al. 1987, Eckersten et al. 1998/, which have been widely used on different ecosystems and climate regions /*e.g*. Espeby 1992, Gärdenäs and Jansson 1995, Eckersten et al. 1995, 1999/. With increasing computer capacity, the simulation period has been extended from decades to 100 years for several boreal forest systems applications such as Jädraås, Forsmark and Simpearp /Gärdenäs et al. 2003, Gustafsson et al. 2006, Karlberg et al. 2007a, b/. *CoupModel* is a one-dimensional, deterministic model with the partial differential equations of water and heat flow solved using an explicit forward difference method called the Euler integration. Plants are divided into the compartments root, leaves, stem and seeds, and soils into a maximum of 100 internally homogeneous layers with specified properties such as hydraulic conductivity, litter content and root density. The technical documentation on *CoupModel* /Jansson and Karlberg 2004/ is regularly updated on the website www.lwr.kth.se/vara%20datorprogram/*CoupModel.*

4.1 Water and heat model

Water flow is estimated by combining Darcy's law for water flow with the law of mass conservation. Similarly, heat flow is estimated by combining Fourier's heat flow law with the law of energy conservation. Soil physical properties can be defined with various degrees of vertical resolution and heterogeneity for a soil profile. Typical characteristics are the water retention curve, functions for the hydraulic conductivity, heat capacity and water uptake response. Water is lost through transpiration, soil evaporation, evaporation of intercepted water (called interception), deep percolation and surface runoff. Potential transpiration is modelled according to the Penman-Monteith equation /Monteith 1965/. Records of air temperature, precipitation, wind speed, relative humidity and global radiation are used as driving variables. Plant development is described with a dynamic behaviour, where height of plant, root depth and Leaf Area Index (LAI, *i.e.* the total leaf area per unit area of soil surface) are described as functions of plant biomass. The canopy conductance is estimated according to the Lohammar-equation /Lohammar et al. 1980/ as a function of the global radiation, saturation deficit and LAI. *CoupModel* is well-known among water balance models for its coupling between heat and water balance processes, including freezing and thawing /e.g. Stähli et al. 2001/. This is of great importance for correct modelling of nitrogen cycling in boreal forests, *e.g.* nitrogen transport with high water flow after snowmelt and the effect of thawing on mineralisation.

4.2 Carbon and nitrogen model

The nitrogen and carbon balances are modelled by dynamic coupling to the simulated daily variation in water and heat flows. The carbon and nitrogen balances strongly interact. Photosynthesis (C assimilation) is driven by global radiation /*cf* De Wit 1965/, and is limited by low leaf nitrogen status /*cf* Ingestad et al. 1981/. Photosynthesis in turn determines the plant nitrogen demand. Available nitrogen for plant uptake depends on the different nitrogen sources, such as nitrogen deposition, nitrogen fertilisation, nitrogen mineralisation, uptake of organic nitrogen through symbiosis with mycorrhizae and nitrogen losses, *e.g*. as nitrogen leaching. Nitrogen mineralisation is governed by soil temperature and moisture, microbial activity and biomass, and soil organic matter. Uptake of organic nitrogen through symbiosis with mycorrhizae is described by a first-order rate coefficient and limited by the amount of soil organic matter and the excess of available mineral nitrogen. Plant characteristics such as radiation use efficiency, litter production rate and allocation pattern to different plant tissues can be parameterised and changed to represent plant age, species and/or climatic region. In particular the plant properties, rooting depth and root distribution are important links between the hydrological conditions and the dynamics of nitrogen and carbon.

The different carbon and nitrogen pools in plant (leaves, stem, root and seeds) and soil (*Litter1, Litter2* and *Humus*) have already been presented in the description of *Tracey*. Microbes can be described by a separate pool or considered part of the soil organic matter, while mycorrhizae can be considered to be incorporated into the root biomass pool.

5 Sensitivity package *Eikos*

The sensitivity analyses were carried out using the software package *Eikos* /Ekström 2005, Ekström and Broed 2006/. *Eikos* includes state-of-the-art sensitivity analysis methods, which can cope with linear, non-linear and non-monotonic dependencies between model inputs and outputs. *Eikos* has been benchmarked, tested and compared with *@Risk* /see www1; Palisade Corporation 2004/, which is a well-established commercial tool, and with test functions that have exact analytical solutions /Ekström 2005/. These comparisons have shown that *Eikos* provides reliable results.

The following sensitivity analysis methods are supported by *Eikos*: Pearson product moment Correlation Coefficient (*CC*), Spearman Rank Correlation Coefficient (*SRCC*), Partial (Rank) Correlation Coefficients (*PCC*), Standardised (Rank) Regression Coefficients (*SRC*), Sobol' method, Jansen's alternative, Extended Fourier Amplitude Sensitivity Test (*EFAST*), the classical FAST method, the Smirnov and the Cramér-von Mises tests. *Eikos* allows Monte Carlo simulations to be performed using either simple random sampling or Latin hypercube sampling. The implementation of these methods in *Eikos* is described in /Ekström 2005, Ekström and Broed 2006/.

In this study, the uncertainty and sensitivity analyses were carried out using Latin hypercube sampling and Spearman Rank Correlation Coefficients respectively. These methods are briefly outlined below. More detailed descriptions can be found in /McKay et al. 1979, Vose 1996, Ekström 2005/ and /Ekström and Broed 2006/.

5.1 Latin hypercube sampling

Latin hypercube sampling (*LHS*) was introduced by /McKay et al. 1979/ and is today considered an essential feature in any risk analysis software package /Vose 1996/. *LHS* is a so-called 'stratified sampling' technique, where the distributions of the random variables are divided into equal probability intervals. As a result, fewer simulations are needed than for simple random sampling. The *LHS* technique used in this study is known as 'stratified sampling without replacement'. This procedure ensures that each sub-interval for each variable is sampled exactly once, in such a way that the entire range of each variable is explored.

5.2 Spearman Rank Correlation Coefficient

As mentioned above, there are several sensitivity analysis methods available in *Eikos*. The choice of an appropriate method depends on several factors, such as the time needed for performing a simulation with the model, the number of uncertain parameters and the type of dependency between the parameters and the simulated variables. For linear dependencies simple methods based on correlations are sufficient, while for complex non-monotonic dependencies more advanced methods, based on decomposition of the variance, are required. Below we describe methods based on correlations that were used in the present study.

The correlation coefficient (CC), usually known as Pearson's product moment correlation coefficient (ρ_{xy}), between two N-dimensional vectors *x* and *y* is defined by:

$$\rho_{xy} = \frac{\sum_{k=1}^{N}(x_k - \bar{x})(y_k - \bar{y})}{\left[\sum_{k=1}^{N}(x_k - \bar{x})^2\right]^{1/2}\left[\sum_{k=1}^{N}(y_k - \bar{y})^2\right]^{1/2}}, \qquad \text{(Eq. 5-1)}$$

where $\bar{x}$ and $\bar{y}$ are defined as the mean of *x* and *y* respectively. The *CC* (ρ_{xy}) could be reformulated as:

$$\rho_{xy} = \frac{\mathrm{cov}(x,y)}{\sigma(x)\sigma(y)}, \qquad \text{(Eq. 5-2)}$$

where $cov(x,y)$ is the covariance between the datasets *x* and *y* and $\sigma(x)$ and $\sigma(y)$ are the sampled standard deviations.

Hence, the correlation coefficient is the normalised covariance between the two datasets and it produces an index between –1 and +1. The *CC* is equal in absolute value to the square root of the model coefficient of determination (R^2) associated with the linear regression. The *CC* measures the linear relationship between two variables without considering the effect that other possible variables might have. Hence, it can be used as a sensitivity measure if the dependency between the inputs and the outputs is linear.

In cases where the relationship between inputs and outputs is not linear, the Pearson Correlation Coefficient performs poorly as a sensitivity measure. Rank transformation of the data can be used to transform a nonlinear but monotonic relationship to a linear relationship. When using rank transformation, the data are replaced with their corresponding ranks. The usual correlation procedures are then performed on the ranks instead of the original data values to obtain the so-called Spearman Rank Correlation Coefficient (*SRCC*), which is calculated in the same way as the *CC*, but on the ranks. The model coefficient of determination R^2 is computed with the ranked data and measures how well the model matches the ranked data. Rank-transformed statistics are more robust and provide a useful solution in the presence of long tailed input-output distributions. The *SRCC* performs well as a sensitivity measure as long as there is a monotonic dependency between the parameters and the simulation results.

6 Technical solutions for linking of models and long-term simulations

The main computational components, *i.e.* the numerical simulation models *Tracey* and *CoupModel* and the sensitivity toolbox *Eikos*, are described in the previous Chapters. This Chapter describes how the different components were linked in practice in this study for the completion of the sensitivity analyses. Appendix II contains a guide to performing a *Tracey*-*Eikos* simulation using the links described below.

The overall scheme can be summarised as follows (see also Figure 2-1):

1) The *CoupModel* simulations of the governing carbon and water variables were generated by stand-alone *CoupModel* runs, where parameters and inputs were modified systematically to represent a variety of ecosystems.

2) The *Tracey* model was created in Simulink, where all inputs are also loaded. A compiled version of the model was created as an exe-file by using Matlab's toolbox Real Time Workshop. This file includes all loaded inputs, including the driving variables simulated by the *CoupModel* and the parameter values generated by the *Eikos* programme. For each *CoupModel* simulation, a new executable version of the Tracey model was compiled. This file was then used in the *Eikos* evaluations.

3) The sensitivity analysis of the trace element model parameters is controlled by *Eikos*. *Eikos* generates parameter sets using Latin hypercube sampling and executes the *Tracey* model using the derived parameter sets, one at a time, as input. This is done in the Matlab environment executing the *Tracey* model as an external exe-file. Through the command line in Matlab the *Tracey* model is executed with a new specific parameter set for each simulation. The results from each *Tracey* model simulation are returned to and stored by *Eikos* in Matlab, where post-analysis is performed as described in previous Chapters.

It is possible to save results from each simulation from *Eikos*, *i.e.* the output data from selected state variables. However, long-term simulations up to 10^4 years with a yearly time step generate large amounts of data. It is therefore necessary to limit the number of time steps saved for each simulation. This requires selection of variables to be saved. For example, saving the results from year 1, 10^1.., 10^4 gives the user an opportunity to track steady state appearances for each simulation and also to determine the number of non-steady state simulations.

The stand-alone runs of CoupModel were initially planned to be made through command-line calls from the Simulink environment. Therefore a command-line interface was implemented in *CoupModel*, which is further described in Appendix III. The advantage of this coupling is that the *Tracey* model can generate its necessary input data without invoking the graphical user interface of *CoupModel*. This command-line interface further makes it possible to run *CoupModel* directly from *Eikos* to include the *CoupModel* parameters in the sensitivity analysis or, if necessary, to correct the simulated carbon and water fluxes using additional plant growth models. However, for practical reasons the final results from the command-line interface were not utilised in this study. On the other hand, the command-line interface has proven very useful in other recent studies using *CoupModel*, for instance the Bayesian calibration analysis presented by /Karlberg et al. 2007b/, where *CoupModel* was run from Matlab.

7 Simulation scheme for *CoupModel*, *Tracey* and *Eikos*

Two forest types with contracting hydrology were studied, a mixed pine-spruce forest typical for recharge areas and a European alder forest typical for discharge areas, located in Forsmark in central Sweden. Recharge areas are high-elevation areas in a landscape, where water is collected, while discharge areas are low-elevation areas, commonly found near a stream or lake, where water leaves a catchment (Figure 7-1). In discharge areas, lateral inflow of the contaminant can be expected to be considerable. For instance, Lidman (pers. comm. 2007-09-13) studied the natural occurrence of radionuclides Sr and To in the soil in a transect along a slope towards a stream in Svartberget and found highest levels of radionuclides close to the stream. Similar results have been found for other solvents e.g. Hg /Bishop et al. 1995/, Pb /Klamninder et al. 2006/ and Al /Cory et al. 2007/ in the same transect. Based on this knowledge, we chose a different contamination approach for the alder ecosystem, in order to also take account of possible lateral inflow of radionuclides in the unsaturated zone.

The alder forest was chosen to represent a natural hardwood forest without management, while the pine-spruce forest was managed in an environmentally friendly way according to the local criteria of the international Forest Certificate Stewardship (FSC). The forest rotation period was set to a 100 years and the forest was thinned according to local practice.

A number of different varieties of the two forest ecosystems were created by varying their root depth and radiation use efficiency in the *CoupModel* simulations. Detailed information on the parameter settings of these varieties, or functional forest types, is given in Chapter 8 (*CoupModel* simulations of carbon and water fluxes). Sixteen functional forest types were created for the pine-spruce forest and 12 for the alder forest (Table 7-1). We chose to vary root depth as it can be expected to interact with passive uptake of trace elements by increased potential water uptake. Similarly, radiation use efficiency (RUE) can be expected to interact with active uptake of trace elements as the potential growth rate increases. Radiation use efficiency can be described as the potential growth rate at a certain level of radiation when all other main factors influencing growth are not limiting.

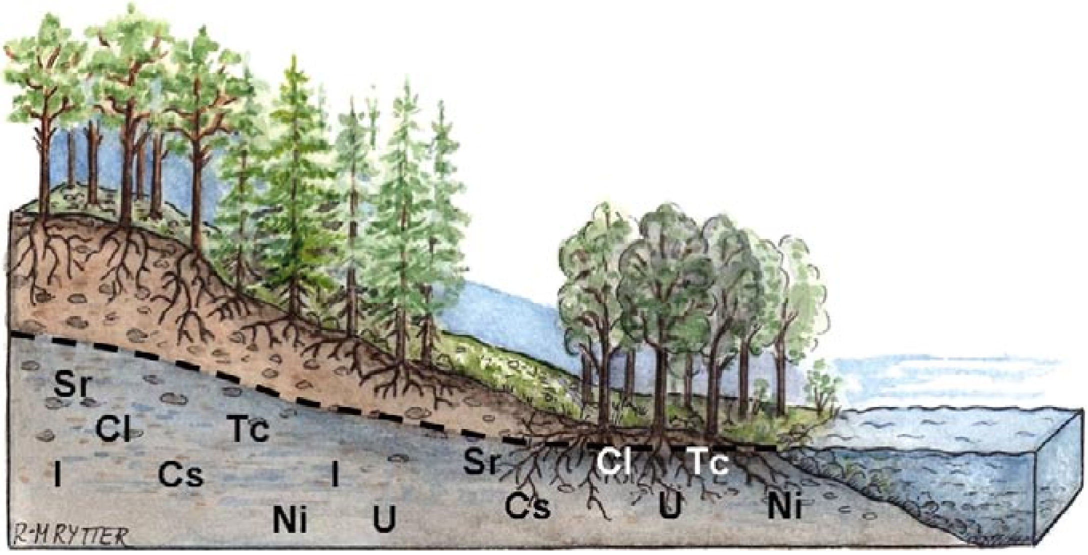


***Figure 7-1.** Schematic overview of possible soil contamination in pine-spruce ecosystems in recharge areas and in alder ecosystems in discharge areas. Dashed line represents groundwater table. Illustration by Rose-Marie Rytter.*

Table 7-1. Simulation scheme of the functional forest type with different root depth and Radiation Use Efficiency (RUE). Of the 16 pine-spruce forest types, passive uptake was only applied on the four with shallow and the four with very-deep roots. Twelve alder functional forest type were created.

Ecosystem	**Pine-spruce**		**Alder**	
***CoupModel*: Functional forest types**	16		12	
***Tracey*: Passive or active uptake**	Active uptake 16	Passive uptake 8	Active uptake 12	Passive uptake 12
***Tracey-Eikos:* 1,000 Monte Carlo simulations per *Tracey* variant**	16,000	8,000	12,000	12,000

Tracey simulations were made using active plant uptake for all the different functional forest types of pine-spruce (16) and alder (12). For alder, *Tracey* simulations were also made using passive uptake for all different functional forest types (another 12 alder). For pine-spruce, the simulations with *Tracey* using passive uptake were limited to the four functional forest types with the deepest roots and the four with the shallowest roots.

These 24 pine and 24 alder *Tracey* varieties were included in the sensitivity analysis using *Eikos*. For each variant, a 1,000 combination of parameter settings was made. The parameter settings of *Tracey* are given in Chapter 9 (*Tracey-Eikos* applications) for the respective forest type. After analysing the results, one functional forest type of the pine-spruce and one of the alder had to be disregarded and thus the overall results for pine-spruce are based on 22 × 1,000 *Tracey* Monte Carlo simulations (of which 7,000 used passive uptake and 15,000 active uptake) and the results of alder are based on 22 × 1,000 *Tracey* Monte Carlo simulations (of which 11,000 used active uptake and 11,000 used passive uptake).

8 *CoupModel* simulations of carbon and water fluxes

8.1 The pine-spruce forest functional types

The mixed pine-spruce ecosystem was represented by a forest in north-east Uppland (Forsmark, 60°22'N, 18°13'E). Weather data (air temperature, precipitation, wind speed, cloudiness and relative humidity) were based on time series for the period 1970–2004 for Forsmark /Gustafsson et al. 2006/. This dataset was compiled from various observations from Forsmark and other weather stations in north-east Uppland, including Uppsala. The annual mean temperature in the final dataset varied between 3.8 and 7.2 °C with an average of 6.0 °C, and the annual precipitation varied between 357 and 740 mm per year with an average of 561 mm per year. Nitrogen deposition was set at 5 kg ha^{-1} yr^{-1}. Water and carbon fluxes were simulated for periods of 300 years with daily time steps, of which the last 100 years, *i.e.* one complete forest rotation period, were used as input for the *Tracey-Eikos* simulations. The forest was thinned at stand age 8, 15, 43 and 76 years and clear-felled at 100 years in accordance with local and regional forest management at Forsmark (Anders Löfgren, pers. comm. 28-5-2005; Forestry Statistical Yearbook, 2000; see www2). Height development was adjusted to the observed rate at Forsmark and given as a driving variable. The early thinnings had clear positive effects on the height development of pine-spruce, with the trees increasing exponentially in height. The development of Leaf Area Index (LAI) was simulated and varied from 0.2 for small plants to 2.5 for old trees. The canopy resistance was described using the Lohammar approach with maximal stomatal conductivity set to 0.012 units. The resulting canopy resistance varied between 100 and 1,000 s m^{-1}, with a mean of around 500 s m^{-1} during the 100 years of a forest rotation period.

The initial groundwater level varied between 20 and 250 cm depth, with a mean at around 125 cm depth during the simulation period. The soil of the pine-spruce forest areas in Forsmark can be characterised as sandy-silty till. Soil physical properties and process descriptions were taken from /Lundin et al. 2004/ and /Gustafsson et al. 2006/ with the exception that drainage was described using the Hooghoudt approach instead of the linear approach /for details see Jansson and Karlberg 2004/. The soil was modelled down to 4 m depth and divided into 10 layers (5, 10, 10, 20, 10, 25, 50, 70, 100 and 100 cm thick respectively). There is a less permeable layer with reduced hydraulic conductivity between 35 and 55 cm depth.

The parameterisation of the carbon and nitrogen processes was based on /Gärdenäs et al. 2003/ and /Gustafsson et al. 2006/. The initial total carbon of the soil was 8 kg C m^{-2} and the total nitrogen content 400 g N m^{-2} and the soil layer content were assumed to decrease exponentially with depth. Three soil organic matter pools were used, *Litter1* for needle and fine root litter with a decomposition rate of 0.01 day^{-1}, *Litter2* for stem litter with a decomposition rate of 0.005 day^{-1} and *Humus* for older soil organic matter with a decomposition rate of 0.01 day^{-1}. The initial C/N ratio of the three soil organic matter pools was 25, 50 and 20 for *Litter1*, *Litter2* and *Humus* respectively.

The simulation period started with a very young forest stand with small plants and an initial total plant carbon and nitrogen content of 400 g C m^{-2} and 5 g N m^{-2} respectively. Plant carbon and nitrogen were distributed between seeds, leaves, old leaves, stems, old stems, roots and old roots. Potential plant growth was estimated using the radiation use efficiency (*RUE*) and global radiation adsorbed. Actual plant growth was estimated from potential plant growth, actual temperature, nitrogen availability and soil moisture. Each plant compartment has an individual mortality rate; these were 0.0027 day^{-1} for leaf, 0.000018 day^{-1} for stem and 0.0054 day^{-1} for roots. It was assumed that 0.001% of the carbon and nitrogen contents of the leaves were translocated to the seeds every day.

On the thinning occasions and at final clear-felling, a percentage of the stem carbon was harvested, a percentage was added to the slow-decomposing litter pool *Litter2* and the remaining percentage stayed in the living stem. At each thinning 30% of the stem was harvested and at clear-felling 99%. At each thinning, 30% of needles and seeds and 25% of roots were transformed to the *Litter1* pool. At clear-felling, 99% of needles and seeds and 95% of roots were transformed to the *Litter1* pool.

8.2 Different pine-spruce functional forest types

Different varieties of the same tree species can take up radionuclides in different rates /Greger 2004/. In order to represent different varieties of mixed pine-spruce ecosystems, two properties, namely maximum rooting depth and radiation use efficiency were varied. These properties were chosen because rooting depth is known to strongly influence the water uptake potential, while radiation use efficiency strongly influences the growth potential. According to our description of passive and active uptake of trace elements, these two ecosystem characteristics are essential for the potential plant uptake of radionuclides. We call the assumed, artificial varieties 'functional forest types' as we focus on how they function instead for to try to represent specific varieties.

Maximum rooting depth of the pine-spruce ecosystem was set to 60, 80,100 and 120 cm and radiation use efficiency to 1.8, 2.0, 2.2 and 2.4 g d.w. MJ^{-1} (see Table 8-1). For comparison, the parameter settings for alder ecosystems are also given. Please note that the root depth classes given for alder do not refer to the same root depth as those for pine-spruce.

The carbon and water fluxes for all combinations of rooting depth and radiation use efficiency were simulated as different functional forest types and given a corresponding code name. For instance, the pine-spruce forest with maximum root depth of 60 cm and Radiation Use Efficiency of 1.8 g d.w. MJ^{-1} was called Pine-Spruce *Rshallow RUElow*.

The *CoupModel* simulations were run for 300 years but only the simulation results for the last 100 years, *i.e*. the last complete forest rotation period, were used as input for the *Tracey-Eikos* simulations. The dynamics of the main water fluxes and carbon pools are shown in Figures 8-1 and 8-2 for the forest functional types with high *RUE* (=2.2 g d.w. MJ^{-1}) and all root depths. Both the water and carbon dynamics fell into two categories, one consisting of shallow and medium roots and one consisting of deep and very deep roots.

Table 8-1. Root depth (*R*) and Radiation Use Efficiency (*RUE*) for the different pine-spruce and alder functional forest types and their nomenclature.

Ecosystem	Root depth, *R* (cm)		Radiation Use Efficiency, *RUE* (g d.w. MJ^{-1})	
Pine-spruce	Shallow	60	Low	1.8
	Medium	80	Medium	2.0
	Deep	100	High	2.2
	VeryDeep	120	VeryHigh	2.4
Alder	Shallow	50	Low	1.125
	Medium	150	Medium	2.250
	Deep	250	High	3.375
			VeryHigh	4.500

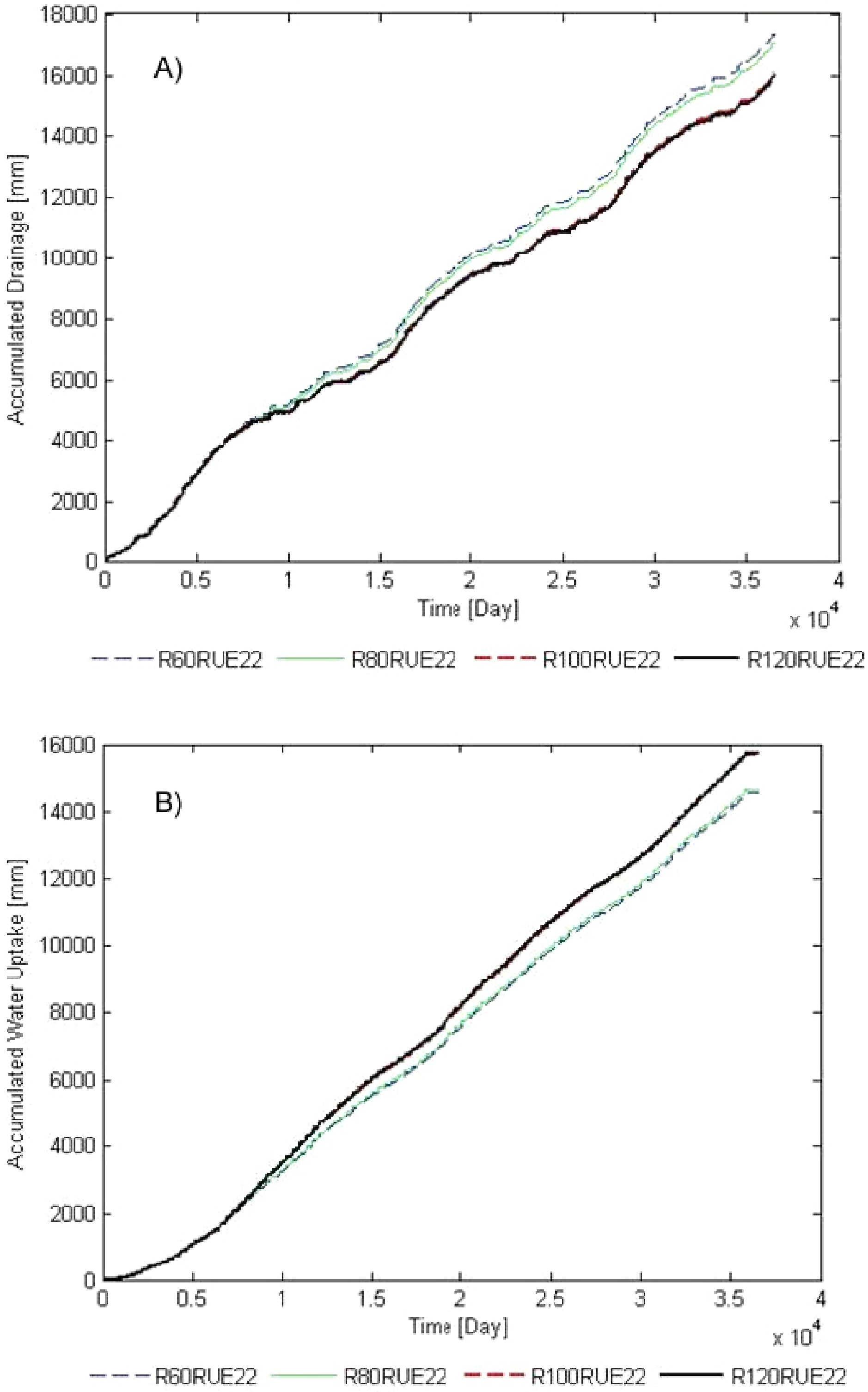


Figure 8-1. *The accumulated drainage (A) and water uptake (B) for the pine-spruce forests with RUEhigh (= 2.2g d.w. MJ*$^{-1}$*) and root depths 60, 80, 100 and 120 cm.*

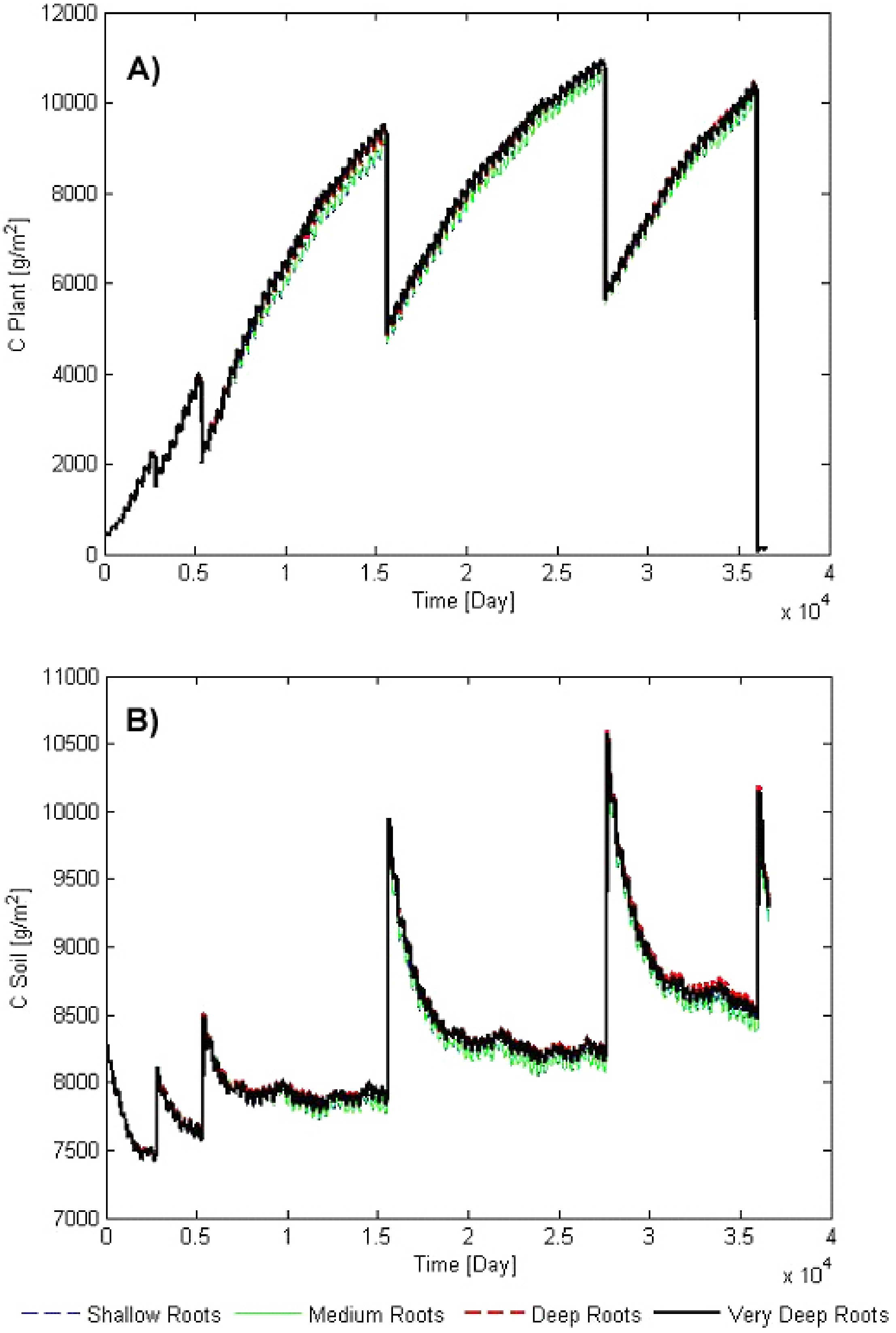


Figure 8-2. *Changes in C content of plant (A) and soil organic matter (B) during one forest rotation period for the pine-spruce forests with RUEhigh (=2.2 g d.w. MJ^{-1}) and root depth 60, 80, 100 and 120 cm.*

8.3 The alder *CoupModel* scenarios

CoupModel was used to simulate carbon and water flows of an alder ecosystem. The purpose was to get simulated outputs of water and carbon states and flows in plant and soil that can represent a non-harvested alder forest in the Uppland region. The outputs also needed to be close to steady state as the relatively short period simulated by the *CoupModel* had to be used in a repeated sequence in the trace element simulations over periods of several thousands of years. A non-steady state would have caused a repeated abrupt change in the mass balance of the carbon pools, which would have caused trace element flows which were not related to any natural carbon flows.

Inputs

The purpose of the parameterisation was to obtain simulated outputs of water and carbon states in plant and soil representative for an alder forest. The focus was to get realistic outputs of water and carbon variables that could become driving variables of the *Tracey* model, rather than to achieve absolutely realistic parameter values derived from the literature or elsewhere. Heat and nitrogen dynamics influence the water and carbon and thus had to be parameterised for the simulations. However, as the focus was on water and carbon outputs, less attention was devoted to the parameterisation of heat and nitrogen processes.

Soil conditions were taken as those of a clay soil at Ultuna, 8 km south of Uppsala. The soil was divided into 10 layers (5, 10, 10, 10, 15, 20, 20, 20, 60, 120 cm thick, respectively), of which eight layers were in the upper 110 cm and the two deepest layers from 110 to 290 cm. Physical conditions were characterised by low total hydraulic conductivity in the top layer but otherwise high and moderate below 90 cm. The porosity was 50% in the top layer but then decreased from 36 to 23% at 1 m depth. More than one-third of the organic matter was in the top 5 cm, about the same amount between 5 and 50 cm, and less than 1% below 1.1 m depth. Total soil organic N was set to about 800 g N m^{-2} and a C/N ratio of 15 was assumed to represent an intermediate soil type between forest and arable, which gave a total carbon pool of 12–13 kg C m^{-2}. In the simulations the total carbon was distributed between humus, fast decomposing litter and slow decomposing litter. These fractions, derived by letting the model run for about ten years, turned out to be 95%, 4.5% and 0.5% respectively.

Weather variables, *i.e.* daily records of global radiation, air temperature, air humidity, wind speed and precipitation, were taken from the Ultuna climate station (8 km south of Uppsala) for the period 1961–87, which was close to the period usually used as a reference period in climatic research.

Reference simulations

The reference simulation represents an alder forest growing on an Ultuna soil during the period 1961–87 in approximate steady state carbon budget both for plant and soil, repeated about three times to give an 80-year simulation period. To cancel out initial transient effects, the first 20 years of the *CoupModel* simulations were removed before the results were used as input to the *Tracey* model.

Gross annual plant growth rate of the reference simulation was about 500 g C m^{-2} y^{-1} (30, 45 and 25% for leaves, stem and roots respectively). However litterfall and respiration were of a similar magnitude, giving no net increase in total plant carbon. Standing plant carbon was about 4,000 g C m^{-2} y^{-1}, of which 60–65% was in stem. Soil humus C pool was approximate stable at 12,500 g C m^{-2}. The fast decomposing litter pool was on average 550 g C m^{-2} but varied from 400 to 650 between years. The slow decomposing litter pool was about 40 g C m^{-2} (variation 10–70 g C m^{-2} between years). Of the total annual precipitation, of about 580 mm y^{-1}, about 395 mm were lost by evaporation and 185 mm were lost by run-off, of which surface run-off comprised only a few percent.

8.4 Different alder functional forest types

Alternative alder ecosystems were adopted to represent systems with different rates of plant growth and different rooting depths. The different growth rates were achieved by changing the radiation use efficiency (*RUE*). The alternative systems were also adopted to be at approximate steady state carbon budget. The different *RUE* values thus represent soil-plant systems of different carbon flows and pool sizes. The larger growth rate (higher *RUE*) gave a larger input of C to the soil. This was balanced by a larger decomposition loss, which was achieved by increasing the initial value of the humus carbon pool. The steady state conditions with the alternative *RUE* value were achieved by making an 80-years-long simulation to get a new value for the humus pool. The humus pool size at the end of this period was then set as the initial state of a repeated 80-year simulation, and the procedure was repeated until the humus pool was in steady state. Thereafter the last 60 years were selected to avoid initial transient effects of the litter pools. This period was used as input to the *Tracey* model. For the low *RUE* ecosystem, *LAI* was assumed to have been lower than in the reference system. To represent systems with different root water uptake, the rooting depth was altered. The soil carbon pools were balanced to be in steady state. In all cases the initial states of the plant C pools were altered to achieve steady state plant pools. The simulation results differed in flows and states in a similar manner. The 100% increase in *RUE* resulted in an approxiamate 100% increase in annual plant gross growth and a slightly more than 100% increase in decomposition losses. The plant carbon stocks doubled as well (see Table 8-3).

Table 8-2. Inputs to the *CoupModel* that differed between the different alder ecosystems functional forest types. *R150RUE2250* denotes root depth =150 cm and *RUE* = 2.250 g d.w. MJ^{-1} and is the reference *CoupModel* simulation.

Functional forest type	Growth	Root depth m	RUE g d.w. MJ^{-1}	LAI (max) m^{2}m^{-2}	Initial root C kg C m^{-2}	Initial stem C kg C m^{-2}	Intial humus C kg C m^{-2}
Shallow roots							
R050RUE1125	Low	0.5	1.125	3	0.5	0.9	4.4
R050RUE2250	Medium	0.5	2.25	5	1.3	2.6	10.5
R050RUE3375	High	0.5	3.375	5	1.6	3.9	15.1*
R050RUE4500	Very high	0.5	4.5	5	2.2	4.4	10.6*
Medium roots							
R150RUE1125	Low	1.5	1.125	3	0.5	1.0	4.8
R150RUE2250 (=Reference)	Medium	1.5	2.25	5	1.3	2.6	12.4
R150RUE3375	High	1.5	3.375	5	1.9	3.9	18.4
R150RUE4500	Very high	1.5	4.5	5	2.6	5.1	24.5
Deep roots							
R250RUE1125	Low	2.5	1.125	3	0.5	1.0	4.8
R250RUE2250	Medium	2.5	2.25	5	1.3	2.6	12.4
R250RUE3375	High	2.5	3.375	5	2.1	4.0	18.8
R250RUE4500	Very high	2.5	4.5	5	2.8	5.4	12.7*

Table 8-3. Average annual flows simulated by *CoupModel* for the different functional forest types of alder (see also Table 8-2). R150RUE2250 denotes z_r =150 cm and *RUE* = 2.250 g d.w. MJ^{-1} and is the reference *CoupModel* simulation.

Ecosystem	Stem growth g C m^{-2} y^{-1}	Photosyn. g C m^{-2} y^{-1}	Decomp. g C m^{-2} y^{-1}	Transpir. mm y^{-1}	Total Evap. mm y^{-1}	Tot Runoff mm y^{-1}
Shallow roots						
R050RUE1125	68–112	373	346	134	301	281
R050RUE2250	149–264	876	810	202	355	228
R050RUE3375	223–394	1,305	1,206	202	355	228
R050RUE4500	298–536	1,775	1,646	202	355	228
Medium roots						
R150RUE1125	82–117	407	379	145	314	268
R150RUE2250 (Reference)	202–309	1,061	987	240	395	187
R150RUE3375	303–464	1,590	1,477	240	395	187
R150RUE4500	406–618	2,118	1,966	240	395	187
Deep roots						
R250RUE1125	82–119	407	380	146	314	267
R250RUE2250	225–315	1,101	1,024	252	407	176
R250RUE3375	338–473	1,652	1,539	252	407	176
R250RUE4500	451–630	2,052	2,203	252	407	176

9 *Tracey-Eikos* applications

9.1 Contamination

The contamination was assumed to take place continuously during the whole simulation period of *Tracey* (10,000 years). The contamination is expressed in mg per year and m^2 as carbon and water flow are expressed in mass per unit time and per unit surface area. The contamination level was set to 0.8 mg per m^2 and year. This roughly corresponds with 1 Bq per m^2 and year for ^{238}U, a major long-living radionuclide in nuclear fuel waste. In the pine-spruce ecosystems, only the saturated soil layers were contaminated, which varied with the daily fluctuations in ground water table as simulated by *CoupModel*. In the alder the whole soil profile was contaminated.

9.2 Pine-spruce

In the sensitivity analysis, 14 different *Tracey* parameters were included to represent different combinations of radionuclides (*e.g.* adsorption coefficient, K_d, and degree of convective transport of trace elements, $TE_{DWaterFlow}$) and ecosystem properties (*e.g.* bulk density, γ, and fraction allocated to leaves, f_{PULeaf}). For each *Tracey* parameter, its distribution was defined based on literature data. For radionuclide properties, we used data of a various radionuclides and/or micro-nutrients. Ecosystem characteristics are based on data from forest research sites in Fenno-Scandinavia. The nominal values and distributions are given in Table 9-1.

Table 9-1. Nominal values and distributions of Tracey parameters for pine-spruce ecosystems in *Eikos* (Appendix 1. contains a list of all abbreviations and symbols).

Parameter	Nominal	Distribution	Mean (μ)	Std (σ)	Min	Max	References
General							
γ (kg m^{-3})	1,180	Uniform	n.u	n.u	400	1,500	1
K_d (m^3 kg^{-1})	0.5	Log-uniform	n.u	n.u	0.002	10	2
$TE_{DWaterFlow}$ (–)	1	Log-normal	0.7	0.4	0	1.5	3
$TE_{DLitter1\rightarrow Solved}$ (–)	0.5	Normal	0.5	0.1	0	1	Assumed
$TE_{DHumus\rightarrow Solved}$ (–)	0.5	Normal	0.5	0.1	0	1	Assumed
Passive uptake							
$TE_{DWUptake}$ (–)	1	Log-normal	0.7	0.15	0	1	Assumed
f_{PULeaf} (%)	0.1	Log-normal	0.05	0.05	0.01	1	4, 5
f_{PUSeed} (%)	0.01	Log-normal	0.01	0.005	0	0.1	4, 5
f_{PURoot} (%)	0.7	Log-normal	0.7	0.35	0.01	1	6, 5
Active uptake							
$\mathrm{TE}_{BioRate}$ (d^{-1})	0.1	Log-normal	0.15	0.25	0.001	0.7	7
$P_{MaxTECLeaf}$ (mg TE g^{-1} C)	5.04	Log-normal	7.29	7.53	0.93	24.79	4, 5
$P_{MaxTECSeed}$ (mg TEg^{-1} C)	0.83	Log-normal	2.09	2.42	0.27	7.06	4, 5
$P_{MaxTECStem}$ (mg TEg^{-1} C)	1.15	Log-normal	1.26	1.05	0.14	3.19	4, 5
$P_{MaxTECRoot}$ (mg TEg^{-1} C)	0.35	Log-normal	0.58	0.78	0.08	2.12	6, 5

n.u.= not used

1= /Lundin et al. 2004/.

2= /Bergström et al. 1999/.

3= /Simunek et al. 2006, Carrillo-González et al. 2006/

7= /Eckersten et al. 2007/.

4= /Helmisaari 1992/.

5= Helmisaari et al. 2002, H-S. Helmisaari, pers. comm. 2006.

6= /Mälkönen and Helmisaari 1999/.

Using Latin hypercube, *Eikos* made 1,000 different combinations of parameter settings for each of the 16 pine-spruce functional forest types produced with *CoupModel*. All sixteen functional forest types were used for modelling active plant uptake, while eight (the four with shallow root depth (60 cm) and the four with very deep root depth (120 cm)) were used for modelling passive uptake. In total, there were 24 pine-spruce varieties of root depth, *RUE* and uptake approach, with 1,000 samples each.

The distribution of bulk density γ was based on /Lundin et al. 2004/ and that of adsorption coefficient, K_d, on values for mineral soils presented in a review of K_d for 40 radionuclides in mineral soils by /Bergström et al. 1999/. $TE_{DWaterFlow}$, the degree of convective transport of radionuclides, mimicked both dispersion and preferential transport. Transport of radionuclides by colloids on dissolved organic matter (DOM) is a very important transport mechanism for some radionuclides /Buddemeier and Hunt 1988, Marley et al. 1993/. Transport of TE_{Solved} can be both slower and faster than mass flow of water /Simunek et al. 2006, Carrillo-González et al. 2006/.

No information was found on parameter values for $TE_{DLitter1\rightarrow Solved}$ and $TE_{DHumus\rightarrow Solved}$. These parameters are difficult, if not impossible, to measure directly, as when analysing soil organic matter, it is difficult to differentiate between trace elements that are part of soil organic matter and trace elements adsorbed on soil organic matter. These parameters could be calibrated when simulating an existing ecosystem for which the contamination rate, the losses and the content of a trace element in all other pools are known. However, this was not the case in this study.

With the parameter $TE_{DWUptake}$ used in passive uptake, we can simulate the degree to which a trace element in soil water solution follows the mass flow of water when water is taken up by plants. If $TE_{DWUptake}$ is lower than one, a fraction will stay in the rhizosphere on the surface of roots rather than being taken up by roots. The assumed values were based *e.g.* on discussions with Yves Tyree (pers. comm. 8/5/2003) and Heljä-Sysko Helmisaari (pers. comm, 12/12/2006). When using active uptake, *i.e.* when the trace element is assumed to be taken up in relation to plant growth, the corresponding parameter is $TE_{BioRate}$. This parameter expresses the fraction of trace element in the soil solution that can be taken up daily and is based on values for macronutrients such as nitrogen, which have relatively low plant availability (*cf* Eckersten et al. 2007).

The fractions of trace element allocated to different plant tissues (f_{PULeaf}, f_{PUSeed} and f_{PURoot}) were based on studies of the content of different micronutrients in pine forests of different ages in eastern Finland by /Helmisaari 1992, Mälkönen and Helmisaari 1999, Helmisaari et al. 2002/ and Heljä-Sysko Helmisaari (pers. comm. 12/12/2006) respectively. Data on macronutrient contents in the same forests were used for the parameters of active uptake, $P_{MaxTECLeaf}$, $P_{MaxTECSeed}$, $P_{MaxTECStem}$ and $P_{MaxTECRoot}$.

9.3 Alder

One thousand simulations were made by *Tracey*-*Eikos* for each of the 12 alder functional forest types produced with *CoupModel*. For alder forest too, the simulation period was set to 10,000 years. Twelve different *Tracey* parameters were varied to represent different combinations of radionuclides (for instance adsorption coefficient, K_d) and ecosystem properties (*e.g.* bulk density, γ, and the degree of mass flow of trace elements during water uptake, $TE_{DWUptake}$). The nominal values and distributions are given in Table 3-3. Allocation pattern for passive uptake was based on /Ingestad 1980/ and for active uptake on /Elowson and Rytter 1988, Wittwer and Immel 1980/ and /Saarsalmi et al. 1985/. The fraction of trace element in soil solution that can be taken up daily, $TE_{BioRate,}$, was fixed to 0.1 (see further Table A2, Appendix V). A separate test of $TE_{BioRate}$ is given in Chapter 10.

Table 9-2. Nominal values and distributions of *Tracey* parameters for alder ecosystems in *Eikos* (Appendix 1. contains a list of all abbreviations and symbols).

Parameter	Nominal	Distribution	Mean (μ)	Std (σ)	Min	Max	References
General							
γ (kg m^{-3})	1,180	Uniform			400	1,500	1
K_d (m^3 kg^{-1})	0.01	Log-uniform			0.00001	10	2
$TE_{DWaterFlow}$ (–)	1	Log-normal	0.7	0.4	0	1.5	3
$TE_{DLitter1 \rightarrow Solved}$ (–)	1	Log-normal	0.5	0.1	0	1	assumed
$TE_{DHumus \rightarrow Solved}$ (–)	1	Log-normal	0.5	0.1	0	1	assumed
Passive uptake							
$TE_{DWUptake}$ (–)	0.7	Log-normal	0.7	0.15	0	1	assumed
f_{PUStem} (%)	0.18	Normal	0.18	0.05	0	1	4
f_{PULeaf} (%)	0.65	Normal	0.65	0.14	0	1	4
f_{PURoot} (%)	0.17	Normal	0.17	0.09	0	1	4
Active uptake							
$P_{MaxTECLeaf}$ (mg TE(g C)$^{-1}$)	74	Log-normal	30	26.75	8	74	5, 6
$P_{MaxTECSeed}$ (mg TE(g C)$^{-1}$)	0	n.u.	n.u.	n.u.	n.u.	n.u.	
$P_{MaxTECStem}$ (mg TE(g C)$^{-1}$)	14	Log-normal	5	5.24	1	14	7
$P_{MaxTECRoot}$ (mg TE(g C)$^{-1}$)	14	Log-normal	5	5.24	1	14	8

n.u.= not used

1= /Lundin et al. 2004/.

2= /Bergström et al. 1999/.

3= /Carrillo-González et al. 2006, Šimunek et al. 2006/.

4=/Ingestad 1980/.

5= /Elowson and Rytter 1988/.

6= /Wittwer and Immel 1980/.

7= /Saarsalmi et al. 1985/.

8= /Elowson and Rytter 1993/.

10 Model response to contamination process

10.1 Contamination level

We applied two approaches for trace element contamination of the soil profile. For pine-spruce, it was assumed that contamination only took place in layers below the groundwater level, i.e. where the soil was saturated with water. In the alder applications, we assumed all soil layers to have been contaminated by a certain amount of trace element per cm depth per day (mg m^{-2} cm^{-1} d^{-1}). In both ecosystems, the total load per ground surface area and day was the same and the differences in approach only concerned the levels that were contaminated. The default approach, as used for pine, was that only soil layers below the saturation level should be contaminated. However in the low-elevated alder ecosystems, considerable lateral inflow of radionuclides can be expected in the unsaturated zone and therefore it was assumed that all layers of the soil profile were contaminated. This assumption was also in line with an important objective of the study, namely to assess the potentially highest contamination of the plant and soil organic material. The alder trace element simulations could then be regarded to represent potentially high accumulation levels in plant and soil of low-lying areas. Different production and transpiration levels related to different water situations were covered by the alternative *CoupModel* simulations.

To demonstrate the sensitivity of trace element uptake by the plant and soil C to the contamination level, a simple test was made for the reference alder *CoupModel* simulation in which a contamination level that was proportional to the groundwater level was introduced. The groundwater level in the reference *CoupModel* simulation was deeper than root depth (1.5–3.5 m compared with 1.5 m; groundwater level of all alder *CoupModel* simulations ranged from 1.0–9.5 m). The test was then made by changing the contamination level from 0.01 times the groundwater level (*i.e.* contamination from the 1.5–3.5 cm layer and below), which was practically equal to all layers of the soil profile, to 0.6 times the groundwater level (*i.e.* contamination below 0.9–2.1 m depth). The other parameter values of the *Tracey* model were kept constant equal to the nominal (reference) values of the *Eikos* simulations (see Table 9-2). The contamination dose of the whole soil profile per unit of time was the same in all simulations (8,030 mg *TE* per 10,000 years).

When using passive uptake and all soil layers were contaminated (loaded) with trace element, about 97% of the accumulated trace element load was adsorbed to soil particles or solved in soil water solution by the year 10,000 (Table 10-1; scale groundwater level = 0.01). The rest mainly left the system by leaching. Very little was found in the soil organic and plant organic material. When the contamination was restricted to progressively deeper layers the accumulation in organic material (plant and soil) and leaching progressively decreased, and at contamination levels close to the root depth (i.e. scaling factor equals 0.01) practically all the trace element load, except for less than 0.1%, was accumulated by adsorption and in soil solution. It should be noted that the only exchange pathway for water in the saturated zone was upwards.

Table 10-1. Trace element (% of load) after 10,000 years for different contamination depths (expressed as fraction of groundwater level). The alder reference *CoupModel* simulation and nominal *Tracey* parameterisation for passive uptake were used. (For absolute values see Appendix 5, Table A5-2).

	Scaling factor of groundwater level					
Variable	**0.01**	**0.2**	**0.4**	**0.5**	**0.6**	**1.0**
Plant	0.02	0.01	0.004	0.001	0.00002	0.00002
Organic Soil	0.4	0.2	0.1	0.03	0.0005	0.0005
Adsorbed & Solution	97.1	98.1	98.9	99.5	100.0	100.0
Leached	2.5	1.7	1.0	0.4	0.03	0.002
Total load	100.0	100.0	100.0	100.0	100.0	100.0

In the active plant uptake simulations a larger fraction of the trace element load was accumulated in the plant and soil organic material (34%, Table 10-2) than in the passive uptake. The fraction of trace element lost by leaching was low, less than 1% by the year 10,000. Of the trace element accumulated in the organic material most was found in humus, and only a few percent in the plant. The sensitivity to the contamination level was similar as for the passive uptake, and the trace element load was almost 100% accumulated as adsorbed and in soil solution when the contamination level was close to the rooting depth.

When the contamination of the root zone and the plant was driven by capillary rise alone it became much lower. By the year 10,000 only parts per million had entered the biota (Tables 10-1 and 10-2; scale groundwater level = 1.0). The upward movement of trace element was assumed to be equal to the product of net vertical upflow of water and trace element concentration of soil water, and the discrimination factor for soil water flow. (This process was not used in the *Eikos* simulations, and is therefore not presented in the *Tracey* model description above).

In conclusion, the trace element accumulation in organic matter was very small when the contamination had to be driven by capillary rise, in comparison with when it was driven by root uptake. Assuming contamination only for layers below the saturation level (which in the current alder simulation was below the rooting depth) resulted in a very low fraction of the load uptake being accumulated in organic matter, compared with assuming a contamination of the whole soil profile. Thus the rooting depth in relation to the saturation level was found to be very important for trace element accumulation in organic matter. In the alder *CoupModel* simulations, the saturation level was almost always below the rooting depth and to reduce the strong influence of the relationship between these two depths on the contamination, we assumed all soil layers below soil surface to be contaminated. In the case of active uptake, this resulted in 33% of the trace element load being accumulated in organic matter, whereas this fraction would have been only 0.1% assuming only capillary rise for contamination. In the case of passive uptake, the choice of contamination level had an even larger influence on the fraction allocated to plant and soil organic matter than for active uptake, although the fractions were much lower.

Table 10-2. Trace element (% of load) after 10,000 years for different contamination depths (expressed as a fraction of groundwater level). The alder reference *CoupModel* simulation and nominal *Tracey* parameterisation for active uptake were used. (For absolute values see Appendix 5, Table A5-3).

	Scaling factor of groundwater level					
Variable	**0.01**	**0.2**	**0.4**	**0.5**	**0.6**	**1.0**
Plant	0.7	0.5	0.3	0.1	0.01	0.002
Organic Soil	33.0	23.7	14.7	6.6	0.5	0.1
Adsorbed & Solution	65.7	75.4	84.7	93.1	99.4	100.0
Leached	0.6	0.4	0.3	0.1	0.01	0.001
Total load	100.0	100.0	100.0	100.0	100.0	100.0

11 Results for pine-spruce ecosystem

11.1 General picture for pine-spruce ecosystems

A general picture of the results was obtained by calculating the average of the simulated harvest, plant, leached and soil of the 1,000 cases for each of the 24 forest functional types (Figure 11-1). For the pine-spruce ecosystems, on average 71–79% of the added radionuclide was leached. The total contamination over 10,000 years was 8,000 mg m^{-2} of an unspecified radionuclide. The functional forest types with deep and very deep roots (i.e. 100 and 120 cm depth) and active uptake had somewhat lower percentage leaching. At the same time, harvest losses were higher for these functional forest types, so that total losses were the highest for these forest types.

The percentages stored in plants were very small, at most 0.05% for the active uptake forest functional types with roots at 100–120 cm, and thus are not visible in Figure 11-1. The low percentage storage in plants is understandable when taking into account that trace element content in plants is the amount stored in a 100-year-old forest (a value of a state variable at year 100), while the other variables, leached, harvested and stored in the soil, represent accumulated amounts over 10,000 years (values of net flow after 10,000 years).

The distribution of trace element within plant and soil is shown in Figure 11-2A and B respectively. By far the most of the trace element stored in plants was found in old stem tissues, 60% for the active uptake forest functional types and 90% for the passive ones. For the active functional forest types, the remainder was stored in old and young leaf tissues. For the passive functional forest types, the remainder was found in roots, both young and old. The amounts in the other plant tissues, *YoungStem* and *Seed*, were very small and are not visible in Figure 11-2A.

On average, between 20 to 25% of total added radionuclide accumulated in the soil of the pine-spruce forest systems. For the distribution of trace element in the soil (Figure 11-2B), a logarithmic scale was used so that all different pools are visible within one diagram. Almost all trace element in the soil, as much as 97–98%, was found as adsorbed. Both the plant uptake approach, passive and active, and the root length affected the distribution in the soil. The passive functional forest types absorbed most and accumulated in total most. Less competition for trace element by plant uptake increased the amount of trace element adsorbed in the passive functional forests.

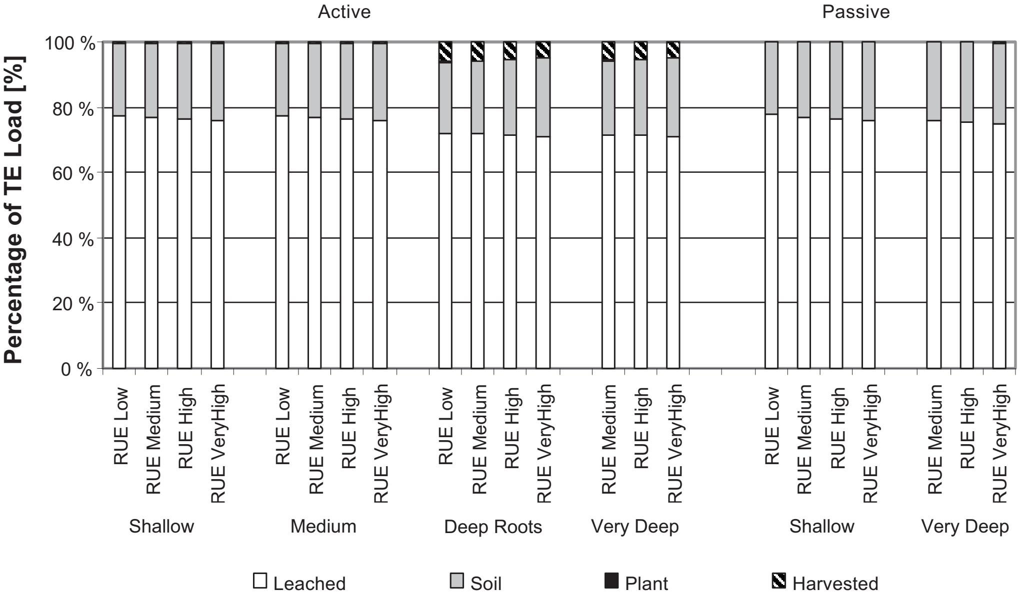


Figure 11-1. *Average percentage of trace element added lost by leaching (white box) and harvest (striped) and accumulated percentage in the soil (grey box) and plant (black) of the 1000 simulations per forest functional type. Active uptake is given on left side and passive on right side. Definitions of root depths and RUE categories are given in Table 8-1 and Appendix 1. Percentage stored in plant is so low (< 0.05%) that it is not visible.*

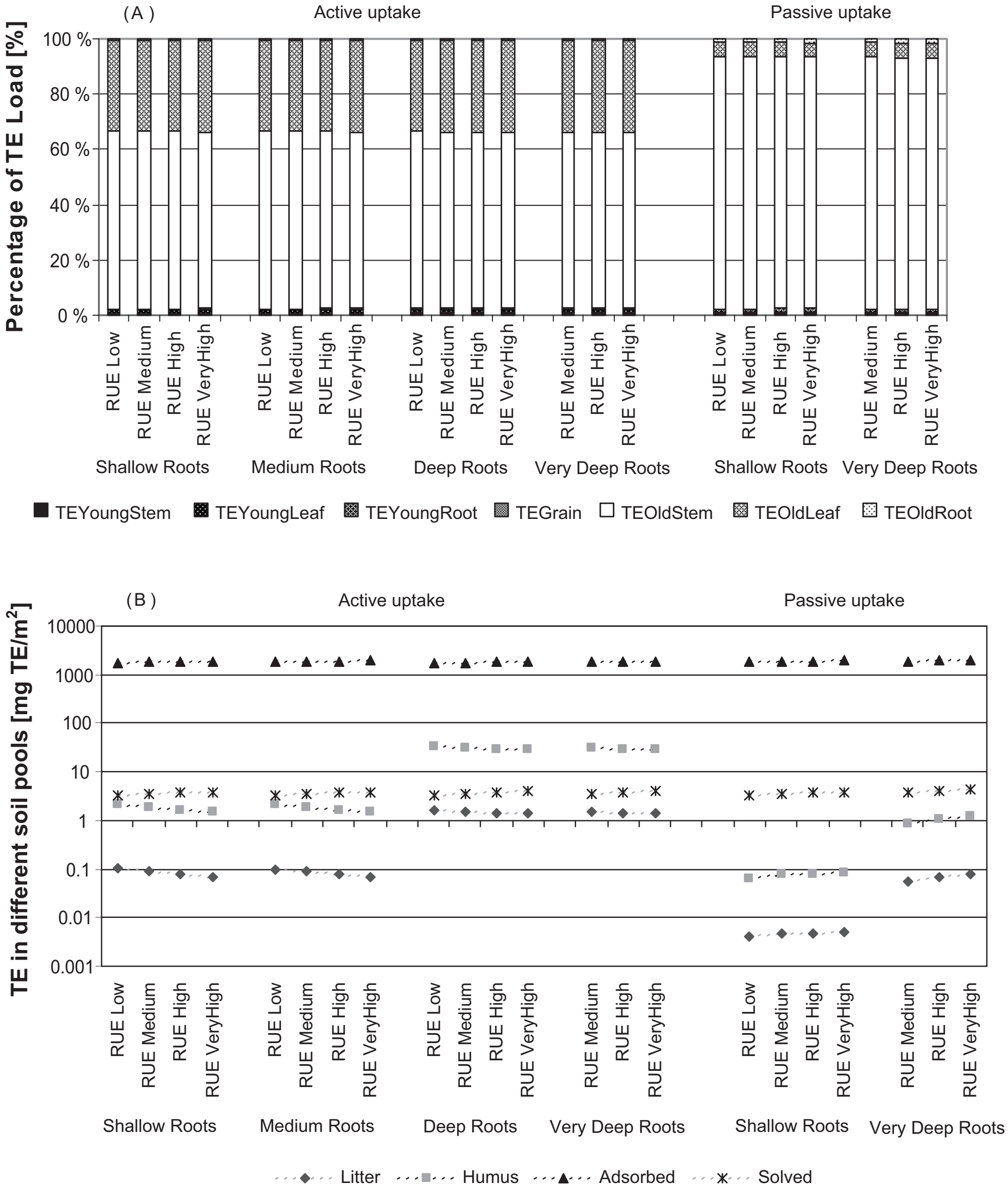


***Figure 11-2** Average distribution of trace element in plant (A) and soil (B) for different RUE and root depths. In figure A, plant, from top to bottom trace element in old root, old leaf, old stem, seeds, young roots, young leaves and young stem are given. The amounts in several plant tissues like young stem, young leaf, young roots and seeds is so small that they are not or hardly visible.*

The active functional forest accumulated most in soil organic matter, one magnitude higher than the passive uptake forest types. Root depths of 1 m or more also increased the trace element content in soil organic matter pools.

Figure 11-3 shows distribution of trace element with soil depth for both the passive and active varieties of the functional forest type with different root depth and a radiation use efficiency of 2.2 d.w. MJ^{-1}. By far most of the trace element was found below 2 m depth, also for the forest types using active plant uptake. The mean groundwater level was 1.3 m. Slightly more of trace element was found close to the soil surface with active uptake and deep to very deep roots.

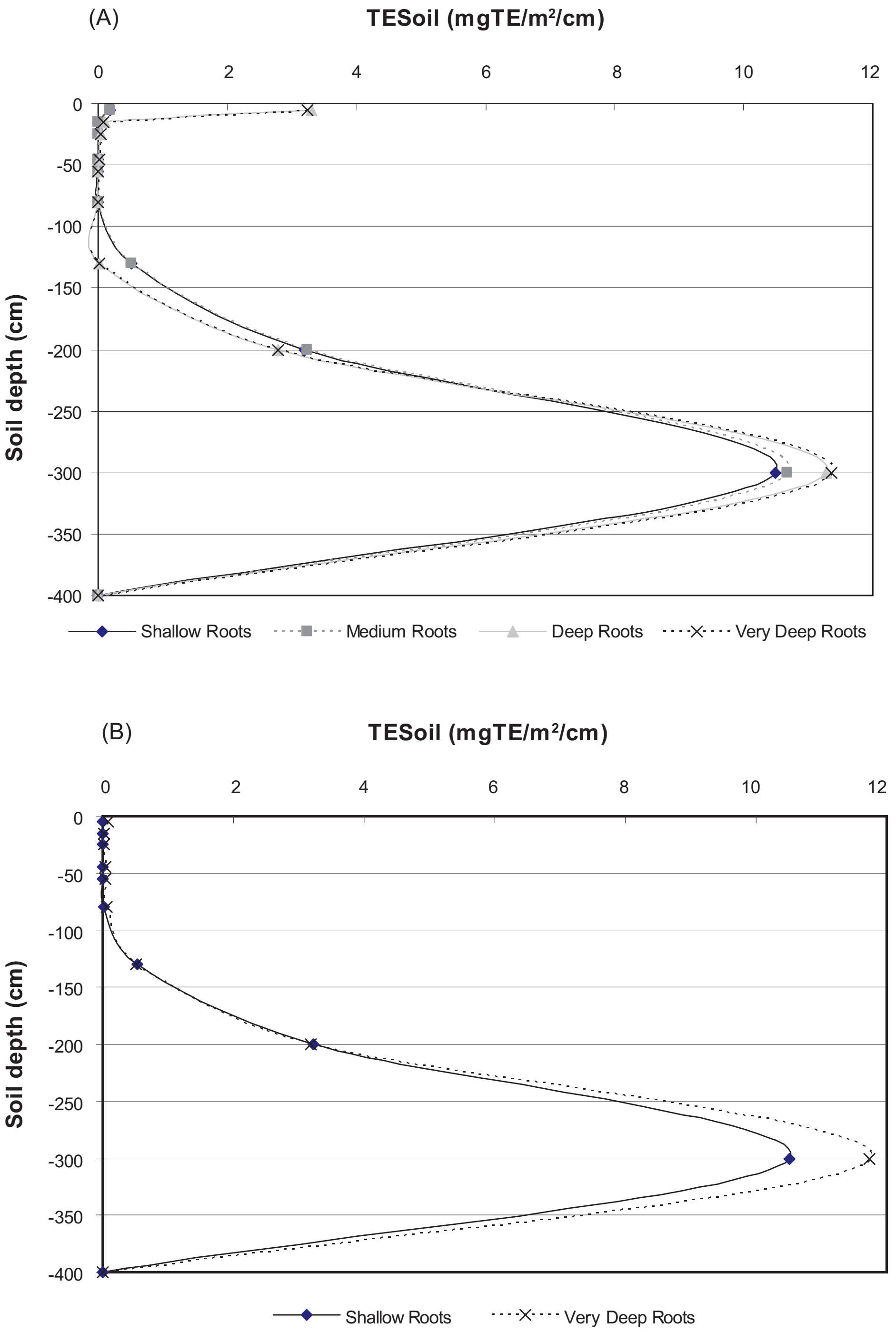


Figure 11-3. *Depth distribution of trace element in the soil for radiation use efficiency (RUE) of 2.2 g d.w. MJ*$^{-1}$*, various root depths and active uptake (A) and passive uptake (B). For definition of root depth see Table 8-1 and Appendix I.*

The amount of trace element leached was clearly lower for the pine forest types with root depths of at least 1 m (Figure 11-4A). The factor here is most likely, not absolute root length, but the increased contact of the roots with the groundwater and thereby the source of contamination, as in the pine-spruce ecosystems contamination only occurred within the saturated zone. The amount of trace element stored in a soil increased somewhat with increased radiation use efficiency, which is a measure of potential growth rate (Figure 11-4B).

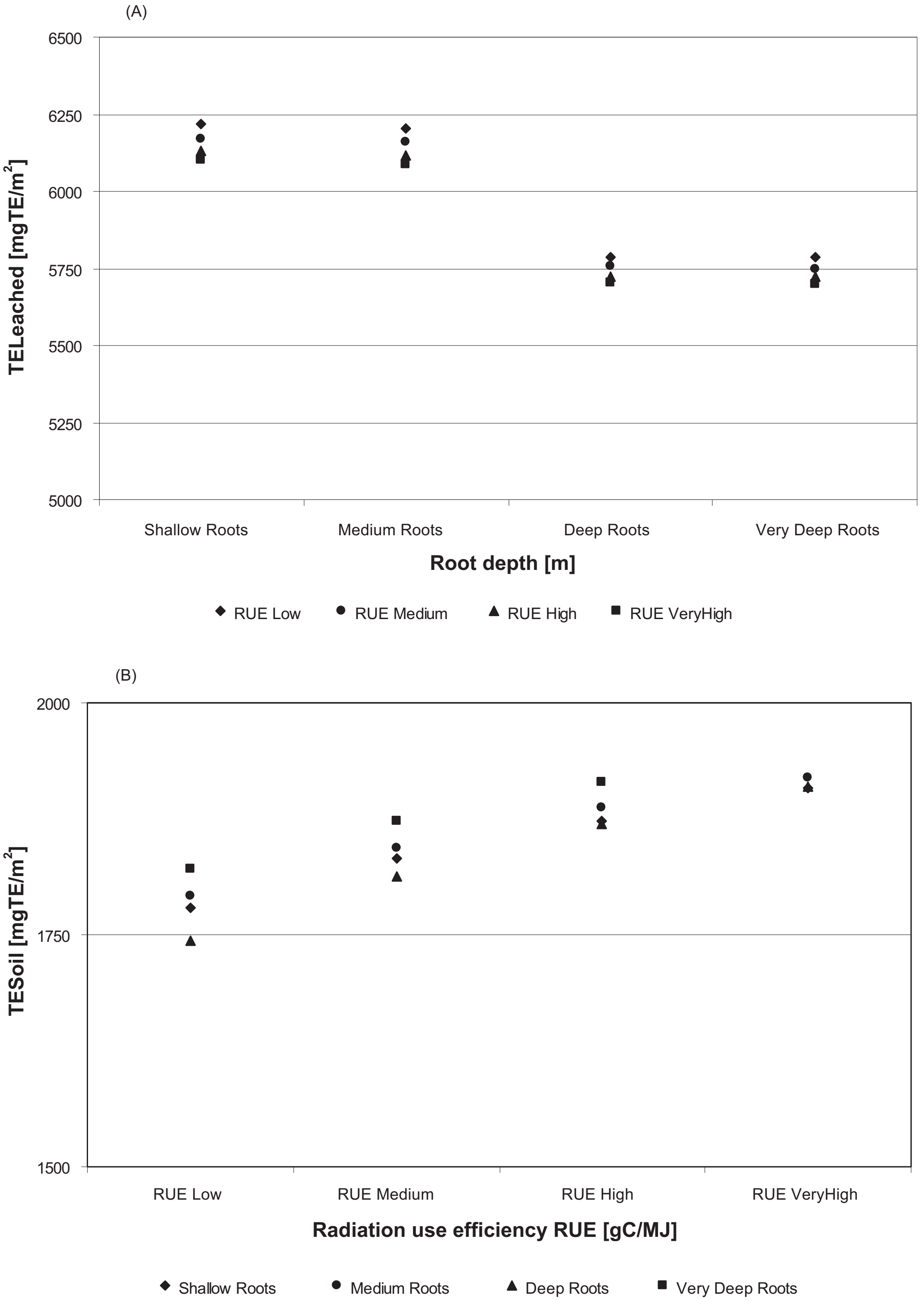


Figure 11-4. *Average accumulated trace element leached (A) and in soil (B) for different root depths and radiation use efficiency using active plant uptake. For definition of root depth see Appendix I.*

11.2 Variation in simulation results

The forest functional types with radiation use efficiency 2.2 g d.w. MJ^{-1} and root depth of 60, 80, 100 and 120 cm for active uptake and root depth 60 and 120 cm for passive uptake were selected to show the variation in simulation results among the 1,000 simulations. The average, standard deviation, median, minimum and maximum of trace element in plant, soil, leaching and trace element harvest of all forest functional types are given in Appendix 4. In general the standard variation was very high compared with the average value, especially for amounts accumulated in the soil and those estimated using passive uptake.

The frequency distribution of the 1,000 simulations for the forest functional types with active uptake and passive uptake are given in Figures 11-5 and 11-6 respectively. The sub-figures on the left-hand side are the losses by harvest and leaching respectively ($TE_{Harvest}$ and $TE_{Leached}$) and on the right-hand side the storage in plant and soil (TE_{Plant} and TE_{Soil}). For instance, the frequency distribution of trace element lost by harvest, $TE_{Harvest}$ in Figure 11-5A, showed that at most 800 mg trace element, *i.e.* 10% of the total added contaminant, was lost by harvest for all 1,000 simulations of the different forest types. Looking more closely at the numbers (not shown here), in fact 100% of the simulations with shallow roots lost less than 1% of the contaminant by harvest, while 80% of the simulations with deep roots lost 5–10% of the contaminant by harvest. The low losses by harvest can be explained by the low total trace element content in plant tissues, TE_{Plant} (Figure 11-5B). Nevertheless, most of the trace element in plants accumulated in old stem tissues, the fraction which is harvested.

Accumulated trace element leached and trace element in the soil, $TE_{Leached}$ and TE_{Soil}, showed more variation and were inversely proportional. Sixty percent of the simulations with shallow and medium roots depths (*i.e.* 60 and 80 cm) and 40% of those with deep and very deep roots (*i.e.* 100 and 120 cm) lost as much as 90–100% of the total added contaminant by leaching (Figure 11-5C). The deeper-rooted forests had a somewhat higher proportion of simulations in the 80–90% category than the shallow-rooted forests (Figure 11-5C). The remaining simulations were quite evenly spread among the 20–80% of total load leached categories.

A few simulations were observed in the lowest category of leaching, *i.e.* at most 800 mg or 10% of the contaminant. These simulation results were found for all types of pine-spruce forest, a few more for forest types with deeper roots than with shallow roots. However, at this point we are unable to identify a specific type of functional forest which leached a very low percentage of the contaminant.

The frequency distribution for trace element harvested, leached, accumulated in plant or soil was very much the same for passive uptake as for active uptake (Figures 11-5 and 11-6).

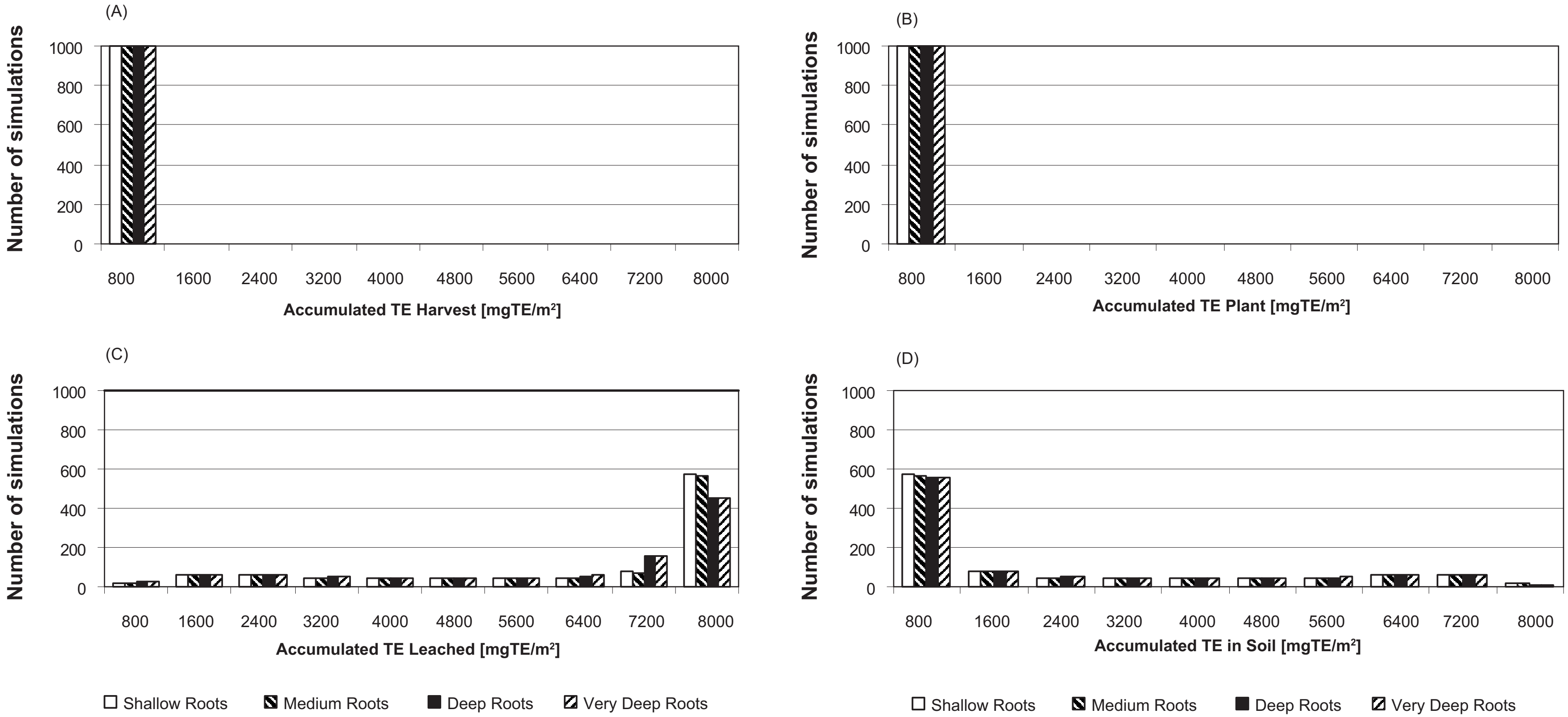


Figure 11-5. *Frequency distributions of accumulated trace element in harvest (A), plant (B), drainage (C) and soil (D) of the 1,000 simulations with active uptake for pine-spruce ecosystem forest functional types with RUE High (i.e. 2.2 g d.w. MJ^{-1}) and different root depths, see Appendix I for definition of root depths). The Y-axis denotes the observed number of simulations within a certain class and the X-axis denotes 10 even classes of total load, so that each class corresponds to 10% of the total load. The different bars represent forest functional types with different root depths, with the shallowest to the left and deepest roots to the right.*

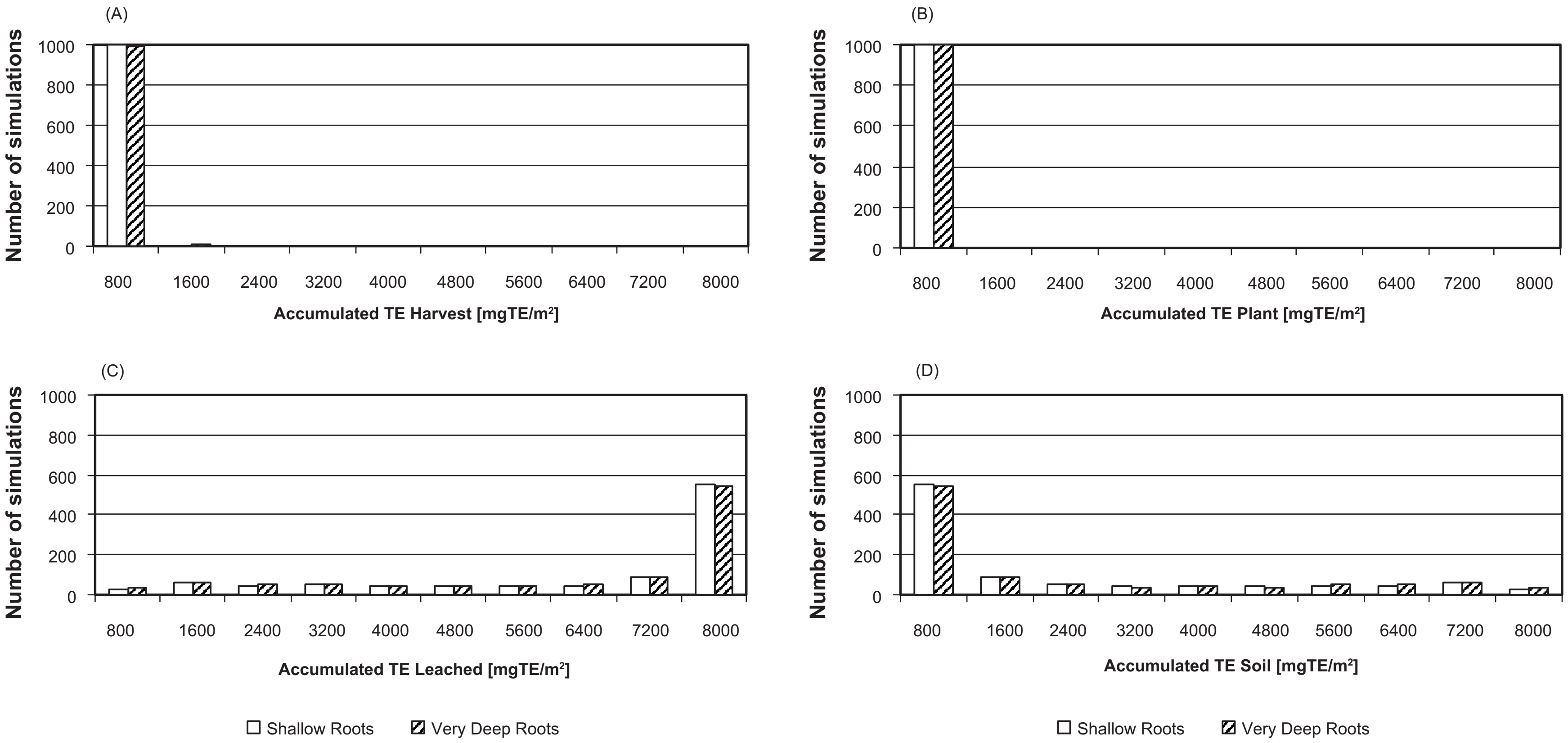


Figure 11-6. *Frequency distributions of accumulated trace element in harvest (A), plant (B), leached (C) and soil (D) of the 1,000 simulations with passive uptake for pine-spruce ecosystem forest functional types with RUE High (i.e. 2.2 g d.w. MJ^{-1} and different root depths, see Appendix I definition of root depths). The Y-axis denotes the observed number of simulations within a certain class and the X-axis denotes 10 even classes of total load, so that each class corresponds to 10% of the total load. The different bars represent forest functional types with different root depths, with the shallowest to the left and deepest roots to the right.*

11.3 Importance of radionuclide properties and ecosystem characteristics for losses and accumulation

In the sensitivity analysis, 10 different explaining variables were included for the active uptake forest types and nine different variables for the passive uptake forest types as one less variable is needed to describe allocation. Simulated leaching and absorption showed inverse patterns. The relationships between leaching and adsorption and their most important explanatory variables are given in the 3D-scatter diagrams in Figure 11-7. Leaching increased with low adsorption coefficient K_d, especially below 4 m^3 kg^{-1}. The corresponding mean Spearman ranking of the adsorption coefficient for leaching was –0.96 for active uptake and –0.97 for passive uptake and thereby adsorption coefficient was by far the most important explaining variable (Table 11-1). Leaching was further increased by a low adsorption coefficient in combination with a soil bulk density < 800 kg m^{-3} or in combination with preferential transport (*i.e.* $TE_{DWaterFlow} > 1$). The corresponding mean Spearman ranking of the soil bulk density for leaching varied from –0.1 for active uptake to –0.17 for passive uptake and for degree of convective transport ($TE_{DWaterFlow}$) it was 0.2 for both uptake approaches (Table 11-1).

The highest adsorption, 90–100% of total load, was found for samples with adsorption coefficient K_d higher than 4 m^3 kg^{-1} and soil bulk density higher than 1,000 kg m^{-3} (Figure 11-7). Low plant availability also stimulated adsorption. The relationship between adsorption and the degree of convective transport $TE_{DWaterFlow}$ was not monotonic (Figure 11-7D). Adsorption was stimulated both by degree of convective transport $TE_{DWaterFlow}$ being as low as 0.6 or less and by enhanced convective transport or preferential transport, i.e. $TE_{DWaterFlow}$ being higher than one. In the cases of low convective transport, the trace element is presumably adsorbed in the layer of contamination, and in the case of preferential transport, the trace element is quickly transported to a layer with low actual adsorption, to be adsorbed there. With deeper roots, the degree of convective transport $TE_{DWaterFlow}$ gained importance at the expense of soil bulk density.

When looking closer at different soil storages pools (not shown here), the amount of trace element in soil water solution was best explained by $TE_{DWaterFlow}$.

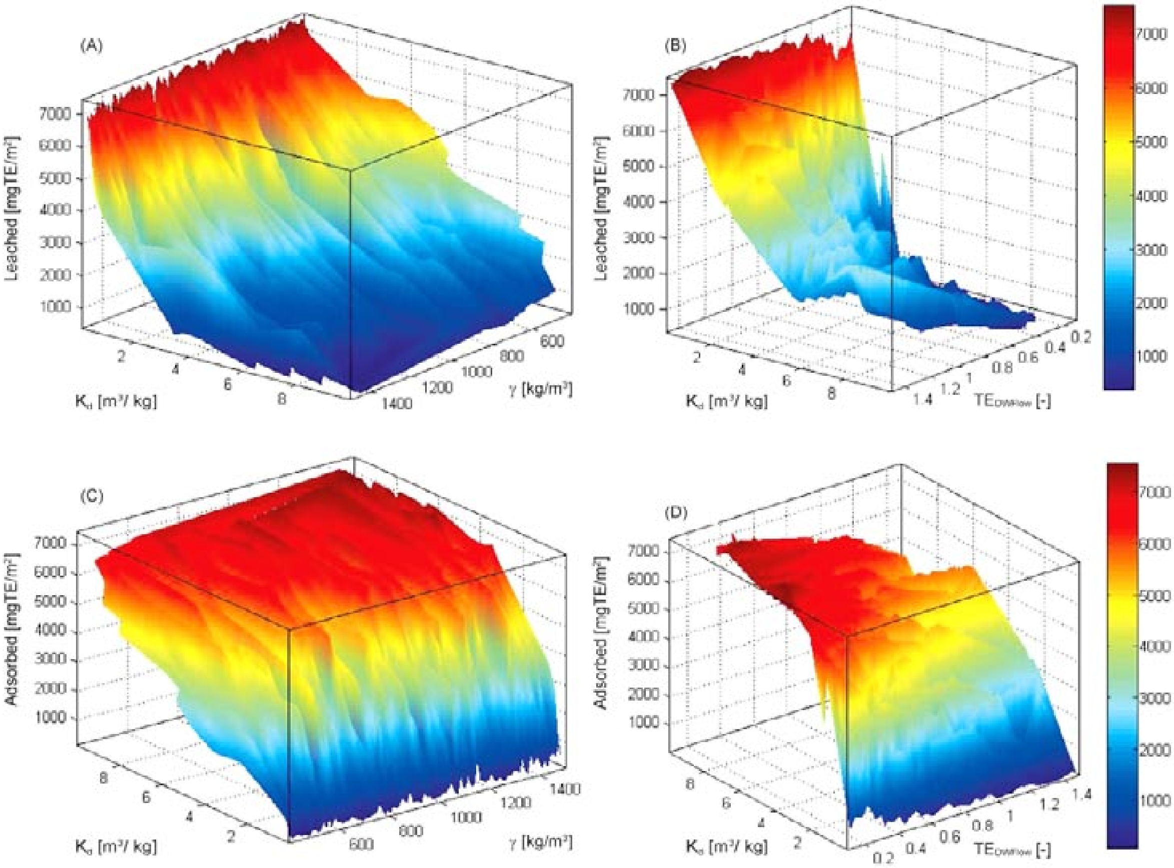


Figure 11-7. *Three-dimensional scatter diagrams of TE leached (A and B) and TE adsorbed (C and D) versus adsorption coefficient* K_d*, soil bulk density* γ *and degree of convective transport* $TE_{DWaterFlow}$ *for scenario with active uptake, medium root depth of 80 cm and radiation use efficiency of 2.2 [g d.w.* MJ^{-1}*]*.

Table 11-1. Average Spearman ranking of *Tracey* parameters for accumulation in soil and plant and losses of radionuclides (see Appendix 1 for definitions).

	Plant		Soil		Leached		Harvested	
Uptake	**Active**	**Passive**	**Active**	**Passive**	**Active**	**Passive**	**Active**	**Passive**
Parameter	Average (STD)	Average (STD)	Average (STD)	Average (STD)	Average (STD)	Average (STD)	Average (STD)	Average (STD)
General								
γ (kg m^{-3})	0.04 (0.00)	–0.03 (0.02)	0.10 (0.00)	0.18 (0.00)	–0.10 (0.00)	–0.17 (0.00)	–0.03 (0.01)	–0.04 (0.02)
K_d (m^3 kg^{-1})	0.01 (0.02)	–0.07 (0.08)	0.97 (0.00)	0.97 (0.00)	–0.96 (0.01)	–0.97 (0.00)	–0.13 (0.04)	–0.19 (0.08)
$TE_{DWaterFlow}$ (–)	–0.16 (0.03)	–0.71 (0.04)	–0.18 (0.00)	–0.18 (0.00)	0.20 (0.01)	0.19 (0.01)	–0.25 (0.03)	–0.58 (0.02)
$TE_{DLitter1\rightarrow Solved}$ (–)	–0.02 (0.00)	–0.06 (0.01)	–0.02 (0.01)	–0.04 (0.00)	0.01 (0.00)	0.04 (0.00)	0.04 (0.01)	–0.05 (0.01)
$TE_{DHumus\rightarrow Solved}$ (–)	–0.01 (0.00)	0.04 (0.01)	–0.03 (0.01)	–0.02 (0.00)	0.01 (0.00)	0.02 (0.00)	0.10 (0.01)	0.04 (0.01)
Active uptake								
$TE_{BioRate}$ (*day*$^{-1}$)	0.36 (0.04)		0.00 (0.00)		–0.04 (0.03)		0.64 (0.04)	
$P_{MaxTECLeaf}$ (mg *TE* gC^{-1})	0.68 (0.02)		0.06 (0.02)		–0.03 (0.00)		–0.31 (0.03)	
$P_{MaxTECSeed}$ (mg *TE* gC^{-1})	–0.04 (0.01)		0.03 (0.00)		–0.04 (0.00)		0.00 (0.00)	
$P_{MaxTECStem}$ (mg *TE* gC^{-1})	0.52 (0.02)		–0.03 (0.03)		0.00 (0.01)		0.44 (0.04)	
$P_{MaxTECRoot}$ (mg *TE* gC^{-1})	0.04 (0.00)		0.05 (0.01)		–0.04 (0.00)		–0.15 (0.01)	
Passive uptake								
$TE_{DWUptake}$ (–)		0.26 (0.02)		–0.02 (0.00)		0.01 (0.01)		0.22 (0.00)
f_{PULeaf} (%)		–0.02 (0.11)		0.02 (0.00)		–0.02 (0.00)		–0.11 (0.00)
f_{PUSeed} (%)		–0.02 (0.00)		0.03 (0.00)		–0.02 (0.00)		–0.02 (0.00)
f_{PURoot} (%)		–0.49 (0.21)		0.00 (0.00)		0.02 (0.01)		–0.60 (0.02)

The most important explaining factors for harvest differed with plant uptake approach. The plant availability $TE_{BioRate}$ and allocation to stem were most important for losses by harvest for the active plant uptake forest functional types. Allocation to roots and degree of convective transport $TE_{DWaterFlow}$ for matter most for harvest losses when using the passive plant uptake forest types (Figure 11-8A, Table 11-1).

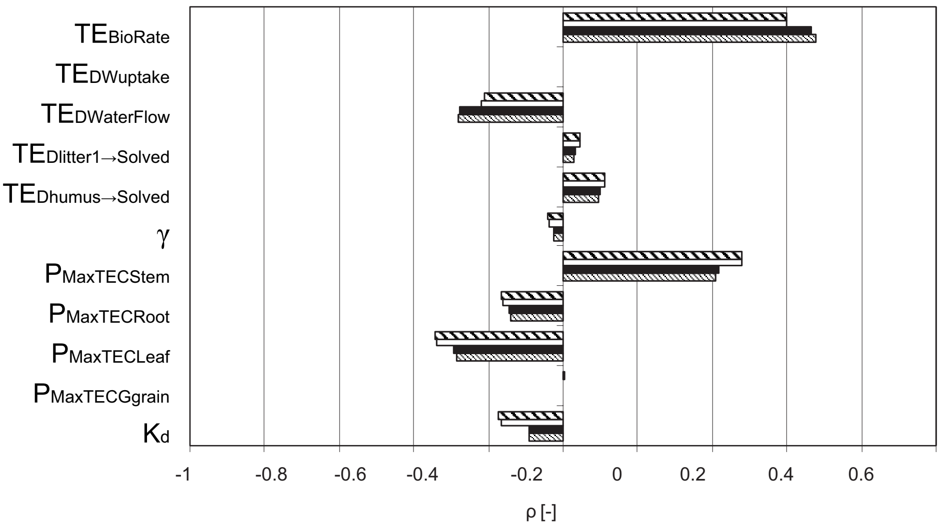
Humus pool was the second most important storage of radionuclides for the active uptake forest functional types with deeper roots. It was positively related to maximum concentration of trace element in leaves and negatively to that in stem (Figure 11-8B). The negative relation with stem may be due to the harvest of stems. The differences in decomposition rates of needle and stem litter might also have an effect. For passive uptake scenarios, humus and soil were negatively related to degree of convective transport $TE_{DWaterFlow}$ and positively to fraction allocated to roots (Table 11-1).

Accumulation in plants was of small magnitude. However, it might be relevant to determine the factors that were most important for other applications, *e.g.* assessments of contamination of animal food or other uses of forest products such as forest energy. Young leaves and stems of pine-spruce are part of the diet of game animals, which eventually can be eaten by humans.

The trace element content of young leaves was very much determined by the maximum concentration of trace element in leaves and stem when trace element was taken up actively (Figure 11-9A). 'Seeds' of pine and spruce are cones, which may be eaten by squirrels, for instance. With seeds, we created a plant compartment that receives trace element content mainly by retranslocation from another plant compartment, in this case leaves. As such, it is understandable that the Spearman ranking coefficients for young leaves and seed are very much alike (Figures 11-9–11-10A and C).

The trace element content in young stems, like that in twigs, showed a different pattern for forests with shallow-medium root depths than for those with deep-very deep roots when using active uptake (Figure 11-9B). The trace element content in young stems in shallow-rooted forests increased with increasing adsorption coefficient K_d, while it decreased in deep-rooted forests with increasing adsorption coefficient K_d. The deeper-rooted forest had better contact with the source of contamination. In

(A) **Spearman coefficients of TE Harvest- Active Uptake**



(B) **Spearman coefficients of TE Humus- Active Uptake**

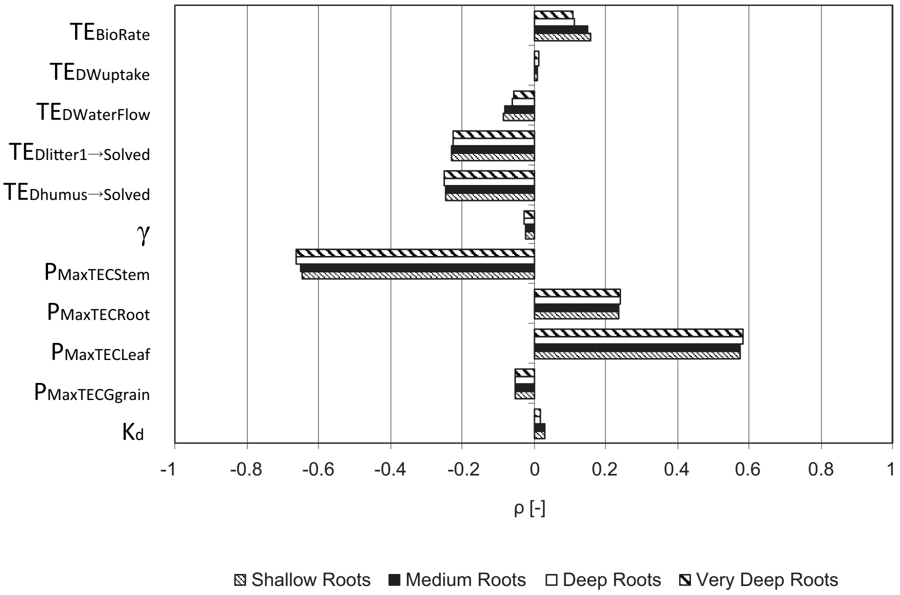


Figure 11-8. *Spearman ranking coefficients for trace elements in harvest (A) and humus (B) using active plant uptake. Parameter names of different symbols are given in Appendix 1.*

such forest types, plant uptake was reduced when adsorption was competitive. In the shallow-rooted forests, plant uptake was enhanced when trace elements were adsorbed instead of leached.

The trace element content of old stem (Figure 11-9D) was mainly dependent on the plant availability $TE_{BioRate}$. Stem had by far the largest carbon pool for most of the simulation periods. The maximum concentration of trace element in stem tissues was rather small, and hence had little effect on accumulation in old stem parts.

Using active uptake, the Spearman ranking coefficients of the different plant compartments were very much dominated by degree of convective transport $TE_{DWaterFlow}$ and the fraction allocated to that compartment (Figure 11-10). The fraction allocated to stem was described as the difference between unity and the sum of the fractions for seeds, leaf and roots. The root fraction was by far the greatest fraction and hence the trace element content of young and old stems was strongly negatively related to the root fraction. The passive uptake forest functional types showed no difference in Spearman ranking coefficients between shallow and deep root depths as the active uptake forest functional types did for trace element content in old stem (Table 11-1).

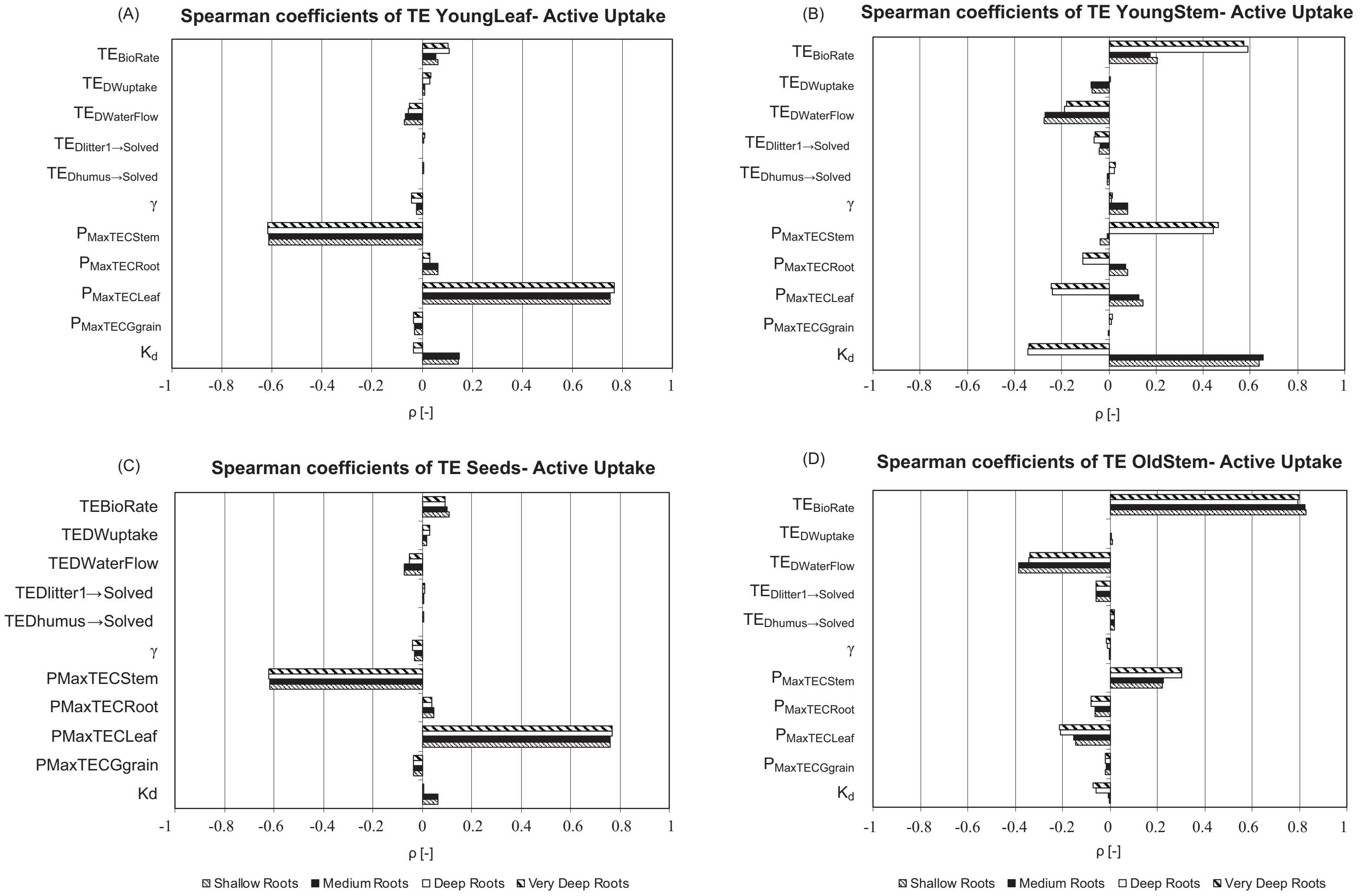
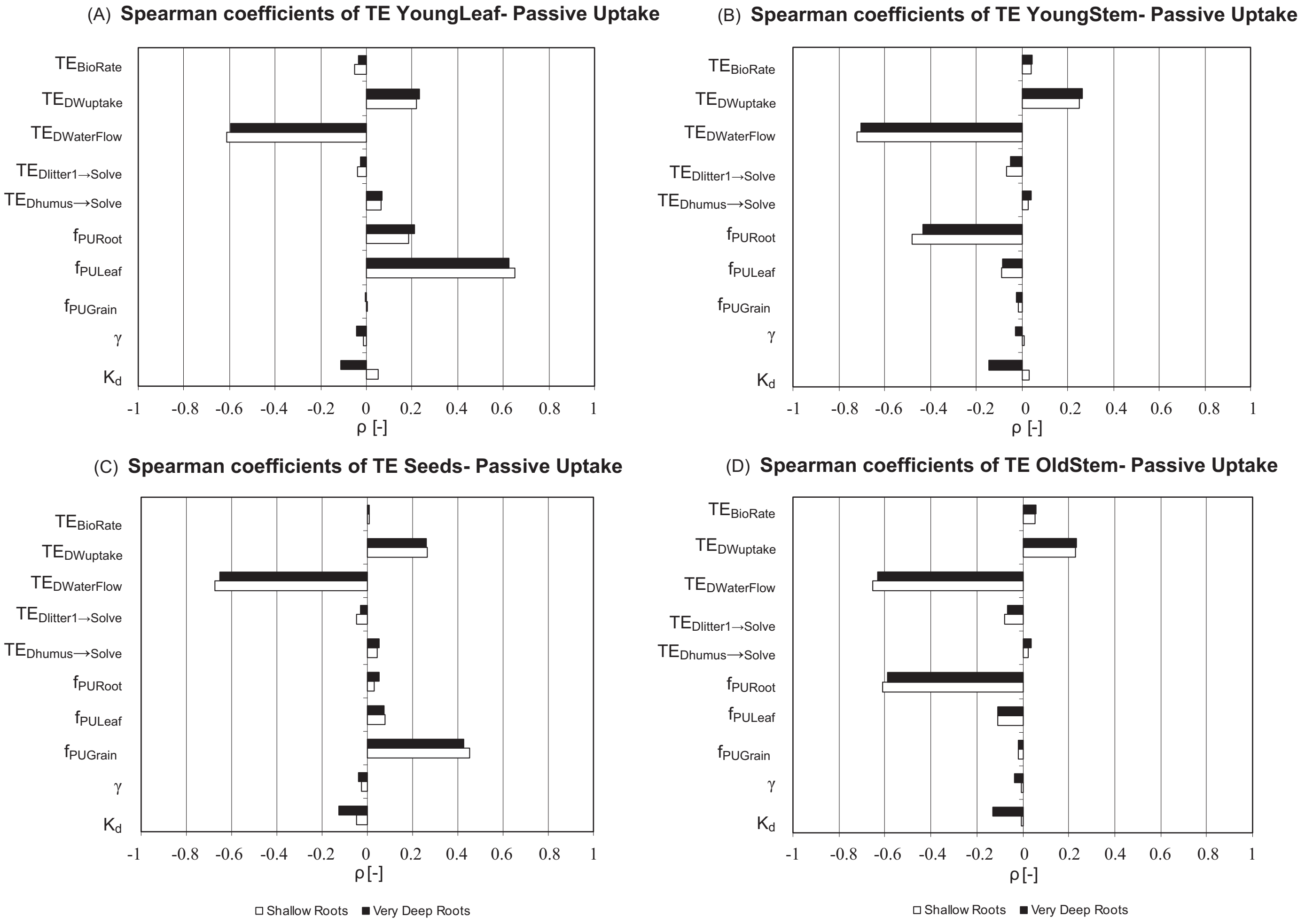


Figure 11-9. *Spearman coefficient for trace elements in Young leaves (A), Young stem (B), Seeds (C) and Old Stem (D) for active plant uptake forest types. Parameter names of different symbols are given in Appendix 1.*


(A) Spearman coefficients of TE YoungLeaf- Passive Uptake

(B) Spearman coefficients of TE YoungStem- Passive Uptake

(C) Spearman coefficients of TE Seeds- Passive Uptake

(D) Spearman coefficients of TE OldStem- Passive Uptake

Figure 11-10. *Spearman coefficients for trace elements in Young leaves (A), Young stem (B), Seeds (C) and Old Stem (D) for passive plant uptake forest types. Parameter names of different symbols are given in Appendix 1.*

11.4 Circumstances increasing leaching losses

In this study we have take into account how daily weather affects leaching. From comparable studies of solute leaching, we know that in addition to plant capacity to take up solutes and soil adsorption capacity, weather conditions are crucial in determining whether leaching will occur or not. For instance, pesticide leaching from arable land has been found to occur only when heavy rainfall occurs within two weeks after pesticide spreading /Lindahl et al. 2005/. Likewise leaching of nitrogen from fertilized forest is limited to short episodes at snowmelt and autumn storms /Gärdenäs et al. 2003/.

We used the water and carbon fluxes of a forest ecosystem for one forest rotation period of 100 years as driving variables. During the regeneration phase (*i.e.* the first 10–15 years), plant capacity to take up radionuclides is limited because of its small biomass, while at the same time water drainage is relatively large. Accordingly, the probability that radionuclides will be leached was highest during snowmelt and autumn storms in the forest regeneration phase. The daily variation in trace element leached, carbon content of plant, soil surface infiltration and water drainage for the forest types with active uptake, high *RUE* and shallow roots as well as the ones with very deep roots are given in Figure 11-11. The nominal values of the *Tracey* parameters were used. Trace element leaching corresponded well with water drainage and showed highest peaks during the regeneration phase, as well as some minor peaks after thinnings.

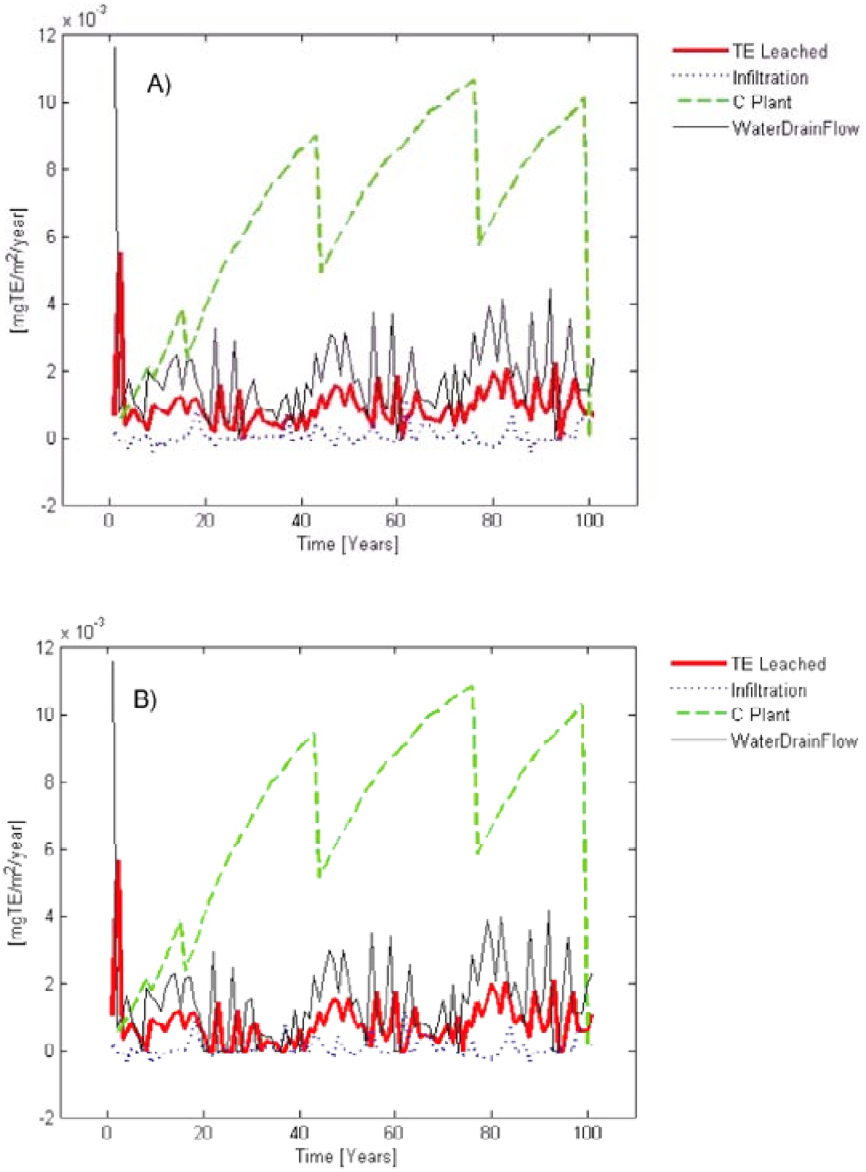


Figure 11-11. *Daily variation in trace element leached (bold red line), water drainage (black line), C plant (dashed green line) and water infiltration (dotted blue line) for the pine-spruce ecosystem forest functional types with RUE High (i.e. 2.2 g d.w. MJ^{-1}) and shallow roots (=60 cm) (A) and very deep roots (=120 cm) (B) for the years 8,000–8,100. Y-axis shows the amount of trace element leached during a day.*

12 Results for alder ecosystems

12.1 Average distribution of trace element

To provide an overview, the trace element accumulation in different parts of the system after 10,000 years is first presented as an average for all 1,000 simulations with different combinations of parameter settings (see Table 9-2.). The alder functional types were categorised from shallow to deep root depth and from low to very high plant growth rate (*i.e.* low and very high radiation use efficiency, *RUE*). For passive uptake, this categorisation had a little influence on the fraction of trace element load allocated to soil and plant versus to leaching. After 10,000 years more than 80% had been leached in all systems (Figure 12-1, right). For active uptake, the accumulation in plant and soil was larger and thus accumulated trace element leaching was smaller (Figure 12-1). For shallow root depth, the accumulation in plant and soil was as small as for passive uptake (*i.e.* about 20%). For medium root depth, about half the total load was accumulated in plant and soil and the other half was leached. For deep root depth, almost all (i.e. about 90%) was accumulated in plant and soil. The plant growth rate (or *RUE*) had a minor influence on the average distribution of the trace elements (Figure 12-1, left).

Of the trace element accumulated in the soil, almost all was adsorbed in the case of passive uptake (Figure 12-2, right). The ecosystems with medium root depth, showed slightly higher trace element accumulation in humus. The distribution in the soil for active uptake differed with root depth. In the shallow root depth systems about half was adsorbed and the other half accumulated in humus. In other ecosystems with a deeper root depth, only 20% was adsorbed and about 80% accumulated in humus (Figure 12-2). The fractions distributed to litter and soil solutions were small. The plant growth rate influenced the pattern slightly but not in a systematic way.

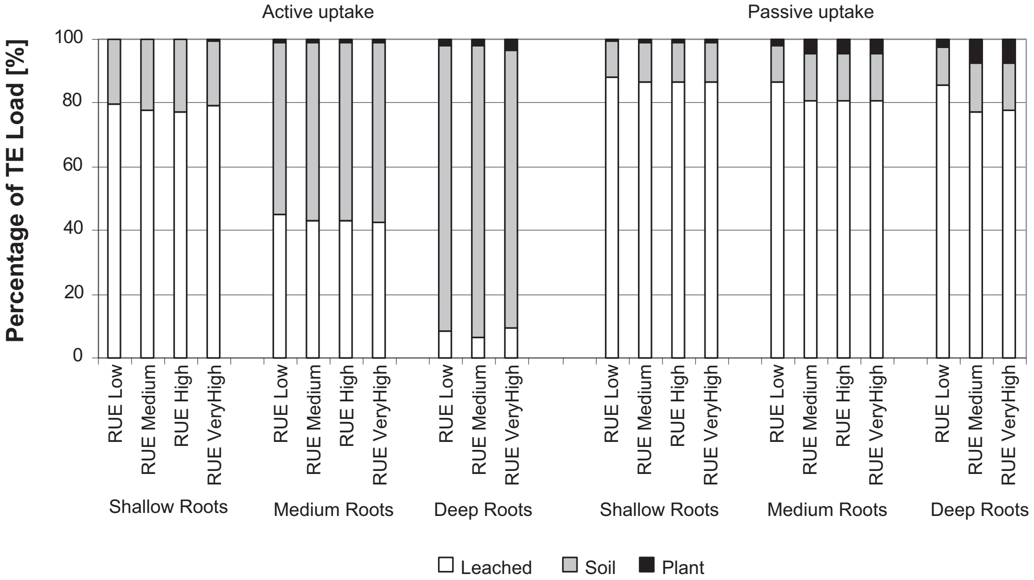


Figure 12-1. Average fractional distribution of trace element in plants and soil, distributed from top to bottom; plant, soil and accumulated leached, respectively, after 10,000 years for different ecosystems based on average values of 1,000 simulations of the alder ecosystem forest functional types with active uptake (left) and passive uptake (right).For definition of RUE and root depth see Appendix 1.

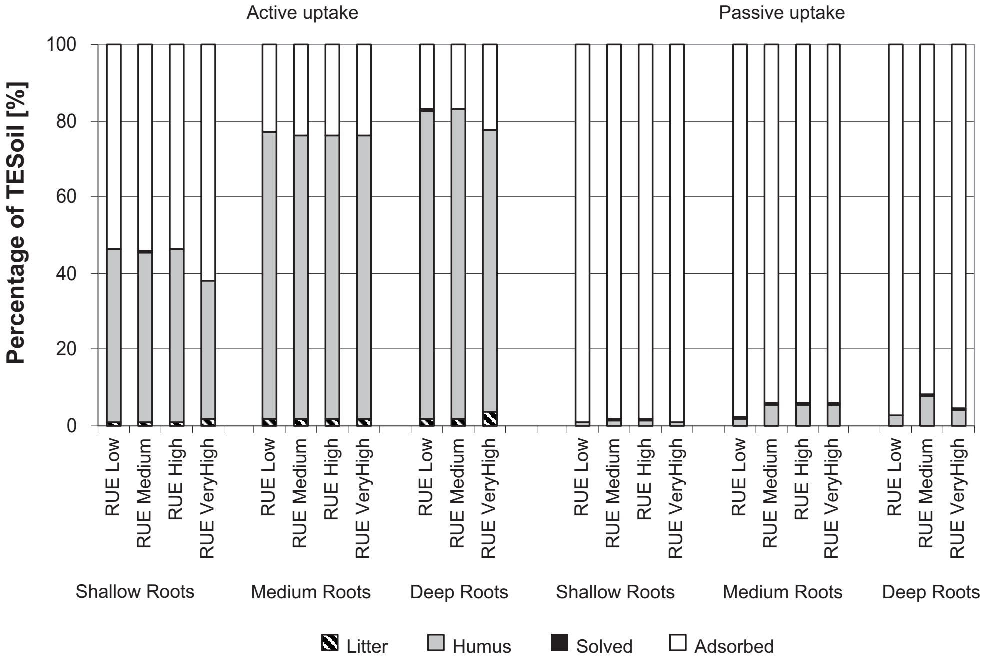


Figure 12-2. Average fractional distribution of trace element in the soil, from top to bottom; adsorption soil solution, humus and litter, respectively, after 10,000 years of alder ecosystem forest functional types with active uptake (left-side) and passive uptake (right-side). Note that amounts in the soil solution are very small. For definition of RUE and root depth see Appendix 1.

Of the trace element accumulated in the plant, practically all (99%) was accumulated in old roots in the case of passive uptake (Figure. 12-3, right). In the case of active uptake, up to 10% was accumulated in young tissues and the rest in old tissues, with old stem being the most important sink. The fraction distributed to old roots was highest for the shallow-rooting systems and somewhat higher for slow growing plants, *i.e.* plants with lower *RUE* (Figure 12-3, left).

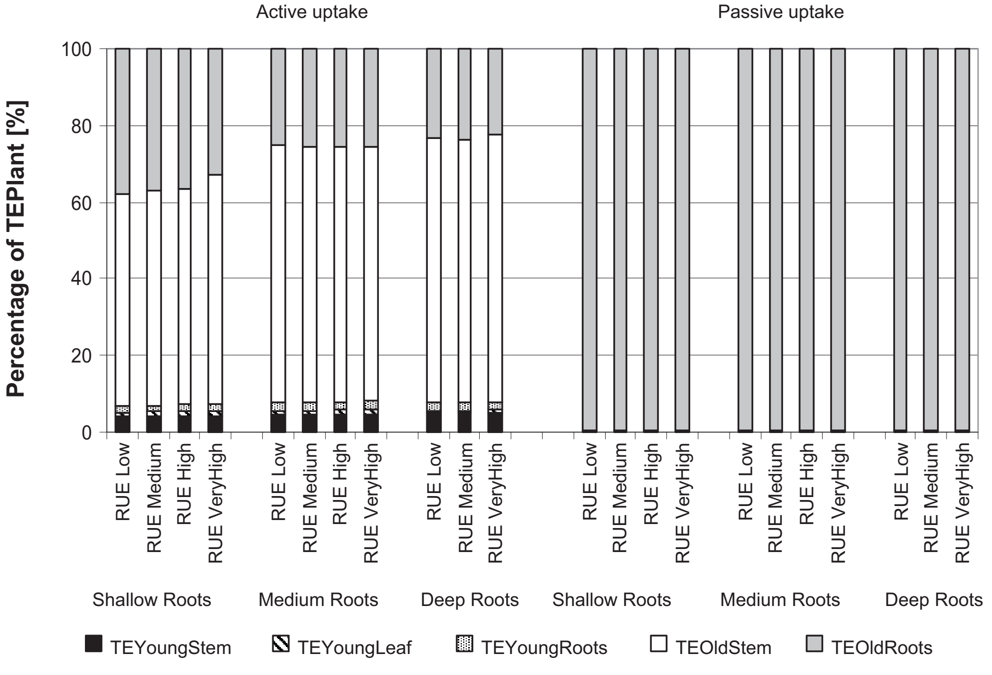


Figure 12-3. Average fraction distribution of trace element in plant, from top to bottom; old roots, old stem, young roots, leaves and young stems, respectively, after 10,000 years for alder ecosystem forest functional types with active uptake (left-side) and passive uptake (right-side). For definition of RUE and root depth see Appendix 1.

Overall for passive uptake, average losses by leaching of total load during 10,000 years was high (about 80–90% of total load) for all types of parameter combinations. Only 10–15% was accumulated in soil, of which most (> 90%) was adsorbed, and less than 5% was accumulated in plants. For active uptake the pattern was similar to that for passive uptake for the shallow root system, but deeper root depths strongly decreased the fraction lost by leaching. Instead, the trace element load was accumulated in soil, mainly in humus, whereas plants accumulated only a few percent of the total load. For active uptake with the deepest root depth, 10% was lost by leaching and almost 90% was accumulated in soil, of which 75% was in humus and less than 3% in plants.

12.2 Trace element amounts

The absolute values of trace element accumulated in a single plant and in soil components are often quite small in comparison with the total load, and are easier seen on a logarithmic scale (Figures 12-4 and 12-5). Similarly to the relative distributions presented above, these figures show that on average for the 1,000 randomly chosen parameter sets, the total amount of trace element distributed to soil was almost independent of root depth in the case of passive uptake (Figure 12-4), and significantly larger than the accumulation in the plant (Figure 12-5).

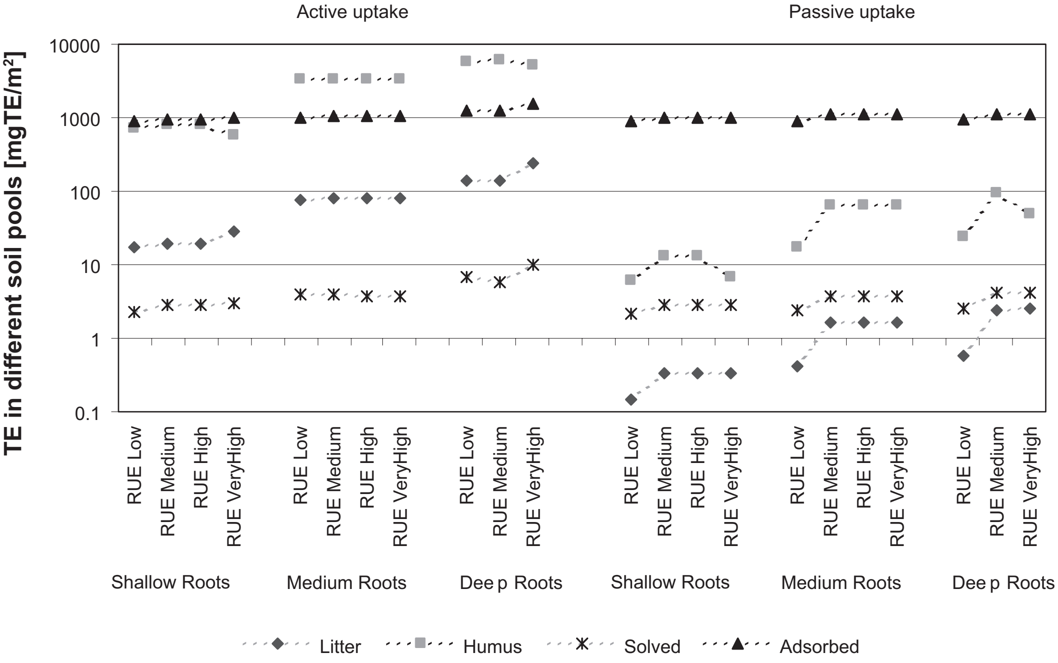


Figure 12-4. *Average amounts of trace element (mg m^{-2}) accumulated in different soil pools; litter, soil solution, humus and adsorbed, respectively, after 10,000 years for alder forest functional types with active uptake (left-side) and passive uptake (right-side). For definition of RUE and root depth see Appendix 1.*

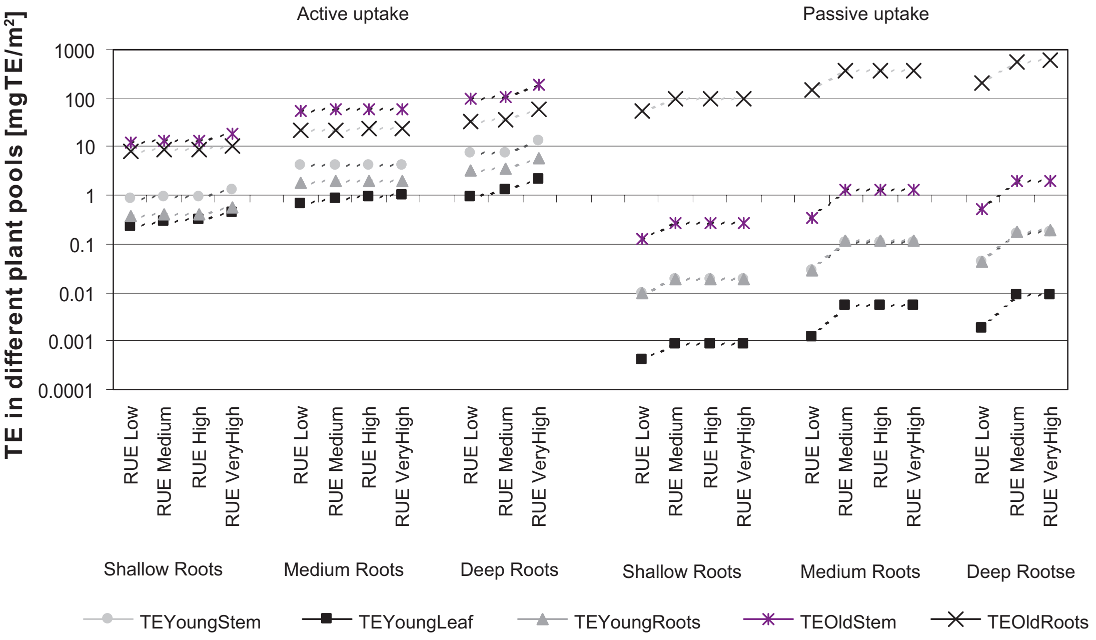


Figure 12-5. *Average amount of trace element (mg m^{-2}) accumulated in plant; in leaf, young roots, young stem, old roots and old stem (young stem and young roots very similar for passive uptake), respectively, after 10 000 years for alder forest functional types with active uptake (left-side) and passive uptake (right-side). TEYoungStem and TEYoungRoots are very similair and hard to distinguish for the passive systems. For definition of RUE and root depth see Appendix 1.*

12.3 Variation in distribution due to parameter variations

For each alder ecosystem, 1,000 simulations were made using different values for 12 parameters of the *Tracey* model, for instance adsorption capacity (K_d) and the discrimination factor in soil water flow ($TE_{DWaterFlow}$, see Table 9-2.). This caused a variation around the average trace element values presented above. The fraction of total load accumulated in the soil plant system varied strongly. For some combinations of parameter values almost all the trace element load was accumulated, whereas for other combinations almost zero was accumulated (see Table 12-1a and b). As shown earlier, this pattern strongly dependend on rooting depth.

Overall for passive uptake the fraction of total load lost by leaching ranged between 5 and 100% depending on parameter setting, but in more than half of cases it was larger than 90%. The fraction adsorbed varied in between the same range, but on average it was 10% and the median was close to zero. The fraction accumulated in humus was at most about 30% in one deep rooting ecosystem, but in most ecosystems it was never above 5%. The accumulation in plants was higher than in humus, and for forest types with deep rooting depths and high growth rate the fraction reached at most 80% (Table 12-1a).

Overall for active uptake the full ranges of variation in the fraction of trace element load lost by leaching or adsorbed were 0–99% and 0–95% respectively, *i.e.* similar to those for passive uptake. The adsorption fraction showed a similar relationship to the variation in parameter values as for passive uptake. However, leaching showed quite a different relationship to rooting depth compared with passive uptake. For deep rooting ecosystems it almost never exceeded 70%, whereas the accumulation in humus in these systems ranged between 2–97%. Accumulation in plants never exceeded 30% of total load (Table 12-1b).

For deep root depth and active uptake, less than 10% of trace element was lost by leaching in more than 80% of all simulations (*i.e.* more than 90% was accumulated in the system), and in no case was the fraction lost by leaching larger than 50% (Figure 12-6A). For the shallow root depth the distribution was also strongly skewed, but in the opposite way, with more than 60% of the simulations having a leaching loss higher than 80%. For the medium root depth (1.5 m) the distribution was more evenly distributed around 50% leaching loss.

In the case of passive uptake the influence of root depth was much less than for active uptake, and for all depths the majority of parameter settings resulted in almost all the trace element load being lost by leaching (Figure 12-6B).

Table 12-1a. Accumulation of trace element in different pools after 10,000 years as a fraction of total load (%) for alder, passive uptake. Values refer to 1,000 simulations with different parameter values. Root depth shallow is 50 cm, medium 150 cm and deep 250 cm respectively. Radiation use efficiency, *RUE* low is 1.125, medium 2.250, high 3.375 and very high 4.5 g d.w. MJ^{-1} respectively.

Root depth	Shallow				Medium				Deep		
RUE	Low	Medium	High	Very high	Low	Medium	High	Very high	Low	Medium	Very high
Leached											
Mean	88	86	86	86	87	81	81	81	85	77	78
Std	23	24	24	24	23	26	26	26	23	26	27
Median	98	98	98	98	97	92	92	92	96	89	89
Min	5	4	4	4	5	4	4	4	5	4	4
Max	100	100	100	100	100	100	100	100	100	100	100
Adsorbed											
Mean	11	12	12	12	11	14	14	14	12	14	14
Std	23	24	24	24	23	26	26	26	23	26	26
Median	0	0	0	0	0	0	0	0	0	0	0
Min	0	0	0	0	0	0	0	0	0	0	0
Max	94	95	95	95	95	96	96	96	95	96	96
Humus											
Mean	0	0	0	0	0	1	1	1	0	1	1
Std	0	0	0	0	0	2	2	2	0	2	1
Median	0	0	0	0	0	0	0	0	0	1	0
Min	0	0	0	0	0	0	0	0	0	0	0
Max	1	4	4	2	4	21	21	21	6	33	19
Plant											
Mean	1	1	1	1	2	5	5	5	3	7	7
Std	1	2	2	2	3	8	8	8	5	12	12
Median	0	0	0	0	0	0	0	0	0	0	0
Min	0	0	0	0	0	0	0	0	0	0	0
Max	11	15	15	15	34	48	48	48	53	79	80

Table 12-1b. Accumulation of trace element in different pools after 10,000 years as a fraction of total load (%) for alder, active uptake. Values refer to 1,000 simulations with different parameter values. Root depth shallow is 50 cm, medium 150 cm and deep 250 cm respectively. Radiation use efficiency, *RUE* low is 1.125, medium 2.250, high 3.375 and very high 4.5 g d.w. MJ^{-1} respectively.

Root depth	Shallow				Medium				Deep		
RUE	Low	Medium	High	Very high	Low	Medium	High	Very high	Low	Medium	Very high
Leached											
Mean	79	78	77	79	45	43	43	43	8	7	9
Std	21	22	22	23	14	14	14	14	10	9	12
Median	86	85	85	88	44	44	43	43	4	3	5
Min	5	4	4	4	5	3	3	3	1	0	0
Max	98	98	98	99	89	85	85	84	68	61	75
Adsorbed											
Mean	11	12	12	13	12	13	13	13	15	15	19
Std	21	23	23	24	22	24	24	23	26	26	30
Median	0	0	0	0	0	0	0	0	1	1	1
Min	0	0	0	0	0	0	0	0	0	0	0
Max	93	94	94	95	91	92	92	92	93	94	96
Humus											
Mean	9	10	10	7	41	41	42	42	73	74	65
Std	5	5	5	5	14	14	14	14	23	23	25
Median	8	9	10	6	46	47	47	48	83	85	75
Min	1	1	1	1	3	3	3	3	5	5	2
Max	20	20	20	19	57	57	57	57	97	97	95
Plant											
Mean	0	0	0	0	1	1	1	1	2	2	3
Std	0	0	0	0	1	1	1	1	2	2	3
Median	0	0	0	0	1	1	1	1	1	1	2
Min	0	0	0	0	0	0	0	0	0	0	0
Max	2	2	2	3	10	10	10	10	17	18	29

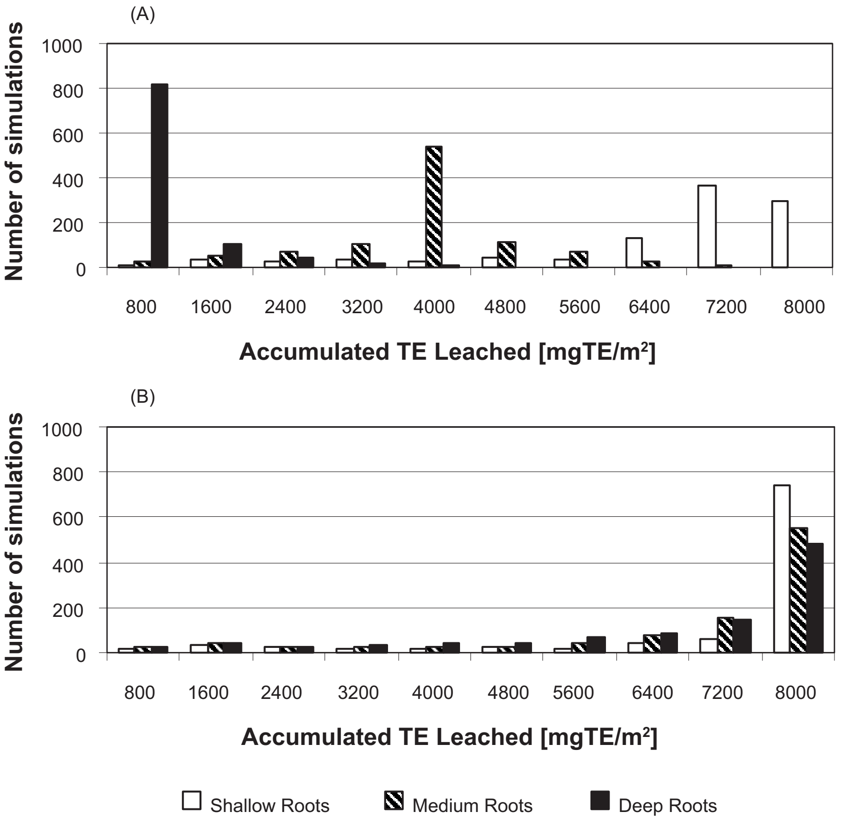


Figure 12-6. *Frequency distribution of the fraction of trace element load lost by leaching by the year 10,000, for alder forest functional types with different rooting depths. The reference radiation use efficiency (2.25 g d.w. MJ^{-1}) was used. (A) Active uptake and (B) Passive uptake. For definition of RUE and root depth see Appendix 1.*

12.4 Relationships between averaged driving variables and trace element pools

The trace element dynamics are driven by carbon and water dynamics of plant and soil as simulated by *CoupModel*. Different functional alder types were simulated characterised by different radiation use efficiency (*RUE*) and root depth (z_r) values. Moreover, the alder forest had to be in a quasi-steady state as regards carbon budget, *i.e.* plant biomass and soil organic C had to fluctuate regularly around a long-term mean. This resulted in alder forests being characterised by different sizes of plant C and soil C pools. Large pools were related to high growth and decomposition rates promoted by high radiation use efficiency and high water availability due to deep root depth. To identify possible simple relationships between trace element dynamics and alder carbon and water dynamics, we evaluated the degree to which the trace element simulations were systematically related to the sizes of the plant and soil C pools, transpiration or run-off (Table 12-2). Hereby the nominal parameter values of the *Eikos* simulation as given in Table 9-2 were used.

Firstly, it could be noted that the carbon and water variables simulated by *CoupModel* were related to each other. High plant C values were correlated with high soil C values (R^2=0.63, n=11), high transpiration rates were correlated with high plant C (R^2=0.60, n=11), and low run-off was strongly correlated with high transpiration rates (R^2=0.99, n=5). However, the trace element accumulation in the system was not correlated with any single carbon or water characteristic, the highest R^2 being 0.07 (n=11, Table 12-2). Among the trace element accumulations simulated by the *Tracey* model, there was a very strong relationship between high trace element in soil organic matter and low values of adsorbed trace element (R^2=0.999, n=11, the relationship to trace element in soil water was similar), whereas the correlation between trace element in soil organic matter and plant trace element was lower, although still high (R^2=0.78, n=11). Consequently, the R^2 value of the relationship between plant trace element and adsorbed trace element was also about 0.8. Accumulated leached trace element was not correlated to any of the other trace element variables (R^2 < 0.07).

Table 12-2. Trace element accumulation (TE mg m^{-2}) at 10,000 years and carbon states (kg C m^{-2}) and annual water flows (mm y^{-1}) at steady state for alder *CoupModel* simulations and active uptake *Tracey* simulations. For the C pools, initial values were used instead of means as they were almost similar to the means.

Alder ecosystem active uptake	Initial plant C	Tranp.	TE Total Plant	Initial humus C	TE Total Soil C	TE Adsorbed & Solution	Total Run off	TE Leached
Shallow roots								
RUE low	1.36	134	10.5	4.4	514	7,414	281	91.5
RUE medium	3.9	202	12.1	10.5	580	7,333	228	105
RUE high	5.5	202	12.3	15.1	591	7,322	228	104.6
RUE very high	6.6	202	14.6	10.6	359	7,544	228	112.3
Medium roots								
RUE low	1.5	145	57.4	4.8	2,755	5,175	268	42.4
RUE medium	3.9							
(Reference)		240	58.0	12.4	2,652	5,274	187	45.3
RUE high	5.8	240	58.3	18.4	2,660	5,267	187	44.9
RUE very high	7.7	240	58.5	24.5	2,666	5,261	187	44.6
Deep roots								
RUE low	1.5	146	113.3	4.8	5,109	2,725	267	82.8
RUE medium	3.9	252	112.8	12.4	5,095	2,738	176	83.5
RUE very high	8.2	252	163.7	12.7	3,805	3,944	176	117.3

From these results, we can conclude that there were strong correlations between single output variables within the models, but none between output variables of different the models. When the fraction of trace element load allocated to the plant, and especially to soil organic matter, was changed, the allocation to adsorption and soil solution changed proportionally.

12.5 Variation among functional forest types

The amount of trace element in plants increased on average for all 1,000 simulations with increasing root depth. The increase was higher for passive uptake than for active uptake, and differed depending on radiation use efficiency (*RUE*, Figure 12-7). For passive uptake, the low *RUE* resulted in a much lower response to root depth (Figure 12-7, right), whereas for the active uptake, the response was almost independent of *RUE*, except that the highest *RUE* caused an increased accumulation of trace element in plants for the deepest root depth (Figure 12-7, left).

Concerning the accumulation of trace element in soil organic matter, neither root depth nor *RUE* influenced the accumulation significantly, in relative terms, for passive uptake (Figure 12-8, right). The reason was that almost all the trace element load was adsorbed (Figure 12-8). For active uptake, increasing root depth strongly increased the accumulation in soil organic matter, whereas *RUE* had almost no influence (Figure 12-8, left).

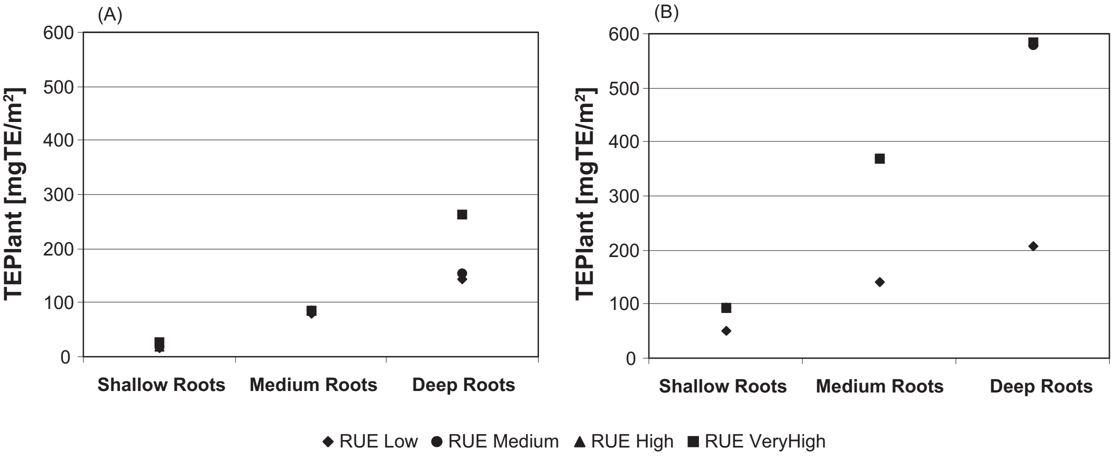


Figure 12-7. *Trace element accumulation in plants after 10,000 years in relation to root depth for different radiation use efficiencies. Average of 1,000 simulation for alder forest functional types with active uptake (A) and passive uptake (B). For definition of RUE and root depth see Appendix 1.*

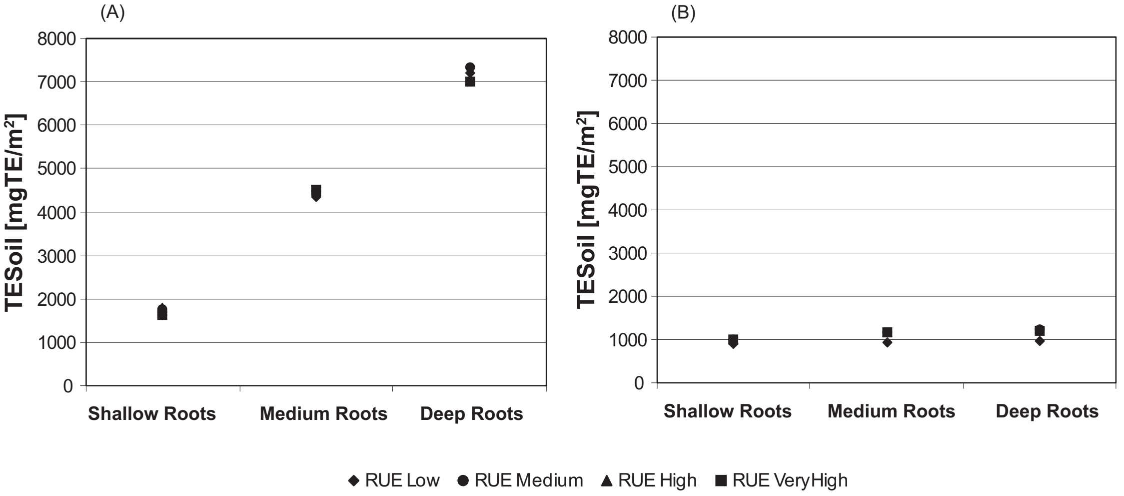


Figure 12-8. *Trace element accumulation in soil after 10,000 years in relation to root depth for different radiation use efficiencies based on averages of 1,000 simulations of alder forest functional types with active uptake (A) and passive uptake (B). For definition of RUE and root depth see Appendix 1.*

12.6 Most influential ecosystem characteristics and radionuclides properties

The accumulated leaching was positively correlated to $\mathrm{TE}_{DWaterflow}$ and negatively correlated to K_d (Figure 12-9A and B). Since the adsorption was the dominant process in the soil system, K_d explained the largest amount of variation. Passive and active uptake showed a similar pattern for these two parameters, except that for active uptake the less important parameters were even less important in explaining the variation in accumulated leaching after 10,000 years (Figures 12-9A and B; the Spearman coefficient expresses the correlation between the variation in simulated accumulated leaching after 10,000 years and the corresponding variation in the parameter values among 1,000 simulations). The variation in adsorption was, just as for the pine-spruce ecosystems, to a large extent determined by K_d alone, both for passive and active uptake (Figures 12-9 C and D).

For passive uptake, the accumulation in humus was negatively influenced by the discrimination in the soil water flow, but positively by water uptake (Figure 12-10B). The discrimination factors for decomposition also mattered. High positive discrimination in the decomposition process resulted in lower accumulation in humus, *i.e.* when there were losses of C from the humus or litter pools, there were higher relative losses of trace element. A high demand for trace element by leaves had a positive influence on trace element in humus. For active uptake (Figure 12-10A), the adsorption coefficient had a strong negative influence on accumulation in humus and all other parameters became small.

The parameter most strongly influencing the variation in trace element accumulation of the old plant was $TE_{DWaterFlow}$ in the case of passive uptake (Figure 12-10D). Preferential transport of trace element decreased the uptake to the plant. Second most important was the discrimination factor in the root water uptake ($TE_{DWUptake}$). For active uptake (Figure. 12-10C) these parameters were not important and instead the maximum trace element concentrations in stem and leaves influenced trace element of old plant most. High stem concentration was positive for the accumulation, whereas high leaf concentration had a negative influence, as the leaves were dropped every year and trace element transferred to litter.

In summary, the most important parameters in terms of high Spearman coefficient were the adsorption coefficient (K_d), the degree of convective transport ($TE_{DWaterFlow}$) and plant water uptake ($TE_{DWUptake}$), and fractions of plant uptake allocated to leaves (f_{PULeaf}) and stems. The fractions allocated to leaf and stem were in the case of active uptake expressed by maximum concentrations in relation to carbon content ($p_{MaxTECLeaf,}p_{MaxTECStem}$). The adsorption coefficient K_d increased adsorption and decreased leaching, but did not significantly influence organic pools in the case of passive uptake, while it decreased the soil organic pool in the case of active uptake. $TE_{DWaterFlow}$ increased leaching and decreased accumulation

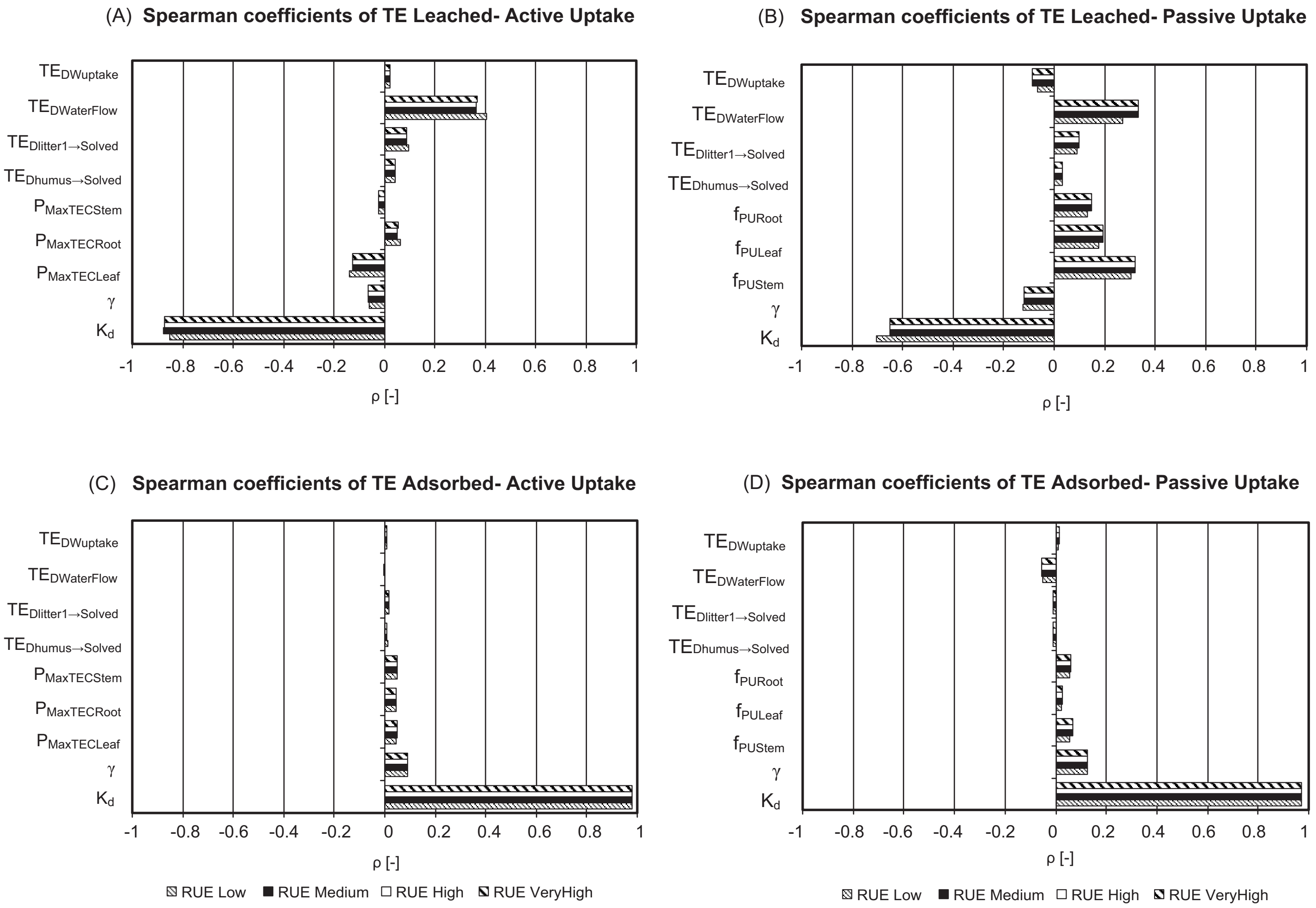


Figure 12-9. *Ranking of parameters in terms of the Spearman coefficient for Leached active (A) and passive uptake (B) and Adsorbed active (C) and passive uptake (D). Bars, from bottom to top, are alder ecosystems with increasing radiation use efficiency (RUE = 1.125, 2.25, 3.375, 4.5 g d.w.* MJ^{-1}*, respectively). Root depth = 1.5 m*

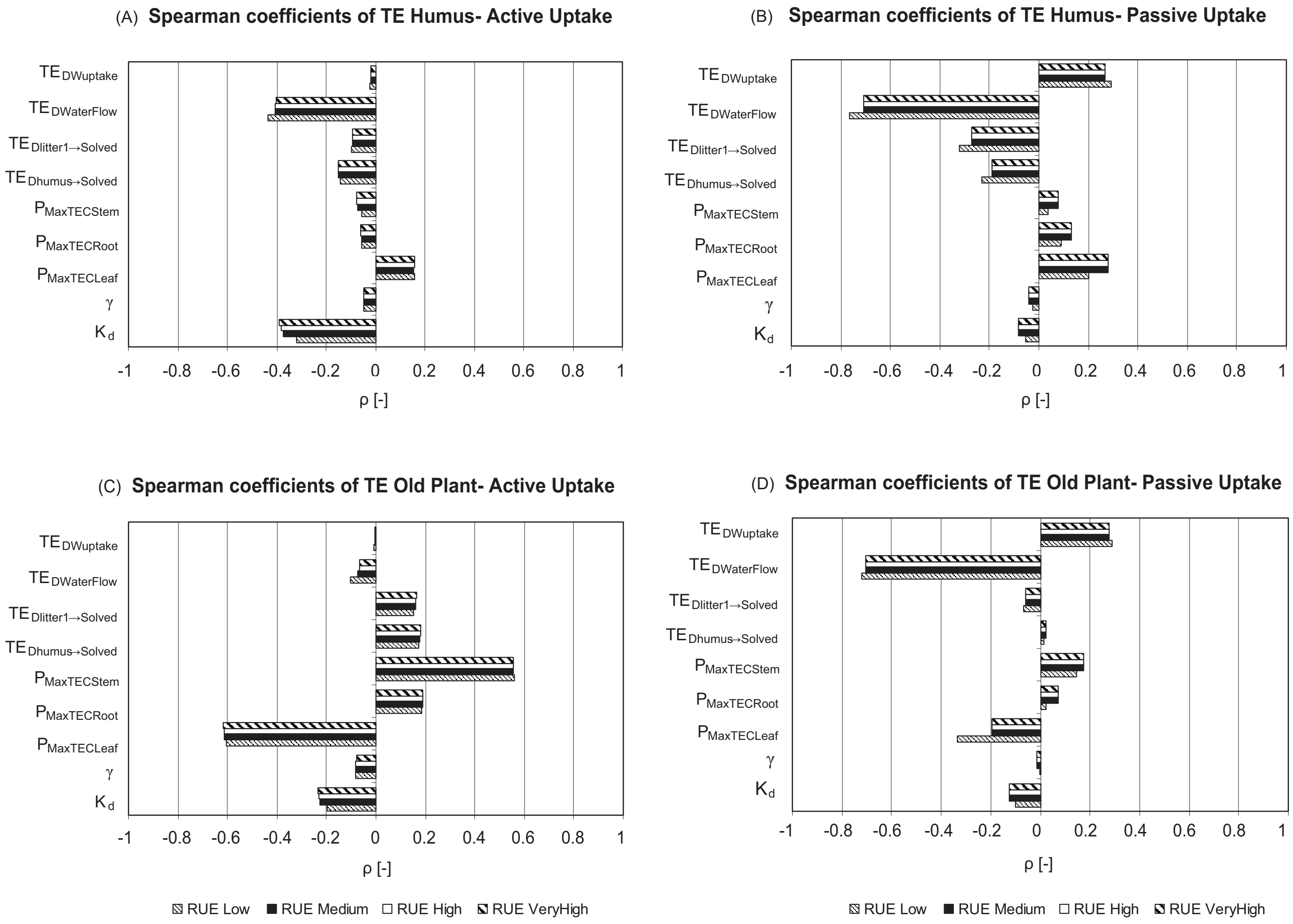


Figure 12-10. *Ranking of parameters in terms of the Spearman coefficients for Humus active (A) and passive uptake (B) and OldPlant active (C) and passive uptake (D). Bars, from bottom to top, are alder ecosystems with increasing radiation use efficiency (RUE = 1.125, 2.25, 3.375, 4.5 g d.w. MJ*$^{-1}$*, respectively and root depth = 1.5 m).*

in organic pools. $TE_{DWUptake}$ increased accumulation in organic pools for passive uptake. For active uptake we would have expected the uptake efficiency ($TE_{BioRate}$, Eq. 3-8) to have a similar effect, but it was not included in the *Eikos* test. Therefore a separate test was carried out, see below. Increased allocation to leaves (f_{PULeaf} and $p_{MaxTECLeaf}$) decreased accumulation in plant and increased it in humus, and in the case of passive uptake it also increased leaching losses. Increased allocation to stem resulted into increased accumulation in plant in the case of active uptake.

A separate test was made regarding how sensitive the accumulation of trace element was to the uptake efficiency (bioavailability $TE_{BioRate}$, Eq. 3-8). In the case of active root uptake, the daily uptake of trace element was proportional to the amount of trace element in soil water, or equal to the plant demand for trace element when the demand was lower than the availability. However, in all cases identified so far the availability of trace element in soil solution was the main limiting factor, and only at low growth rates close to winter and during winter was the demand limiting. The plant ability to take up trace element was determined by the parameter $TE_{BioRate}$ defining the fraction of trace element in soil water that can be taken up per day. Often used values for macronutrients range from 0.01 to 0.2 d^{-1}, *i.e.* 1–20% of trace element in soil solution could be taken up per day. In the reference simulation the 'nominal' value of 0.1 d^{-1} was used. For the reference *CoupModel* simulation and the nominal *Tracey* parameters (Table 9-2), we tested the influence of different uptake efficiencies on the trace element dynamics (Table 12-3).

The accumulation of trace element in organic matter was quite sensitive to $TE_{BioRate}$ and especially the soil organic matter. In the reference case ($TE_{BioRate}$ = 0.1 d^{-1}), one-third of the trace element load was accumulated in soil organic matter, but this fraction was increased to one-half by assuming that the root system was able to take up practically all trace element in soil solution within one day ($TE_{BioRate}$ = 0.8 d^{-1}). Reducing $TE_{BioRate}$ below 0.1 d^{-1} strongly decreased the uptake and at c_{Uptake} equal to 0.01 d^{-1}, which is a value in the lower range estimated for macronutrients /*cf* Eckersten et al. 2007/, the fraction accumulated to soil organic matter decreased to only 3% of accumulated trace element load, and instead trace element was adsorbed to soil particles or stored in soil water. The leached fraction, which was about 0.5%, increased to a few percent. In conclusion, the nominal value chosen for $TE_{BioRate}$ (0.1 d^{-1}) resulted in a high availability. Although the availability could have been even higher, lower values of the uptake efficiency would have influenced the results much more.

Table 12-3. Trace element (% of load) after 10,000 years for different uptake efficiencies of trace element in soil solution. Alder reference *CoupModel* simulation and nominal *Tracey* parameterisation for active uptake were used. (Only one simulation was made for each value; for absolute values see Table A5-1 in Appendix 5).

	$TE_{BioRate}$ (d^{-1})					
Variable	**0.001**	**0.01**	**0.1**	**0.2**	**0.4**	**0.8**
Plant	0.002	0.1	0.7	0.9	1.0	1.1
Organic Soil	0.1	2.8	33.0	40.4	45.4	48.4
Adsorbed & Solution	97.5	94.5	65.7	58.4	53.4	50.5
Leached	2.4	2.7	0.6	0.3	0.2	0.1
Total load	100.0	100.0	100.0	100.0	100.0	100.0

12.7 Single simulations

The variation in the distribution of total load among single simulations of the 1,000 *Eikos* simulations was high. We selected ecosystems with high accumulation rates such as those indicating the occurrence of high maximum or average values in the *Eikos* test (see Table 12-13). The trace element accumulations of each single simulation were plotted (Figure 12-11) against the values of the parameter that had the highest influence according to the Spearman coefficient ranking (see Figure 12-9). The adsorption coefficient (K_d), the discrimination factors for vertical soil water flow between layers ($TE_{DWaterFlow}$) and plant water uptake ($TE_{DWUptake}$), and the soil bulk density (γ) were selected, the latter similarly to the pine-spruce evaluation. It emerged that the passive and the active uptake showed similar patterns and thus in Figure 12-11 only the responses of the passive uptake are presented. Accumulated leaching strongly decreased for increasing values of K_d below about 3 m^3 kg^{-1}, and was most pronounced for low values of $TE_{DWaterFlow}$. Increasing $TE_{DWaterFlow}$ had in general an increasing effect on leaching for all ranges of K_d (Figure 12-11A). Adsorption increased strongly with increasing K_d, especially for high values of γ, and γ had an increasing effect on adsorption, especially for middle range values (around 5 m^3 kg^{-1}) of K_d (Figure 12-11B). The accumulations of trace element in humus and plant were very irregularly related to the parameter values and no general patterns were found, indicating a strong non-linearity of the *Tracey* model response to soil conditions as regards predictions of trace element accumulation in organic matter (Figures 12-11C and D).

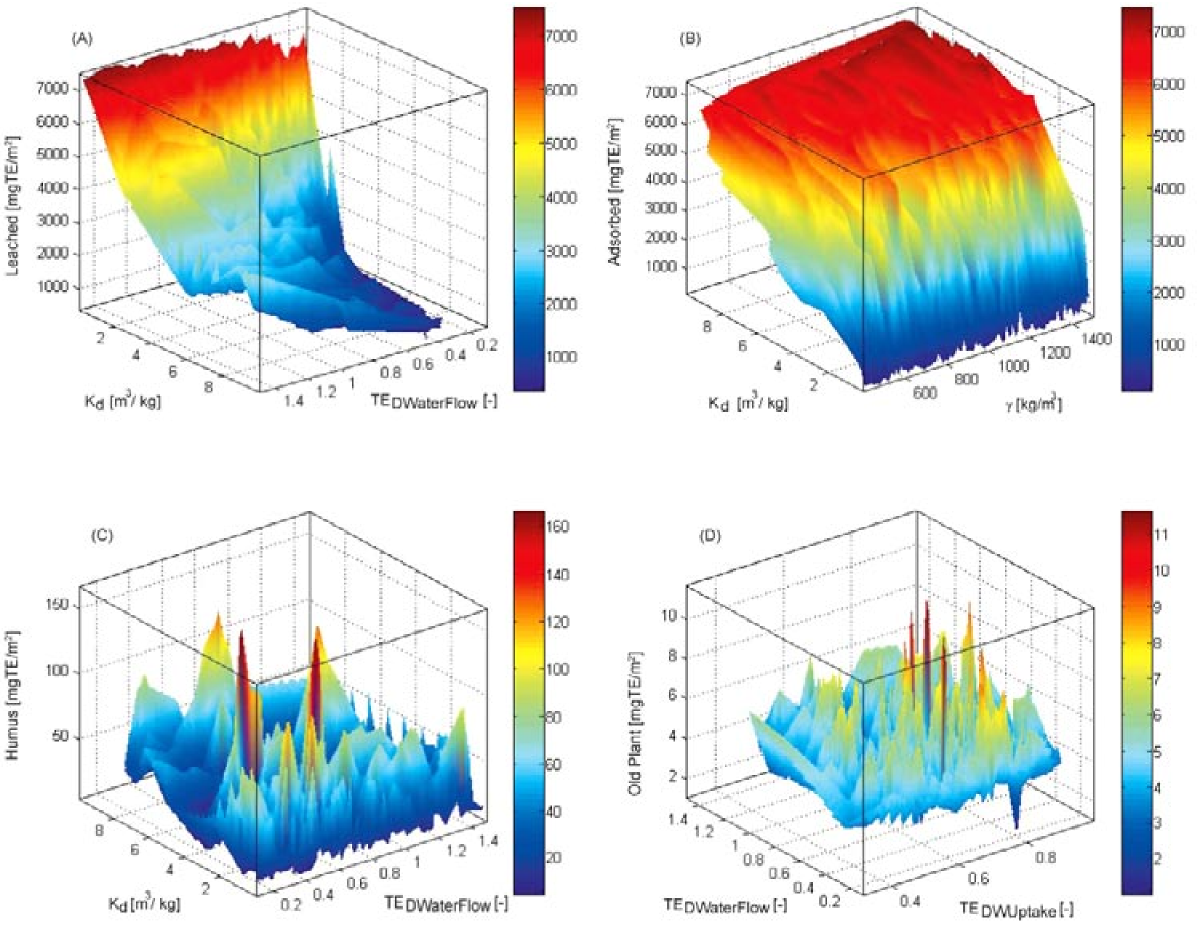


__Figure 12.11.__ Simulated accumulated TE values after 10 000 years versus different parameter values for 1000 Eikos simulations. The ecosystem was: Alder, passive uptake, medium root depth (150 cm) and RUE medium (2.250 g C MJ^{-1}). (A) Leached vs adsorption coefficient K_d & degree of convective water flow TE_{DWFlow}, (B) Adsorbed vs. K_d & soil bulk density γ, (C) Humus vs K_d &TE_{DWFlow} and (D) Old Plant vs. TE_{DWFlow} & discrimination factor for concentration of water uptaken up by plants $TE_{DWUptakee}$

13 Sources of uncertainties

The *Tracey* model includes a large number of sub-models, which involved a risk of mistakes in programming the code. Two such mistakes were discovered concerning the carbon driving variables after the majority of simulations had already been made. To examine the effects on the simulation results and conclusions, a separate test was made comparing simulations made using the corrected model with those presented above in the result Chapters of this report. First, the old root litterfall was erroneously not distributed among soil layers and instead accumulated into the uppermost soil layer. For the alder reference simulation with the nominal parameter values (Table 9-2) this resulted in a small (1–5%) overestimation of the trace element accumulation to plant and soil organic matter, and a small underestimation (0.5%) of trace element adsorbed and in soil solution. The accumulated leaching was only slightly underestimated (1%) in the case of passive root uptake but more markedly underestimated (9%) in the case of active root uptake, although by less than 0.1% of total load.

The second mistake concerned the trace element transfers of C from *Litter1* and *Litter2* to humus and soil water solution, due to decomposition, *i.e.* both humification and mineralisation. The driving variable used for the transfers represented C mineralisation only. However, in the simulations presented in previous Chapters it was assumed that this variable represented decomposition, including the C to be allocated to humus. For this reason the trace element transfer out of *Litter1* and *Litter2* was underestimated, resulting in an overestimation of the trace element accumulation in the litter pools. Compared with the model corrected for both errors, the model used here overestimated trace element accumulation in soil organic matter of the alder reference simulation by 16–46% (mostly for passive uptake), and overestimated trace element in plant by 6% for passive uptake, but underestimated it by 16% for active uptake. The adsorption and accumulated leaching were almost unaffected (–0.13% and –0.05%, respectively) for passive uptake but significantly underestimated for active uptake (6% for the large adsorption pool and 24% for the small accumulated leaching; Table 13-1).

Overall for alder, in relation to total trace element load only the redistribution between adsorption and soil solution on the one hand, and organic matter on the other, were significantly influenced by the mistakes in the model formulation, and only for the cases with active uptake (Table 13-1). For the active uptake there was a significant overestimation of the distribution of trace element to the soil organic matter, but almost no influence on total accumulation of the plant-soil system. The influence of the mistake relating to old root litterfall distribution among soil layers alone had a very small impact on the relative distribution of trace element in the system, as well as on the total accumulation of the system. Concerning passive uptake the effects of the mistakes were small, except that there was a large relative overestimation of trace element in the soil organic matter. However, this was related to the pool being very small.

Table 13-1 Trace element (% of total load) after 10,000 years for two different *Tracey* model versions (Used = used in result Chapters; Corrected = corrected for two errors). The alder reference *CoupModel* simulation and nominal *Tracey* parameterisation were used. (Only one simulation was made for each value).

	Passive uptake		Active uptake	
Variable	**Used**	**Corrected**	**Used**	**Corrected**
Plant	0.02	0.02	0.7	0.9
Organic Soil	0.4	0.3	33.0	28.4
Adsorbed & Solution	97.1	97.2	65.7	70.0
Leached	2.5	2.5	0.6	0.7
Total load	100.0	100.0	100.0	100.0

To examine the influence of the incorrect model formulation not only on the nominal *Tracey* model parameter values but also on the full range of variability in the parameters, the test was also run for 1,000 *Eikos* simulations. This test was made for two pine-spruce ecosystems, one assuming active uptake, a rooting depth of 1 m and a radiation use efficiency of 2.2 g d.w. MJ^{-1}. For each of the 1,000 simulations (*i.e.* different parameter combinations), the incorrect model gave exactly the same accumulated leaching as in the correct model, showing that the total trace element accumulation of the ecosystem was unaffected by the model error (Table 13-2). The same was true for the amount of trace element adsorbed and stored in the soil water. The only changes were in the organic matter. The trace element accumulation in organic matter was small (5.8%) in comparison with the total load, as accumulated leaching accounted for 71% and adsorption plus soil water for almost 23%. Of this 5.8% of total load, less than 10% was stored in soil organic matter and the rest allocated to accumulated harvest. In comparison with the correct model this was a slightly higher fraction of total load allocated to the soil organic matter and slightly lower fraction allocated to harvest. Thus the incorrect model favoured the accumulation to soil organic matter in the pine-spruce simulations, similarly to the results of the alder simulation although much less pronounced, at the expense of trace element accumulated in harvest (compare with Table 13-1). However, the relative overestimation of soil organic matter was high, on average about 40%. The accumulated harvest was on average underestimated only by 2%. The changes in variability within the 1,000 simulations were approximately similar (see further Table 13-2).

A pine-spruce *CoupModel* simulation with passive root uptake was also tested for effects of the incorrect model version on *Eikos* simulations. This *CoupModel* simulation represented an ecosystem with a very deep root depth (120 cm) and radiation use efficiency (2.4 g d.w. MJ^{-1}) compared with that of active uptake. In the 1,000 *Eikos* simulations with the passive uptake, only 0.3% of the trace element load was allocated to organic material (Table 13-2). About 75 % of total load was leached and the rest went to adsorption and storage in soil water (25%). Similarly to active uptake, the incorrect model gave almost exactly the same result as the correct model as concerns the amounts leached, adsorbed and in soil solution, but considerable changes in the amounts of trace element in organic matter. Among trace element allocated to organic matter, only 6% was allocated to soil and the rest to the plant, of which practically all was harvested. The accumulated harvest was overestimated by on average 10%. The very small soil organic trace element pool was overestimated by more than 70% and the variation among the 1,000 simulations increased considerably (Table 13-3).

Overall for alder and pine-spruce, the effect of the errors in the incorrect model on accumulated leaching, and thus total accumulation of trace element of the ecosystem, was zero for alder passive uptake and pine-spruce active uptake and very small for the other two ecosystems. The adsorbed trace element and trace element in soil water were the same for both models for pine-spruce active uptake, whereas for the passive uptake and alder they changed in relation to changes in trace element in the organic matter. However, the changes were usually very small as trace element in the organic matter pools was small in comparison with that in the pools of adsorbed and soil water.

Table 13-2. Trace element (% of total load) after 10,000 years for two different *Tracey* model versions. Averages of 1,000 *Eikos* simulations with pine-spruce *CoupModel* simulation for passive uptake, z_r=1.20 m and *RUE*=2.4 g d.w.MJ^{-1}, and for active uptake, root depth=1.00 m and *RUE*=2.2 g d.w.MJ^{-1}.

	Active uptake		Passive uptake	
Variable	**Used**	**Corrected**	**Used**	**Corrected**
Plant	5.4	5.5	0.3	0.2
Organic Soil	0.4	0.3	0.02	0.01
Adsorbed & Solution	22.9	22.9	25.0	25.0
Leached	71.3	71.3	74.7	74.8
Total load	100.0	100.0	100.0	100.0

For both pine-spruce and alder, the incorrect model greatly overestimated the soil organic matter in relative terms. For pine-spruce it was also shown that the variability increased for trace element in organic matter, especially for passive uptake. The model error thus significantly influenced the trace element content in organic matter in relative terms, but not the distribution between organic matter, adsorption, soil water and accumulated leaching. The alder active uptake simulation formed an exception, as in this case the trace element soil organic pool was overestimated significantly.

Table 13-3. Relative changes (%) in pine-spruce trace element distribution fractions after 10,000 years for the incorrect model in relation to the correct *Tracey* model version. Values are relative changes compared with values given in Table 13-2.

	Active uptake				Passive uptake			
Variable	Mean	StdDev	Min	Max	Mean	StdDev	Min	Max
Plant	–2	+3	–0.5	–0.3	+10	+10	+21	+13
Organic Soil	+41	+39	+30	+21	+78	+118	+47	+144
Adsorbed & Solution	–0.0	–0.0	+0.0	–0.0	–0.0	–0.0	–0.0	–0.0
Leached	+0.0	–0.0	+0.0	–0.0	–0.0	–0.0	–0.0	–0.0
Total load	0	0	0	0	0	0	0	0

14 Discussion

We analysed the importance of various radionuclide properties and ecosystem characteristics for accumulation of radionuclides after 10,000 years of contamination. Two ecosystems with contrasting hydrology were studied, a pine-spruce ecosystem representing hydrological recharge areas and an alder ecosystem representing hydrological discharge areas in a landscape.

Proportion of the contamination accumulated in the ecosystem, where is it stored and importance of uptake approach

The pine-spruce ecosystems accumulated on average 20–25% of the contamination in the soil and the alder ecosystems accumulated on average 20–90% of the total load. Trace element in the soil was predominately found adsorbed below 2 m depth in low-accumulating ecosystems (*i.e.* ≤ 25% of the contaminant was stored in the soil), while it was predominately stored in humus in the upper soil in the high-accumulating ecosystems (i.e. ≥ 75% of the contaminant was stored in the soil). Accumulation in humus in alder systems was stimulated by active plant uptake and increasing root depth. The same trend was seen in the pine-spruce systems, although much less pronounced. The lower effect in the pine-spruce ecosystems can be explained by the lower degree of contamination within the root zone. Pine-spruce roots are only in contact with the contamination source for limited periods and then mainly outside the growing season, when water uptake and growing rate are reduced. It was concluded that the combination of uptake approach and rooting depth influenced the amount accumulated in soil and where it was accumulated, and that the influence was more distinct in ecosystems where the whole rooting zone was contaminated during the growing season.

The accumulation *in* the plant was small, for the pine-spruce a maximum of 0.5% of the contamination and for the alder at most 10%. Even though the total storage *in* plants was small, as discussed above the uptake *by* plants was important for the total accumulation in an ecosystem. Radionuclide would never end up in humus if not first taken up by the plant. It is our understanding that accumulation *in* plants is merely limited by the limited life-time of different plant parts. While the soil accumulated radionuclides over 10,000 years, most of the trace element content in leaves of alder had already returned to the soil as litter after one year. The stem of both forest types had the longest life time and largest biomass of the plant parts and could accumulate most if not limited by the low allocation to stem. Indeed, most of the trace element did accumulate in the stems of pine-spruce ecosystems and as well in the stem of alder ecosystems using active uptake.

In summary, accumulation of radionuclide *in* plants is low, but uptake *by* plants is important for total accumulation in ecosystems. The other factors determining accumulation *by* plants, such as allocation pattern, water uptake rate and growth rate, were included in the sensitivity analysis and are discussed in more detail below.

Proportion of the contaminant lost, how it is lost and circumstances stimulating losses

Pine-spruce ecosystems lost on average 70–80% of the contaminant by leaching and alder ecosystems 10–90%. Leaching was highest for the ecosystems with passive uptake and shallow roots. Leaching from the pine-spruce ecosystem occurred all the time, but especially during the regeneration phase of the forest when plant biomass was small, and thus the plant capacity to take up water and solutes was reduced, and at the same time water drainage flow high.

Losses by harvest were in general small, at most 10% of the contaminant for forest types with active uptake and deep roots. The pine-spruce ecosystems that lost more by harvest lost less by leaching, so that the total losses of the pine-spruce forests varied little. However if there had been no harvest, accumulation in the soil might have been somewhat higher for pine-spruce ecosystems with active uptake. Today, there seems to be a revived interest in bio-energy from forest, which would mean increased harvest of twigs and increased losses of radionuclides by harvest compared with the conventional harvesting assumed in our study. We found that the plant uptake approach, passive or active uptake, and root depth interacted and influenced not only the distribution of trace element within the soil, but also the percentage lost by leaching. This was most pronounced in the alder ecosystem, where the whole root zone was contaminated.

Most important radionuclide properties and ecosystem characteristics for accumulation and losses

The adsorption coefficient K_d, was the single most important factor for the low-accumulating systems, the alder passive uptake and pine-spruce ecosystems. This is understandable as in these systems trace element is predominately found adsorbed in deeper soil layers. Absorption was stimulated by an adsorption coefficient of ≥ 4 $m^3 kg^{-1}$ in combination with a soil bulk density of ≥ 1,000 kg m^{-3}. This is because mineral soils with high soil bulk density enhances adsorption capacity.

The degree of convective transport $TE_{DWaterFlow}$ in combination with high adsorption coefficient could also stimulate adsorption, but this relationship is not monotonic, as both a $TE_{DWaterFlow}$ less than 0.6 and a $TE_{DWaterFlow}$ equal to 1.4 stimulated adsorption. Low $TE_{DWaterFlow}$ is the most important factor and it can be expected to stimulate adsorption in the contamination layer. The trace element is adsorbed to soil particles before it can be washed out. In the case of a $TE_{DWaterFlow}$ higher than one, i.e. preferential transport, the increased adsorption can be explained by amounts of trace element being quickly transported to other soil layers with high adsorption capacity, to be adsorbed there.

In the high-accumulating systems, alder with active uptake and deep roots, most of the trace element is stored as humus. In these systems, the determining factor is the competition for trace elements between plants and adsorbing particles. A low degree of convection $TE_{DWaterFlow}$ and low adsorption capacity favoured high uptake by plants and accumulation in humus.

In summary, adsorption coefficient is by far the single most important factor. High adsorption coefficient increases accumulation. When competition by plants for trace elements is high, a low degree of convective transport $TE_{DWaterFlow}$ in combination with low adsorption capacity favours high uptake by plants and accumulation in humus.

Evaluation of the degree of complexity of Tracey model

Within this project, we developed the dynamic trace element multi-compartmental model *Tracey*, which describes the main processes determining the fate of a trace element in the soil-plant system. We established links to the dynamic carbon-water flux model *CoupModel* and the sensitivity simulation toolbox *Eikos*. *Tracey* has the advantage that the soil can be divided into different layers such that a realistic root uptake distribution and groundwater fluctuations are modelled, two features that are very important for risk assessments of contaminants in the soil-plant system. /Skagg et al. 2007/ showed that accumulation within an ecosystem can be overestimated as much as two-fold when using a one-compartmental soil model. This is in agreement with the differences in results we found for the pine-spruce and the alder ecosystem. The alder can be compared with a one-compartmental soil model as the whole root zone is contaminated, while the pine-spruce ecosystems were only contaminated in the saturated zone.

We also showed that peaks in leaching were highly episodic and related to the daily dynamics in water drainage. We concluded that use of multi-compartments soil model and the time resolution of the driving variables were relevant for the objectives of this study.

We made a simplification in the description of trace element uptake by plants. In reality, plants take up trace elements passively and at the same time actively to various degrees. In the model, plants take up trace element either passively *or* actively. We made this simplification as we only know the sum of both pathways from the content of macronutrients in different plant parts. If instead we had modelled active uptake to take place in addition to passive uptake, we would have been forced to make an estimation of the contribution of passive uptake to total uptake in advance, whereas in fact it was one of our objectives to analyse the potential contribution of passive plant uptake. A more sophisticated model can only be validated when more knowledge is available about the degree to which radionuclides are taken up actively. We simply state this simplification explicitly to avoid any possible misinterpretation.

The dispersion-convection process is known to be a very important transport process when explaining actual distribution of solutes in a soil. /Kirchner 1998/ warns that multi-compartmental soil models can overestimate transport of radionuclides, if dispersion-convection is not taken into account. In this model, it is described very simplistically by multiplying water flow by only one discrimination parameter $TE_{DWaterFlow}$, which may be the appropriate level for a sensitivity analysis like this study. When *Tracey* is being used to explain the actual occurrence of different radionuclides in an ecosystem, we anticipate that this approach might be too simplistic. /Buddemeier and Hunt 1988, Marley et al. 1993/ showed that some radionuclides are predominately transported by forming colloids with dissolved organic carbon. We would like to suggest for applications of *Tracey* on actual occurrence of different radionuclides a comparison of different approaches describing dispersion-convection and the inclusion of dissolved organic carbon as a driving variable, which very conveniently can be simulated by *CoupModel*.

The linear description of adsorption used in the *Tracey* model is appropriate when contamination levels are low or the simulation period not too long, as in this study, since otherwise this process also might need to be more sophisticated described.

Uncertainties

The model applications of this time horizon cannot be validated. Instead, its reliability is based on the model's mechanistic approach and the assumptions that the trace element flows are in proportion to the carbon and water flows and that trace elements do not influence the carbon and water flows. We evaluated the influence of these assumptions indirectly by means of a comprehensive sensitivity analysis of parameters relating the trace element flows to the carbon and water flows for a large number of alternative ecosystems representing a large variation in carbon and water dynamics. Nevertheless, there are plenty of reasons for validation of the *Tracey* model. It should be tested for its suitability to model measured dynamic of trace elements for short-term simulations. The uncertainty in the simulation results can only be assessed by performing comparisons between modelled and measured dynamics.

Another uncertainty was introduced due to mistakes in the model formulation, although these apparently had no significant influence on the total fraction of trace element load accumulated in the ecosystem. However, for alder the model seemed to have overestimated the amount of trace element accumulated in humus instead of being adsorbed, by as much as 15% in one simulation. For the distribution of trace element between soil organic matter and plant the error seemed to be greater, and re-simulations would be preferred for more for comprehensive analyses of these parts.

We tested adsorption coefficient and soil bulk density as two separate factors, while in fact adsorption coefficient is related to soil bulk density. High adsorption coefficients are found both for soils with very low soil bulk densities (*i.e.* organic soils) and for soils with very high soil bulk densities (*i.e.* mineral soils with high clay content). In performing Monte-Carlo simulations with 1,000 combinations of parameter settings it is difficult to completely avoid unrealistic parameter combinations, but we tried to limit their number by Latin hypercube sampling.

Possibilities for future applications

The *Tracey* model has great potential in risk assessment studies of hypothetical contaminants, as in this study, and of actual contaminants. *Tracey* can be applied to all kinds of waste deposits, from municipal waste to residual nuclear waste. There are other situations where *Tracey* can make a useful contribution to predicting more accurately the transport and accumulation of radionuclides. *Tracey* could be used to analyse how different processes govern naturally-occurring radionuclides in various ecosystems. Understanding today's abundance of various radionuclides in different soil layers and plant compartments and being able to reconstruct past fluxes of radionuclides would certainly lead us further in predicting more accurately what might happen in the event of a groundwater contamination.

15 Acknowledgements

We wish to acknowledge Ulrik Kautsky for fruitful discussions during the whole project. Heljä-Sysko Helmisaari provided unpublished data of plant uptake of various elements. Anders Löfgren provided data of Forsmark forest management. Peter Roberntz made the illustration of the spruce tree and Rose-Marie Rytter the illustration of the landscape with pine-spruce and alder ecosystems. Lund University provided computer facilities. Mary McAfee checked the language. Swedish Nuclear Fuel and Waste Management Co. (SKB) funded the project. All are kindly acknowledged.

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Appendix 1

Definitions of abbreviations, functional forest types and soil layers

Table A1-1. Definitions of abbreviations.

Symbol or abbreviation	Description	Units	Equation no.
γ	Soil bulk density	kg m^{-3}	16
AU	Active uptake	–	
f_{PUSeed}	Specific allocation fraction for seed using PU	%	4
f_{PULeaf}	Specific allocation fraction for leaf using PU	%	4
f_{PURoot}	Specific allocation fraction for root using PU	%	4
f_{PUStem}	Specific allocation fraction for stem using PU	%	4
K_d	Soil adsorption coefficient	M^3 kg^{-1}	16
LHS	Latin hypercube sampling	–	
$p_{MaxTECSeed}$	Maximum concentration of *TE* allocated to seed using AU	mg TE g^{-1} C	6
$p_{MaxTECleaf}$	Maximum concentration of *TE* allocated to leaf using AU	mg TE g^{-1} C	6
$p_{MaxTECRoot}$	Maximum concentration of *TE* allocated to root using AU	mg TE g^{-1} C	6
$p_{MaxTECStem}$	Maximum concentration of *TE* allocated to stem using AU	mg TE g^{-1} C	6
PU	Passive uptake		
q_{Drain}	Water flux lost by drainage	mm day^{-1}	18a
q_{Perc}	Water flux lost by percolation	mm day^{-1}	18b
$q_{WaterFlow}$	Water flow from one layer to another layer	mm day^{-1}	17
q_{TEIn}	Daily addition of contamination	mg TE m^{-2} day^{-1}	1
q_{TEout}	Daily loss of contamination	mg TE m^{-2} day^{-1}	1
RUE	Radiation use efficiency	g d.w. MJ^{-1}	
$SRCC$	Spearman Rank Correlation Coefficient	–	
TE	Trace element		
$TE_{Adsorbed}$	TE in adsorbed pool	mg TE m^{-2}	16–17
$TE_{BioRate}$	The *TE* bioavailability, fraction of the trace element the plant can take up in one day	day^{-1}	8
$TE_{DHumus\rightarrow Solved}$	Discriminating factor for the decomposition of humus	–	14c
$TE_{DLitter1\rightarrow Solved}$	Discriminating factor for the decomposition of fine litter	–	14a
$TE_{DWaterFlow}$	Degree of convective transport	–	18
$TE_{DWUptake}$	Discriminating factor for plant water uptake	–	2
TE_{Seed}	TE in seed	mg *TE* m^{-2}	5 (PU) or 9 (AU)
$TE_{Harvest}$	Accumulated *TE* lost through harvest	mg *TE* m^{-2}	20
TE_{Humus}	TE in humus	mg *TE* m^{-2}	13
TE_{In}	Accumulated load of *TE*	mg *TE* m^{-2}	1
$TE_{Leached}$	Accumulated *TE* lost through leaching	mg *TE* m^{-2}	19
TE_{Litter}	TE as the sum of $TE_{Litter1}$ and $TE_{Litter2}$ pools	mg *TE* m^{-2}	12
$TE_{Litter1}$	TE in fine litter	mg *TE* m^{-2}	12
$TE_{Litter2}$	TE in coarse litter	mg *TE* m^{-2}	12
$TE_{OldLeaf}$	TE in old leaf pool	mg *TE* m^{-2}	
$TE_{OldPlant}$	TE in old plant pools	mg *TE* m^{-2}	
$TE_{OldRoot}$	TE in old root pool	mg *TE* m^{-2}	
$TE_{OldStem}$	TE in old stem pool	mg *TE* m^{-2}	

Symbol or abbreviations	Description	Unit	Equation no.
TE_{Plant}	TE in plant as the sum of young and old plant pools	mg TE m^{-2}	
TE_{Soil}	TE in soil as the sum of all soil pools (Litter, Humus, Adsorbed, Solved) from all soil layers	mg TE m^{-2}	
TE_{Solved}	TE in solved pool	mg TE m^{-2}	16–17
$TE_{YoungLeaf}$	TE in young leaf pool	mg TE m^{-2}	5 (PU) or 9 (AU)
$TE_{YoungPlant}$	TE in young plant tissues	mg TE m^{-2}	5 (PU) or 9 (AU)
$TE_{YoungRoot}$	TE in young root pool	mg TE m^{-2}	5 (PU) or 9 (AU)
$TE_{YoungStem}$	TE in young stem pool	mg TE m^{-2}	5 (PU) or 9 (AU)

Table A1-.2. Root depths and radiation use efficiency for the different pine-spruce and alder varieties and their nomenclature.

Ecosystem	Root depth, R (cm)		Radiation Use efficiency, RUE, (g d.w. MJ^{-1})	
Pine-spruce	Shallow	60	Low	1.8
	Medium	80	Medium	2.0
	Deep	100	High	2.2
	VeryDeep	120	VeryHigh	2.4
Alder	Shallow	50	Low	1.125
	Medium	150	Medium	2.250
	Deep	250	High	3.375
			VeryHigh	4.500

Table A1-3. Definitions of soil layers in *CoupModel* and *Tracey.*

	Pine-Spruce (cm)	Alder (cm)
Layer 1	0–5	0–5
Layer 2	5–15	5–15
Layer 3	15–25	15–25
Layer 4	25–45	25–35
Layer 5	45–55	35–50
Layer 6	55–80	50–70
Layer 7	80–130	70–90
Layer 8	130–200	90–110
Layer 9	200–300	110–170
Layer 10	300–400	170–290

Appendix 2

Guide to performing Tracey-Eikos simulations

The following text and scheme are a guide to how to install files and how to simulate with *Tracey* and *Eikos*. This version model of *Tracey* is written in Matlab/Simulink and uses interfaces from where many different selections are possible. If a selection has been made, as for example, loading a parameter setting, an internal command string will be given in the Matlab Command Window, "fm_red". This line will then correspond to an executed and performed task (*i.e.* fm_ RED = ready).

First to install the farm menu system (*Tracey* model menu):

A: Copy to C:\Matlab71\WORK-directory: farm.m, farm_skb.m, farmskb.m

B: Change in the files to the drive you will run the application on (c is used below)

C: Create Application directory: c:\simulink\farm_skb\farmskb\submexe\spruce

D: In Directory c:\simulink\farm_skb\farmskb
-Unfold the following file: af_skb_dirstucture.zip, and then
-Unfold af_skb.zip, af_skb_tmp.zip, af_skb_*Eikos*.zip, af_skb_out.zip

E: In Directory c:\simulink\farm_skb\farmskb\submexe
-Unfold af_skb_exe_spruce.zip

Second:
Stop all automatic shut down or updates that include restart.

Third:
When you have started Matlab (after point 2 below), set path to: c:\simulink*Eikos*\ and subdirectories (File(set path(add with folders(Save)

1. Unzip the files and copy files into directive (folder).

C:\Simulink\FARM_SKB\FARMSKB\SUBMEXE\SPRUCE

The zipped file is named AR120RUE24.zip or AR120RUE22.zip. The zipped files contain a folder with files:

- Mat-files: *CoupModel* Driving variables of water and C fluxes
- tmp_run.mdl (*Tracey*)
- LI_RN: (Library for this *Tracey* model)
- AUSpruce_Param_070808.txt: Parameter settings in *Eikos*
- fm_param.m: Parameters settings for *Tracey*
- *Eikos_CoupModel*.m: M-file for creating ESA
- Nomenclature Spruce variables 070808.doc

All of these files must be placed in the above-mentioned directive.

2. Start Matlab R2007a and change Matlab current directory to C:/
3. Type “**farm**” in Matlab Command Window. An interface appears and **press buttons as follows.**
4. “**Farm_SKB**”
5. “**FARMSKB**”
6. “**RUN MODEL**”
7. “**SPRUCE**”: now a big red interface appears named fm_exe.
8. “**Edit**”: Edit fm_param.m, for instance set values of SWACTIVE and SWACTIVESOIL switches.
9. **“Load param”** (by pressing load button on the interface named fm_exe).
10. **“Open tmp_run.mdl”**, by click button.
11. Select and click on “**Simulation**” in the upper left corner.
12. Mark and click on “**Configuration Parameters**”, a new window appears.
13. Click on “**Build**”. This building procedure takes about 2–3 minutes. When building is done the following text appears in the Matlab Command Window.

    ```
    …
    ** Created executable: tmp_run.exe
    ### Successful completion of Real-Time Workshop build procedure for model: tmp_run
    >>
    ```

    Close “**Configuration Parameters”** window by clicking **OK.**
    Close model.
14. Click on “**run tmp_run.EXE + load**”. This takes about 10 minutes and it’s about time for a coffee. When the EXE-file is finished, the Command Window will state: fm_ RED
15. “**Edit**”: Edit *Eikos_CoupModel*.m so that it is similar to fm_param.m.
16. Click on “**eikos2, eikos_*CoupModel*_run**” and now the creation of ESA-file takes place and when this is done the following text appears in the Matlab Command Window. fm_RED

    An *Eikos* interface named *Eikos* v.2-Simulation Toolbox for Sensitivity Analysis is now displayed. It takes some minutes before you can continue (look at busy in lower left corner of Matlab).
17. **File\Load Assessment:** The next step is to load the previously made ESA-file (from step 14). This is done by clicking on “**File**” in the upper left corner and then “**Load Assessment…**” and choosing file named.
    Eikos_CoupModel.esa
18. **File\Import Parameters:** Buttons in the *Eikos* interface lighten up, that is “**Select model**” and “**Parameters(Outputs**”. But instead of selecting which parameters and so on, we can import the Parameter settings by clicking on “**File**” and select “**Import Parameters…**”
19. Select following file: ASpruce_Param_070808.txt and click on “**Open**” and now a little window appears and states:
    Updated 35 Parameters
    Click on “**OK**”.
20. Click on “**Parameters\Outputs**” and mark all (21) output variables in the lower left corner then **“>>”**, and finally “**OK**”.
21. Click “**Select SA Method**” and mark “**Probabilistic**” in the new interface named *Sensitivity Analysis Method*.
22. Click on “**Method Settings**” and yet another interface appears. Here, type 1,000 in the *Number of iterations* and click on “**Latin Hypercube Sampling**” and finally “**OK**”.
23. Then this interface will disappear and click “**OK**” in the interface named *Sensitivity Analysis Method*.

24. Click on “**Generate Sample**” and now 1,000 samplings of each *Tracey* parameter will be made.

25. In order to save each iteration/sample write in Matlab Command Window:

    global indexIterator < press enter>
    indexIterator = 1; < press enter>

    This procedure will save each sample as a Matlab data file (for example tmp_run1.mat) where each selected output is stored for the selected time steps. A simulation of 1,000 samplings will give the amount of data files (i.e. tmp_run1.mat,…,tmp_run1000.mat).

26. Go back to *Eikos* interface and press “**Simulate**”.

27. Now a little window appears and this will now indicate how many samplings are made and the estimated time of the whole simulation.

28. When the simulation is done (after ~194 hours), the little window is gone and then press “**Compute Results**”.

29. **File\Export to File:** Now it is possible to view results in the *Eikos* interface but we also want to save results together with the ESA-file. So now go to “**File**” and select “**Export to File**”.

30. Create or use the unzipped folder: “AR120RUE24”

31. Click on “**All Info**” and click on “**Export**”. Save it under the scenario name, for example AR120RUE24.xls. Save the file in folder “AR120RUE24”

    <u>**NB!** Set the type of format from txt to **xls** in the “**Save as Type”.**</u>

32. Click on “**Save**” and hopefully a little window appears stating:
    Successfully exported to *.xls

where * means the name of the file. Click “**OK**” and then “**Close**”

33. **File/Save Assessment:** In order to save this ESA-file, go to “**File**” and “**Save Assessment**”. Save under scenario name, for example AR120RUE24.esa.

34. **Quit *Eikos* and Exit Matlab**

35. <u>**Collect result files:**</u> Now we are done with *EIKOS* and we can view all Matlab files of the 1,000 samplings. These are named tmp_run1.mat, tmp_run2.mat,…., tmp_run1000.mat. The files are found in the same directory. Create a new folder named “simres” and copy or move these files into the new folder. The “simres” folder can then be moved into the “AR120RUE24” folder. Store to the directory also some files that documents the simulations: tmp_run.mdl, li_RN.mdl, fm_param.m, *Eikos_CoupModel*.m, ASpruce_Param_070808.txt.

The end!

Appendix 3

Command-line arguments

A command-line interface has been implemented in *CoupModel* that makes it possible to run *CoupModel* and modify parameter values and model settings without invoking the graphical user interface. This command-line interface makes it possible to run *CoupModel* directly from any programme such as *Eikos* or *Tracey* and facilitates efficient sensitivity or model calibration exercises.

The command-line interface to *CoupModel* is based on a number of command-line arguments defined below. The most fundamental command-line argument is the path and name of a so-called sim-file, which is a binary file containing all information needed to execute a simulation with *CoupModel*. This file has a binary format and can only be created using the ordinary graphical user interface of *CoupModel*. The sim-file could be a base-simulation of a specific system, and the command-line model is a practical way to control variations of this base-simulation in terms of specific parameter values, model structures, or inputs. Another important command-line argument is thus the name and path of an ASCII text file, containing parameter values and model settings that should be changed compared with the content of the specified sim-file.

The syntax of the command line mode of *CoupModel* is:

CoupModel [/R] [/S] [/Q] [/N] runid [/P] parfile [/F] simfile

where the meaning of the optional flags are:

/R	Run the simulation (a new document with an updated run-number will be created if the sim-file has already been running).
/S	Save sim-files after simulation.
/Q	Exit application after executing command-line arguments.
/N	Indicates the position of the simulation run number in the command-line.
/P	Indicates the position of the parameter ASCII file in the command-line.
/F	Indicates the position of the *.sim file in the command-line and where:

runid	prescribed simulation run number to be used in the present simulation,
parfile	specifies the path to the ASCII -file with additional parameter values and model settings,
simfile	specifies the path to the *.sim-file to be opened.

If no optional flags are present in the command line arguments, the sim-file specified by filename will be opened in the usual way. The ASCII text file with parameter values should be formated in the following way:

Groupname;Parametername;Parametervalues;index

where the last variable *index* indicates which type of model input according to the following list:

0 represents parameters that do not have model layer index or plant layer index

>0 represents indexes in parameter tables related to soil layers, or multiple plants

-1 represents model switches

-2 represents file names

Group names and Parameter names should be specified according to the internal *CoupModel* convention, and can be found either by using the *CoupModel* interface, or by the summary output files. See further details in /Jansson and Karlberg 2004/.

Appendix 4

Plant, soil, accumulated leached and harvest – average, StD, median, min and max of all iterations for Pine-Spruce scenarios

	Active Uptake											
Roots	**Shallow**				**Medium**				**Deep**			
RUE	**Low**	**Medium**	**High**	**Very high**	**Low**	**Medium**	**High**	**Very high**	**Low**	**Medium**	**High**	**Very high**
TE_{Plant}												
Average	0.318	0.279	0.235	0.212	0.317	0.277	0.235	0.215	5.077	4.725	4.452	4.274
STD	0.123	0.106	0.090	0.081	0.122	0.105	0.090	0.082	1.860	1.723	1.625	1.561
Median	0.286	0.250	0.210	0.190	0.284	0.248	0.210	0.192	4.503	4.194	3.942	3.779
Min	0.041	0.036	0.031	0.028	0.043	0.037	0.032	0.029	0.663	0.617	0.581	0.556
Max	1.169	1.016	0.865	0.778	1.167	1.013	0.867	0.789	18.298	16.923	15.973	15.334
TE_{Soil}												
Average	1,779	1,833	1,873	1,908	1,792	1,843	1,888	1,919	1,743	1,812	1,870	1,910
STD	2,324	2,364	2,393	2,418	2,334	2,372	2,403	2,426	2,217	2,272	2,316	2,346
Median	440	470	493	514	447	476	502	521	487	522	555	578
Min	2	2	2	2	2	2	2	2	9	9	9	9
Max	7,520	7,553	7,577	7,596	7,527	7,558	7,585	7,602	7,462	7,504	7,536	7,557
$TE_{Harvest}$												
Average	31.19	27.12	22.96	20.58	31.15	26.96	23.00	20.90	492.24	455.93	428.95	410.51
STD	6.19	5.32	4.45	3.97	6.01	5.15	4.35	3.94	85.44	78.40	73.21	69.88
Median	33.06	28.71	24.26	21.72	32.98	28.47	24.24	22.03	519.50	480.75	452.49	433.10
Min	1.34	1.24	1.09	1.01	1.43	1.29	1.14	1.06	34.51	33.55	31.50	29.99
Max	38.73	33.60	28.38	25.40	38.39	33.16	28.21	25.63	588.00	543.43	510.26	487.97
$TE_{Leached}$												
Average	6,218	6,168	6,132	6,100	6,205	6,158	6,118	6,088	5,788	5,756	5,725	5,704
STD	2,323	2,364	2,393	2,417	2,333	2,371	2,403	2,425	2,195	2,251	2,296	2,326
Median	7,559	7,533	7,514	7,495	7,552	7,527	7,505	7,487	7,064	7,058	7,048	7,043
Min	475	446	426	410	467	441	419	404	431	400	376	361
Max	8,015	8,016	8,017	8,018	8,014	8,016	8,017	8,018	7,735	7,748	7,758	7,764

Roots shallow=60 cm, medium=80 cm, deep=100 cm and very deep=120 cm respectively while RUElow =1.8, RUEmedium=2.0, RUEhigh=2.2 and RUEVeryhigh =2.4 g d.w. MJ^{-1} respectively.

Plant, soil, accumulated leached and harvest – average, StD, median, min and max of all iterations for all Pine-Spruce forest functional types (continuation from previous page)

	Active uptake			**Passive Uptake**						
Roots	**Very deep**			**Shallow**				**Very deep**		
RUE	**Medium**	**High**	**Very high**	**Low**	**Medium**	**High**	**Very high**	**Medium**	**high**	**Very high**
TE_{Plant}										
Average	4.693	4.451	4.262	0.009	0.011	0.011	0.011	0.118	0.144	0.167
STD	1.706	1.626	1.556	0.009	0.010	0.010	0.010	0.114	0.137	0.156
Median	4.163	3.934	3.767	0.007	0.008	0.008	0.009	0.088	0.108	0.126
Min	0.629	0.596	0.568	0.000	0.000	0.000	0.000	0.002	0.003	0.003
Max	16.795	16.055	15.305	0.072	0.080	0.080	0.088	1.067	1.405	1.686
TE_{Soil}										
Average	1,821	1,873	1,915	1,797	1,851	1,891	1,925	1,916	1,966	2,006
STD	2,279	2,318	2,349	2,341	2,379	2,406	2,429	2,422	2,454	2,480
Median	527	557	581	410	437	459	479	474	504	529
Min	9	9	9	3	3	3	3	4	4	4
Max	7,509	7,537	7,559	7,659	7,682	7,697	7,710	7,707	7,725	7,738
$TE_{Harvest}$										
Average	453.18	429.33	409.80	1.18	1.38	1.41	1.46	15.05	18.11	20.82
STD	76.84	72.26	68.91	1.14	1.31	1.31	1.33	14.89	17.57	19.83
Median	477.86	452.67	432.03	0.87	1.03	1.06	1.11	11.00	13.19	15.34
Min	34.42	32.42	30.79	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Max	537.96	508.61	485.38	9.72	10.93	10.66	10.62	141.61	160.33	173.54
$TE_{Leached}$										
Average	5,749	5,722	5,699	6,230	6,176	6,136	6,102	6,097	6,044	6,001
STD	2,258	2,298	2,330	2,341	2,379	2,406	2,429	2,419	2,451	2,476
Median	7,055	7,046	7,041	7,616	7,587	7,565	7,546	7,537	7,504	7,477
Min	396	375	358	369	346	331	318	320	302	288
Max	7,742	7,752	7,760	8,026	8,026	8,025	8,025	8,024	8,024	8,023

Roots shallow=60 cm, medium=80 cm, deep=100 cm and very deep=120 cm respectively while RUElow =1.8, RUEmedium=2.0, RUEhigh=2.2 and RUEVeryhigh =2.4 g d.w. MJ^{-1} respectively.

Appendix 5

Alder and uncertainty

Table A5-1. Trace element (mg m^{-2}) after 1,000 and 10,000 years for different uptake efficiency of trace element in soil solution, Active uptake.

		$TE_{BioRate}$ (d^{-1})					
Variable	**Year**	**0.001**	**0.01**	**0.1**	**0.2**	**0.4**	**0.8**
Total Plant	10,000	0.20	4.9	58	71	79	85
Total Organic Soil	10,000	7.2	222	2,652	3,248	3,649	3,886
Adsorbed & Solution	10,000	7,828	7,588	5,275	4,687	4,290	4,053
Leached	10,000	195	215	45	24	13	6.7
Total load	10,000	8,030	8,030	8,030	8,030	8,030	8,030
Total Plant	1,000	0.14	1.5	6.8	8.3	9.3	9.9
	max,year	0.20, 9,947	5.1, 9,947	60, 9,961	73, 9,961	81, 9,961	87, 9,961
Total Organic Soil	1,000	5.6	57	272	333	375	401
	max,year	7.7, 3,466	222, 9,946	2,655, 9,979	3,251, 9,979	3,651, 9,979	3,887, 9,979

Contamination level

Table A5-2. Trace element (mg m^{-2}) after 1,000 and 10,000 years for different contamination levels expressed as a fraction of groundwater level, Passive uptake.

		Scale Groundwater level (–)					
Variable	**Year**	**0.01**	**0.2**	**0.4**	**0.5**	**0.6**	**1.0**
Total Plant	10,000	1.7	0.78	0.36	0.12	0.002	0.001
Total Organic Soil	10,000	31.3	14.4	6.65	2.21	0.037	0.024
Adsorbed & Solution	10,000	7,799	7,878	7,943	7,992	8,028	4,442
Leached	10,000	198	137	79.8	35.8	2.09	0.067
Total load	10,000	8,030	8,030	8,030	8,030	8,030	4,442
Total Plant	1,000	1.12	0.55	0.29	0.16	0.03	
	Max	1.96	0.97	0.52	0.26	0.039	
Total Organic Soil	1,000	18.8	9.2	5	2.6	0.52	
	Max	32.9	16	8.5	4.2	0.63	
Total Plant	Maxyear	4,850	4,190	3,590	2,930	1,550	10,000
Total organic soil	Maxyear	5,026	4,366	3,766	3,106	1,726	10,000

Table A5-3. Trace element (mg m^{-2}) after 1,000 and 10,000 years for different contamination levels expressed as a fraction of groundwater level, Active uptake.

		Scale Groundwater level (–)					
Variable	**Year**	**0.01**	**0.2**	**0.4**	**0.5**	**0.6**	**1.0**
Total Plant	10,000	58	42	26	12	1.0	0.096
Total Organic Soil	10,000	2,652	1,902	1,178	530	44	3.49
Adsorbed + Solution	10,000	5,274	6,051	6,803	7,478	7,984	4,438
Leached	10,000	45	36	23	11	0.9	0.04
Total load	10,000	8,030	8,030	8,030	8,030	8,030	4,417
Total Plant	1,000	6.8	5.0	3.3	1.8	0.4	0.001
	max	60,	43	27	12	1.0	–
	year	9,961	9,961	9,961	9,961	9,947	
Total Organic Soil	1,000	272	201	133	71	14	0.035
	max	2,656	1,905	1,180	531	44	–
	year	9,979	9,979	9,979	9,979	9,979	
Variable	**Year**	**0.01**	**0.2**	**0.4**	**0.5**	**0.6**	
Plant Old C	1,000	6.1	4.5	3.0	1.6	0.3	
	max,year	–	–	–	–	–	
	10,000	52.2	37.4	23.2	10.5	0.9	
Soil humus C	1,000	265	196	129	70	14	
	max,year	–	–	–	–	–	
	10,000	2,587	1,855	1,149	517	43	

Uncertainty due to programming

Table A5-4. Trace element (% of total load) after 10,000 years for the correct Tracey model version. Pine CoupModel simulations were used. For passive uptake zr=120 cm and RUE =2.4 g d.w. MJ^{-1} and for active uptake zr=100 cm and RUE =2.2. g d.w. MJ^{-1} Values are averages of 1,000 Eikos simulations.

	Passive uptake				Active uptake			
Variable	**Mean**	**StdDev**	**Min**	**Max**	**Mean**	**StdDev**	**Min**	**Max**
Plant	0.24	0.23	0.00	1.94	5.51	0.88	0.40	6.42
Organic Soil	0.01	0.01	0.00	0.23	0.28	0.28	0.03	2.75
Adsorbed + Solution	24.98	30.90	0.05	96.39	22.90	28.85	0.03	93.82
Leached	74.77	30.85	3.59	99.95	71.31	28.60	4.69	96.65
Total load	100.00	0	100.0	100.0	100.00	0	100.0	100.0

ISSN 1404-0344
CM Gruppen AB, Bromma, 2009