Appendix B Substance-independent data

In this Appendix, the derivation of the spatially-resolved information necessary for the methodological framework is described. The focus is on the spatial information necessary to run the environmental fate model for soil and water, i.e., the spatial differentiation of the continental areas into zones or compartments and the derivation of parameter values varying spatially. However, section B.6 is also dedicated to the exposure as well as to the impact assessment. These follow a spatial differentiation based on administrative units mostly according to the Nomenclature of Territorial Units for Statistics (Nomenclature des Unités Territoriales Statistiques, NUTS) used by the Statistical Office of the European Communities (EUROSTAT).

In the following, first the geographical scope of the external cost assessment methodology is defined (section B.1). Secondly, the spatial differentiation of the 'continental environment' comprising the non-marine environment into zones is presented (section B.2). After the zones have been defined, their constituents namely the compartment entities need to be defined. This will be done separately for the soils and/or land uses on the one hand (section B.3) and freshwater bodies on the other hand (section B.4). In these sections, the dimensions of the different compartments will be defined. What remains to describe are the ways how the other environmental properties including fluxes of water are derived.

Generally, one may distinguish four different kinds of parameters in the spatially-resolved environmental fate model:

1. those that are invariant: such as universal or molar gas constant; a default ambient air temperature
2. those that vary by compartment (and not by zone): erosion rate; fraction of runoff being quick/direct flow; fraction of rain rate being preferential flow; depth (of soils, glaciers and sediment); sedimentation velocity lake; sedimentation velocity stream; sediment resuspension rate lake; sediment resuspension rate stream; net sediment burial rate; sediment burial rate lake;

sediment burial rate stream; volume fraction of sediment, ground water or soil that is solid phase; volume fraction of soil that is gas phase; density of the solid phase (default value); overall mass transfer coefficient diffusion at sediment-water interface; fraction of discharge in lake circulation; density of the organic solid phase; density of the mineral solid phase; density of water; mass fraction of organic carbon (Corg) in organic matter; pH (default values); volume fraction of freshwater that is stagnant water; volume fraction of freshwater that is stagnant water at large river mouth; fraction of sedimentation rate being resuspended; fraction of sedimentation rate finally buried

3. those that vary by region: most hydrology-related data fall into this category such as discharge, runoff, precipitation rate, evapotranspiration rate, temperature, fraction of runoff being quick/direct flow, and fraction of rain rate being preferential flow; furthermore: area of the different zones, area fraction of permeable soils, temperature
4. those that vary by region and compartment: depth (of freshwater bodies and impervious areas), volume (depending on the area of a compartment as the product of the zone, the corresponding compartment's area fraction and the depth), area fraction of a compartment, flow rate of lake water circulation, area fraction of total freshwater sediment lying below stagnant waters, volume fraction of freshwater that is stagnant water; parameters only varying for the different types of soils are density of the solid phase (depending on the organic carbon content), pH and Corg; density of suspended matter; concentration of suspended matter in freshwater bodies.

In section B.5, the spatially variable data of category 3 and 4 for the terrestrial environment as well as the hydrological cycle will be presented.

B.1 Defining the geographical scope of the model

The EcoSense model for stationary sources for Europe (European Commission, 1995; Krewitt et al., 2001) covers most of Europe and small parts of Asia (parts of Turkey) and Africa (parts of Morocco, Algeria, Tunisia and Libya; see Fig. B-1). For consistency reasons, the same geographical coverage is selected.

B.2 Spatial differentiation into zones

In site-dependent modelling, the whole area covered by the model needs to be distinguished into sub-areas. These sub-areas will be called 'zones' in this text.

For the definition of the zones, one has principally to distinguish between two environments: the terrestrial domain and the marine domain.

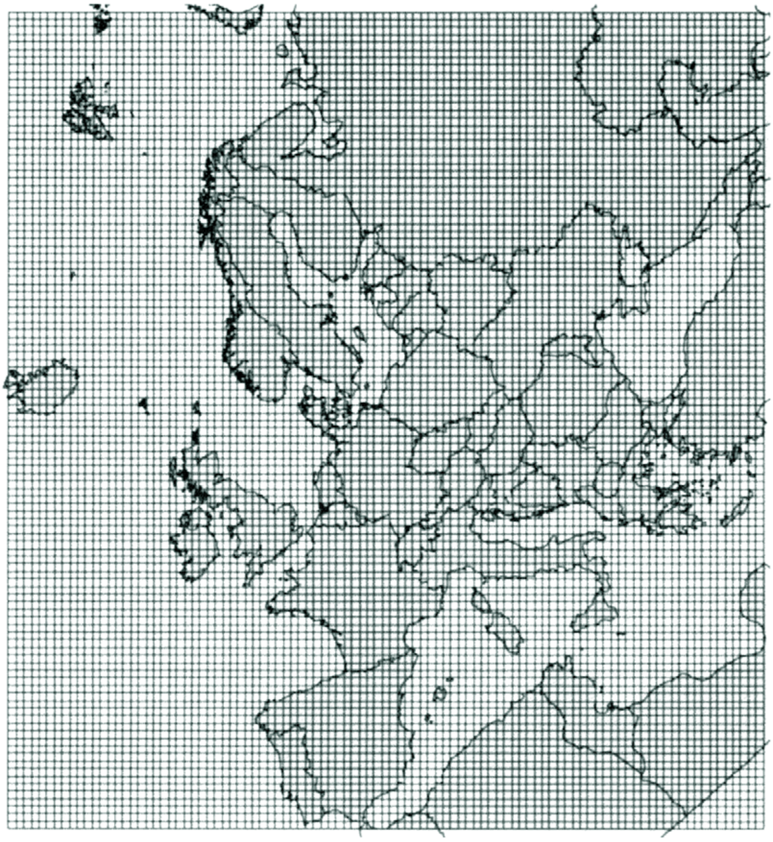

Fig. B-1: Area for which concentrations and depositions are calculated on the EMEP 50 km grid within the single and multi source EcoSense Europe version (European Commission, 1999a; Friedrich and Bickel, 2001a)

For the terrestrial regions to which also rivers, lakes and swamps are counted, the different zones are distinguished according to the drainage basins to which they contribute. These drainage basins were taken from the HYDRO1k geographic database developed at the EROS Data Center (1996). The European basin dataset as well as parts of the Asian and African basin datasets after conversion of their coordinate systems have been used.

The HYDRO1k database consists of topographically derived datasets, including streams, drainage basins and ancillary layers based on the USGS' 30 arc-second digital elevation model of the world (GTOPO30). Within this dataset, the drainage basins are organized following the Pfafstetter code (cf. Verdin, 1997).

This code allows to identify whether and where a zone is situated within a drainage basin. According to this code, each drainage basin of larger rivers is subdivided into nine sub-basins if at least four larger tributaries can be identified. These are coded with even numbers from downstream to upstream. The drainage areas between these basins (called interbasins) assume the respective odd numbers and constitute the main stem of the subdivided river. This procedure can be repeated for each basin and interbasin if again at least four tributaries can be identified. The Pfafstetter code can also be applied starting at the continental level. For Europe, the Rhine catchment, for instance, is identified at the third subdivision level by the code '914' (cf. Fig. 4-4). A further subdivision is also possible at least at the fourth level (as indicated in Fig. 4-4), and for some (inter)basins even below. As a result, the Pfafstetter code allows to identify the connectivities of zones by water currents as provided by the HYDRO1k dataset (EROS Data Center, 1996).[42]

Although a resolution of 1 km^2 is fairly high in a continent-wide analysis, this abstraction might lead to wrong descriptions of the real watersheds (cf. Fekete et al., 2001) and, thus, to the imprecise assessment of the environmental fate of pollutants. Therefore, a qualitative comparison of the drainage basins of the HYDRO1k dataset with the European rivers and catchments database (ERICA Version 1998, European Environment Agency Data Service, 1998) was performed. This database at scale 1:1,000,000 contains over 1500 catchments to river confluences for the largest rivers in the European Environment Agency (EEA) member states. These are located in western Europe (from Portugal through to Germany), Sweden, Greece, parts of Finland, Norway, Italy, England, Ireland and Iceland.

Another comparison was conducted between the HYDRO1k dataset and the Britannica Atlas (Cleveland et al., 1984). In the first place, this was undertaken in order to assign names to the different zones.

The comparison between the HYDRO1k dataset and the other two data sources showed generally good agreement. However, a few significant deviations became obvious which were taken into account (see Table B-1). From these deviations, the assignment of large lakes (with long residence times) to wrong drainage basins was deemed particularly severe. This is especially the case for the Lake Geneva area. However, also further differentiation possibilities have taken into account. Particularly these adaptations may not always result in a subdivision of a (sub-) catchment into 5 interbasins and 4 basins following the Pfafstetter code.

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[42] The Pfafstetter code is to some degree similar to the official German codification of drainage basins which has been in use for some decades already (Länderarbeitsgemeinschaft Wasser (LAWA), 1993).

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Area between Ljusnan (95576) and Indalselven (9556)	Sweden, river mouth near Sundsvall	Upper part of river identified by '95572' is assigned to Indalselven	955660	955723
			955720	955721
Area between Tana-Elv and Muonioelv	Norway, Finland	Correct northern Scandinavian coastal area	957367	357359
			957368	957359
			957369[c]	957359
			957369[c]	954400
Axios/Vardas (91116)	Serbia, Macedonia	Head waters of the southern Morava (tributary to the Danube) falsely assigned to the upper part of the Vardas (tributary to Axios); parts of the (White) Drin falsely assigned to Vardas	911166[c]	838800
			911166[c]	911166
			911169[c]	911169
			911169[c]	911180
Bann (913774)	Ireland, United Kingdom	Adjusting the proper outflow of the Bann river to the sea	913773[c]	913773
			913773[c]	913774
Caspian Sea (02)	Kazakhstan	The lowest region with Pfaffsteter code '021000' falsely located within the Caspian Sea	021000	020300
	Turkey	Tuz gölü lake	355010	355020
			355070	355020
			355080	355020
			355090	355020

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Caspian Sea (02) (continued)	Turkey (continued)	Eber Gü	355040	355060
			355050	355060
		Beysehir Gölü	355061	355040
			355062	355040
			355063	355040
			355064	355040
			355065	355040
			355066	355040
			355067	355040
			355068	355040
			355069	355040
Danube (8)	Germany	Parts of the Danube river falsely assigned to the Neckar river (west) or Main river (north, both tributaries to the Rhine)	914698[c]	899500
			914699[c]	899500
			914760[c]	899900
Dolelv (9558)	Sweden	The main two tributaries which after their confluence build the Dolelv are not well represented	955820	955830
			955830	955820
			955840	955820
			955850	955850
			955860	955850
			955870	955850
			955880	955850
			955890	955850

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Douro/Duero (9118)	Portugal	Parts have not been correctly assigned	911790[c]	911790
			911790[c]	911813
	Spain	Parts were not correctly assigned	911880[c]	911858
			911880[c]	911880
Duna (936)	Russia, Belarus	Subdivision into uppermost tributary and headwaters could not be identified; most of the headwater area (936900) actually belongs to the Dnjepr (see below)	936800	936900
Duna (936), Dnjepr (6)	Russia, Belarus	Most of the headwater area (936900) belongs to the Dnjepr	936900[c]	936900
			936900[c]	662400
Glomma, Glåma (9572)	(mostly) Norway	Upper parts of Glomma river could not be identified to follow disaggregation given by HYDRO1k dataset	957240	957290
			957250	957290
			957260	957290
			957270	957290
			957280	957290
			957290	957250
Guadalquivir (91174)	Spain	Part of the river mouth area falsely assigned to adjacent zone	911739[c]	911739
			911739[c]	911741
Guadiana (91176)	Portugal, Spain	River mouth area is not complete	911750[c]	911741
			911750[c]	911750

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Guadiana (91176) (continued)	Portugal, Spain (continued)	River mouth area is not complete (continued)	911750[c]	911761
			911770[c]	911761
			911770[c]	911770
Kalixälven (95512)	Sweden (border to Finland)	Upper part of the Kalixälven falsely assigned to the Torneälv	954600	955123
			955120	955121
Kemijoki (9538)	Sweden, Finland, Norway	Upper part of the Ounaskjoki (tributary of the Kemijoki) is assigned to the Torneelv	954200[c]	954200
			954200[c]	953810
			954400[c]	953810
			954400[c]	954400
Loire (912)	France	The following tributaries to the Loire had not been distinguished prior to the adjustment: Mayenne and Loie to Sarthe; Creuse to Vienne; Indre	912200[d]	912210
			912200[d]	912220
			912200[d]	912230
			912200[d]	912240
			912200[d]	912250
			912400[d]	912410
			912400[d]	912420
			912400[d]	912430
			912500[d]	912510
			912500[d]	912520
			912500[d]	912530

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Minho/Miño (91192)	Spain, Portugal	Subdivision into one tributary 'Sil' and two interbasins introduced	911920[d]	911921
			911920[d]	911922
			911920[d]	911923
Neva (94), Vuoksi (942)	Finland, Russia	According to HYDRO1k, the Vuoksi river (942) and, hence, the Ladoga lake are not fed by Saimaa lake catchment (952); instead the latter area is supposed to be completely drained by the Saimaa canal to the Gulf of Finland; it is assumed here that hardly any water flow occurs via the Saimaa canal and most of the water from the Saimaa lake catchment flows through the Ladoga lake	942400	942411
			952100	942413
			952210	942421
			952220	942422
			952230	942423
			952240	942423
			952250	942423
			952260	942423
			952270	942423
			952280	942423
			952290	942423
			952300	942430
			952400	942440
			952500	942450
			952600	942460
			952700	942470
			952800	942480
			952900	942490

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Oulujoki (95374)	Finland	Upper part of Oulo river including Oulujärvi lake falsely placed in another zone	953600	953743
			953740	953741
Pasvikelv (95738)	Norway, Finland, Russia	Lower parts including river mouth of Pasvikelv are falsely set to be further east; these areas are assigned to the area in between the new Pasvikelv's lower parts and the Tana-Elv	957384	957383
			957392	957381
			957381	957370
			957382	957370
			957383	957370
Rhine (914)	Germany, France	Moselle, Saar adjustments River mouth of Saar represented by new code: 914421 Saar + Blies + Schwarzbach represented by new code: 914423 Seille represented by new code: 911460	914420	914421
			914460[c]	914423
			914460[c]	914460
	Germany	Lahn is a tributary to the Rhine, there is no closed basin in central Germany	915000	914500
	Netherlands, Germany	Only part of the area belongs to the Vechte	915200[c]	914310
			915200[c]	915200

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Rhine/Meuse (914)	France, Belgium	Parts of the upper Meuse river are assigned to the Oise river, a tributary to the Seine; the Meuse river confluences with the Rhine river (Meuse represented by leading code: 9142)	913245	914293
			913246	914294
			913247	914295
			913248	914296
			913249	914297
			914100	914210
			914290	914291
Rhone (9114)	France, Switzerland	Area around lake Geneve region is falsly assigned to the Rhine catchment	914980	911473
			914990	911475
	France	River mouth is shifted to West	911396[c]	911396
		Durance (tributary to the Rhone river) is partly assigned to the Côte d'Azur coastal area	911396[c]	911420
			911398[c]	911398
			911398[c]	911420
			911399[c]	911399
			911399[c]	911410
			911399[c]	911420
			911399[c]	911510
			911410[c]	911410
			911410[c]	911510

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Rhone (9114) (continued)	France (continued)	Rearrangement of first order sub-basins Ain represented by new code: 911471; in this zone also the main stem of the Rhone river (at least in terms of the name) is situated Saone represented by new code: 911461	911460	911471
			911470	911461
			911480	911462
			911491	911463
			911492	911463
			911493	911463
			911494	911464
			911495	911465
			911496	911466
			911497	911467
			911498	911468
			911499	911469
Scheldt (9134)	Belgium, Netherlands, France	Joining two zones into one	913500	913400
Segre (91162)	Espana	Subdivision into uppermost tributary and headwaters could not be identified	911628	911629
Seine (9132)	France, Belgium	Oise	913242[c]	913243
		Sambre	913242[c]	914270
	France	Joining two zones to identify the Aisne and to distinguish the Oise	913243	913242
			913244	913242

Table B-1: Adjusted representation of catchments as given by the HYDRO1k dataset (EROS Data Center, 1996)

Drainage basin (identification code)	Country or region	Description[a] / tributary	Original code	Adjusted code[b]
Skellefteelv (95518)	Sweden	Upper parts of the Skelleftelv including the Uddjaur lake is falsely assigned to the Vindelelv	955180	955181
			955240	955183
Weser (9158)	Germany	Parts of the Elbe river belong to the Weser	916300[c]	915840
			916440[c]	915840
			916490[c]	915860

a.Note: The way how the Pfafstetter code is employed did not allow a further subdivision of catchments within the HYDRO1k dataset in some cases. Therefore, the HYDRO1k basins should not be considered as incorrect in those cases in which further, partly 'incomplete' subdivisions are introduced in this work (see also footnote b).

b.Note that the adaptations made may not always result in a subdivision of a (sub-) catchment into 5 interbasins and 4 basins following the Pfafstetter code.

c.The zone has only in parts been newly allocated.

d.The whole zone has been further sub-divided.

Two identified irregularities could not be adjusted. One is the Adige river in northern Italy which confluences with the Po river according to the GIS dataset although discharging into the Adriatic Sea in parallel channels. The second is the Kokemäenjoki in southern Finland which partly drains to the Gulf of Finland according to the HYDRO1k dataset.

The areas of the zones were determined from the respective GIS dataset resulting after correction and joining the European, Asian, African and a lake GIS datasets. The derivation of this latter lake dataset is described in the following section.

B.2.1 Definition of large lakes

The lake coverage mentioned above was yielded by taking the geo-datasets on land uses into account presented in section B.3. These were updated by the WELAREM dataset (Lehner and Döll, 2001) where information on the so-called global lakes exist. From this geo-dataset, all water bodies were extracted that are larger than 100 km^2. As mentioned in section B.4.1, these lakes are assumed to have a depth of 74 m.

Some corrections have been made in order for some resulting lakes not to be considered as such. This is because these either do not constitute pure freshwater bodies or do not have a depth as large as 74 m. These are

- the Elbe estuary,
- the bay at the Rügen island,
- the river mouth of the Odra river,
- wetland in southern Finland,
- wetland in northern Denmark and Ringkoebing fjord,
- part of the Mediterranean northwest of Cyprus,
- bay in Tunisia,
- bay in southern France (however keeping the Camarque as wetland with a smaller depth),
- river mouth of the Rhine, and
- bay in northern Ireland.

Some of these larger lakes are fully contained within the zones identified by the HYDRO1k basin dataset (EROS Data Center, 1996; cf. Fig. 6-2). These are only considered in terms of a larger depth. However, many of these lakes spread over different zones. All of these lake portions which are connected by the downstream flow of water constitute separate zones in the proposed methodology (cf. the example of lake Vänern in Fig. 6-2).

B.3 Distinction of different compartments

For the definition of different terrestrial compartments, three sources have been used:

1. one GIS dataset covering some of the EU countries (European Environment Agency, 2000) with a resolution of 250 m and distinguishing 44 land use classes as given in Table B-2 (base year 1990),
2. one GIS dataset covering the whole globe (EROS Data Center et al., 2000) with a resolution of 1 km and distinguishing 24 land use classes as given in Table B-3 (base year April 1992-March 1993),
3. one GIS dataset covering the whole globe (Hansen et al., 1998) from the University of Maryland with a resolution of 1 km (base years 1981-1994, average values used); this is basically used for the definition of the arable land compartment outside the CORINE land cover dataset termed 'cropland' which is why the full set of 14 distinguished land use classes are not shown here.

Additionally, a GIS dataset on lakes, reservoirs and wetlands (Lehner and Döll, 2001) has been used for a better definition of lakes.

Note that these datasets contain information on the different land covers existing in the respective areas. Although land use and land cover are different concepts (e.g., grasslands can or cannot be used as pastures; cf. Moore et al., 1993), these two terms are mostly used synonymously in the present work.

The usage of three datasets was necessary as the one by the EEA has a higher spatial resolution and - more importantly - a more comprehensive set of land uses distinguished than the one by the USGS and GLCF (44 towards 24 and 14, respectively). The distinction of different agricultural land uses with the EEA dataset is a major advantage of this dataset over the other two especially when dealing with human exposures via food. While the USGS dataset has the advantage to be more detailed in terms of land uses distinguished, it does not provide explicit information on crop lands. Due to this shortcoming, the third dataset by the GLCF was used to identify those and 'update' the USGS dataset. The translation of the originally distinguished land covers by the EEA and USGS datasets into the different compartments distinguished by WATSON (cf. sections 5.1.1 and B.3) is given in Tables B-2 and B-3 (see also section B.4 for the treatment of water bodies). The area shares of all compartments present in a zone have been extracted from the resulting GIS dataset.

B.3.1 Considerations with respect to depths of terrestrial compartments

Above, the areas of the different compartments have been defined. In order to arrive at volumes, also the depths need to be known (cf. section A.4). These are defined in the main text for the terrestrial compartments (cf. section 5.1) and are not repeated here.

B.3.2 Considerations with respect to soil depths of volatile substances

Potentially different from exposure models, pure environmental fate models try to capture as much of a substance as possible. This has bearings on the subdivision of these models in terms of compartments as is discussed in the following.

Table B-2: Translation of CORINE land uses (European Environment Agency, 2000) into WATSON land uses

CORINE land use class	Land use type	Assigned compartment type
1.1 Urban fabric	Continuous urban fabric	urban areas
	Discontinuous urban fabric	urban areas
1.2 Industrial, commercial and transport units	Industrial or commercial units	urban areas
	Road and rail networks and associated land	urban areas
	port areas	urban areas
	Airports	urban areas
1.3 Mine, dump and construction sites	Mineral extraction sites	non vegetated land
	Dump sites	non vegetated land
	Construction sites	non vegetated land
1.4 Artificial non-agricultural vegetated areas	Green urban areas	semi natural ecosystems
	Sport and leisure facilities	semi natural ecosystems
2.1 Arable land	Non-irrigated arable land	arable land
	Permanently irrigated land	arable land
	Rice fields	arable land
2.2 Permanent crops	Vineyards	arable land
	Fruit trees and berry plantations	arable land
	Olive groves	arable land
2.3 Pastures	Pastures	pasture
2.4 Heterogeneous agricultural areas	Annual crops associated with permanent crops	arable land
	Complex cultivation patterns	arable land
	Land principally occupied by agriculture	arable land
	Agro-forestry areas	semi natural ecosystems

Table B-2: Translation of CORINE land uses (European Environment Agency, 2000) into WATSON land uses

CORINE land use class	Land use type	Assigned compartment type
3.1 Forests	Broad-leaved forest	semi natural ecosystems
	Coniferous forest	semi natural ecosystems
	Mixed forest	semi natural ecosystems
3.2 Shrubs and/or herbaceous vegetation associations	Natural grassland	semi natural ecosystems
	Moors and heathland	semi natural ecosystems
	Sclerophyllous vegetation	semi natural ecosystems
	Transitional woodland-shrub	semi natural ecosystems
3.3 Open spaces with little or no vegetation	Beaches	non vegetated land
	Bare rocks	non vegetated land
	Sparsely vegetated areas	non vegetated land
	Burnt areas	non vegetated land
	Glaciers and perpetual snow	glacier snow
4.1 Inland wetlands	Inland marshes	semi natural ecosystems
	Peat bogs	semi natural ecosystems
4.2 Coastal wetland	Salt-marshes	semi natural ecosystems
	Salines	non vegetated land
	Intertidal flats	non vegetated land
5.1 Inland waters (cf. footnote 43)	Water courses	water course
	Water bodies	water
5.2 Marine waters	Coastal lagoons	(nothing assigned)
	Estuaries	water
	Sea and ocean	(nothing assigned)
	no information (terrestrial)	(nothing assigned)
	no information (aquatic)	(nothing assigned)

Table B-3: Translation of USGS land uses (EROS Data Center et al., 2000) into WATSON land uses

Land use type	Assigned compartment type
Urban and Built-Up Land	urban areas
Dryland Cropland and Pasture	arable land / pasture
Irrigated Cropland and Pasture	arable land / pasture
Mixed Dryland/Irrigated Cropland and Pasture	arable land / pasture
Cropland/Grassland Mosaic	arable land / pasture
Cropland/Woodland Mosaic	semi natural ecosystems
Grassland	semi natural ecosystems
Shrubland	semi natural ecosystems
Mixed Shrubland/Grassland	semi natural ecosystems
Savanna	semi natural ecosystems
Deciduous Broadleaf Forest	semi natural ecosystems
Deciduous Needleleaf Forest	semi natural ecosystems
Evergreen Broadleaf Forest	semi natural ecosystems
Evergreen Needleleaf Forest	semi natural ecosystems
Mixed Forest	semi natural ecosystems
Water Bodies	water
Herbaceous Wetland	semi natural ecosystems
Wooded Wetland	semi natural ecosystems
Barren or Sparsely Vegetated	non-vegetated land
Herbaceous Tundra	semi natural ecosystems
Wooded Tundra	semi natural ecosystems
Mixed Tundra	semi natural ecosystems
Bare Ground Tundra	non-vegetated land

Table B-3: Translation of USGS land uses (EROS Data Center et al., 2000) into WATSON land uses

Land use type	Assigned compartment type
Snow or Ice	glacier / snow
no data	(not assigned)
Interrupted areas (global Goodes homolosine projection)	(not assigned)

With respect to soils, Mackay (1991) found out that a single soil layer may underestimate volatilisation of those substances for which this process is relevant. There exist different recommendations in order to cope with this underestimation (Cowan et al., 1995b) of which a substance-dependent soil compartment depth (e.g., Brandes et al., 1996) as well as distinguishing at least two soil layers are most often used (e.g., McKone, 1993a). In a recent work, McKone and Bennett (2003) give the recommendation based on theoretical considerations to represent the soil compartment at least as two layers one of which consisting of a thin surface layer in order to properly account for the air-soil mass transfer coefficient of (semi-) volatile compounds. The layer below this should be adjusted to the chemical-specific penetration depth (derived by means of the so-called Damkoehler number). One shortcoming of this adjusted compartment depth, however, is that it may range from 0.1 to several metres (see Table 4 in McKone and Bennett, 2003). When implementing a variable soil depth in a model which is not parameterised for a specific site, this may lead to erroneous assumptions with regard to the structure of the subsurface (e.g., unweathered solid rock, ground water) where penetration is unlikely or at least substantially reduced. This is why in SimpleBox 2.0 the maximally allowed soil depth is set to 1 m (Brandes et al., 1996). The implementation of the effective penetration depth would also have implications on the data needs if one was to represent this part of the terrestrial environment appropriately. This is because the two soil layers would have different characteristics depending on the chemical's effective penetration depth. This shall be illustrated with a rough example. Consider a soil that has a humus rich surface horizon ('layer') of 20 cm followed by 1 m of unconsolidated sand layer which in turn is followed by a consolidated rock layer (e.g., shale). It is assumed here that the surface soil layer is always 2 cm deep and the soil layer below is referred to as 'rooting layer'. If the effective penetration depth was 20 cm the soil layers in the multimedia model could be delimited at 2 cm and 20 cm soil depth having the same properties. However, if the effective penetration depth was

40 cm the rooting layer would have mixed properties of the humus rich soil horizon and the underlying sand rock. This would especially concern the organic carbon content in the case of lipophilic compounds. The situation would be even worse if the effective penetration depths was larger than 1.2 m extending into the shale.

When deriving a Damkoehler number-based effective penetration depth of organic compounds, one has to bear in mind that chemical transformation ('degradation') in soils is mostly dependent on the activity of microorganisms although abiotic transformation processes may also be of importance (McBride, 1994; Alloway et al., 1996), especially photodegradation at the soil surface. Degradation is, thus, mostly confined to areas of biological activity in soils. Correspondingly, it is deemed reasonable principally not to assume Damkoehler number-derived penetration depths larger than 1 m which conforms with SimpleBox 2.0 (Brandes et al., 1996).

In general, however, there are two aspects that suggest not to include a variable soil depth. First, in the context of a spatially-resolved model of continental scope such detailed information on all relevant soil properties (such as partitioning influencing key parameters like organic carbon content for organics and pH for dissociating substances, impermeable subsurface layers) for several decimetres or even metres is not available. Second, if these information became available the averaging of the properties would need to be done for each substance to be modelled separately requiring additional algorithms and a longer computation time. The distinction of several soil layers, thus, touches upon implementation constraints. These are storage of information as well as the dimension of the set of linear differential equations to be handled and, thus, computation time.

Another aspect is to what degree terrestrial vegetation can compensate for the underestimation of volatilisation of a single layer soil compartment. Bennett et al. (1998) used a multimedia model whose soil compartment is two-layered and has an 'effective soil depth' in order to investigate the vegetation influence. They found for TCDD that vegetation is more important on the regional fate of this compound than the soil compartment: the Characteristic Travel Distance (CTD) decreased by an order of magnitude when introducing a vegetation compartment. However, it cannot be assessed what CTD would have resulted if the soil had been represented to consist only of one layer. Nevertheless, vegetation significantly enhances a substance's retention (also supported by findings of Wania and McLachlan, 2001) possibly exerting even a higher effect than does a single soil layer multimedia model. This could mean that the underestimation of the volatilisation from soil may no longer be effective.

Overall, the recommendations with respect to layers and also to variable penetration depths apply to (semi-) volatile organic compounds and are neither feasible (in terms of environmental data acquisition) nor scientifically defendable in terms of potentially allowing unrealistically deep soil compartments in a non-site-specific multi-zonal model of a rather large geographical scope. One also has to keep in mind that even more sophisticated models seem to fail to model more than one zone appropriately (del Re and Trevisan, 1995).

B.4 Dimensions and spatially invariant properties of freshwater compartments

Surface water bodies containing freshwater can roughly be classified into lakes and streams. These show particularly differences in terms of their morphology (depth and width) and flow velocity. Whereas the land use and lake geo-datasets described in a previous section allow for the distinction of larger lakes, reaches (stream extents) are usually too narrow to be represented in such large scale mapping exercises.[43] Nevertheless, one needs to define water volumes for the compartments in order to perform a mass balance based on concentrations. The volumes of unregulated water bodies vary according to the meteorological conditions. In WATSON, however, climatological data are used. Therefore, one needs to base the water volume calculations on long-term averages that are assumed to be constant in time.

As hydrologists usually are more interested for example in flood prevention or drinking/irrigation water supply assessments there is no need to determine such static (long-term) volumes of water bodies from their point of view. Also concentration calculations are usually performed by building the quotient of a mass emission rate (e.g., in kg/s) and the discharge of a stream (e.g., in m^3/s). This may serve as an explanation why no data source on water volumes has been found. The only source found that deals with average volumes is Korzun et al. (1974) cited in Baumgartner and Liebscher (1990) on a global scale.

B.4.1 Dimensions of lakes

According to Korzun et al. (1974) cited in Baumgartner and Liebscher (1990), freshwater lakes globally cover $1.24 \cdot 10^6$ km^2 while containing 91000 km^3 of water. This means lakes are on average 74 m deep. This value is used as a default depth unless other values are provided.

This depth, however, will only be reached by rather large lakes. For the definition of large lakes, a cut-off value of 100 km^2 was used based on a GIS dataset

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[43] Note that in Table B-2 water courses are distinguished from other water bodies; this is because the resulting geo-dataset is also used to determine lake zones.

on lakes which was specifically created for the purpose of this work (cf. section B.5.2).

B.4.2 Dimensions of streams

Korzun et al. (1974) cited in Baumgartner and Liebscher (1990) also estimated the freshwater volume contained in streams. It amounts to 2 120 km^3. As they did not estimate the land area covered by streams and due to lack of such data, it is necessary to estimate the stream water volume as well as its area for the catchments within the geographical scope of the model. Data on area (section B.2) as well as on runoff and discharge (section B.5.2) are readily available on a per zone basis. In order to make a valid water mass balance, however, information on either the residence times of the water or the flow velocities are necessary. These are difficult to obtain.

In order to distribute the global stream freshwater volume, a more pragmatic estimation method is, thus, followed by deriving a continent- and area-specific water volume. The global stream freshwater volume is distributed to the different continents weighted by the total discharge from each continent divided by the global discharge from land (discharge weights in Table B-4). The area-specific stream water volume (per continent) is yielded by dividing this value by the continental area. It is assumed that within one catchment the total stream freshwater volume is given as the product of the total drainage area of the catchment and the area-specific stream water volume:

$$V_{\text{total freshwater volume of catchment c}} = A_{\text{area of catchment c}} \cdot emp_{\text{stream freshwater volume per area}} \cdot \qquad \text{(B-1)}$$

If the catchment consists of more than one zone, the water volume is, furthermore, distributed to the different zones as a function of the total contributing catchment area per zone according to the general observation for rivers in humid areas (Finlayson and McMahon, 1995). As the zones may vary considerably in terms of their spatial extent, the total contributing drainage area per zone is further weighted by the area share of the zone with respect to the total catchment area. The total weight for the water volume distribution within catchment *c* is, hence, given for zone *i* according to Eq. (B-2).

Table B-4: Deriving stream freshwater volumes per catchment area depending on the continent (drainage areas and discharges in the peripheral and central regions of the world taken from Baumgartner and Liebscher, 1990)

Continent	Area $[10^6\ km^2]$		Discharge $[10^3\ km^3/yr]$		Discharge weights	Discharge-weighted stream freshwater volume	Stream freshwater volume per area
	peripheral	central	peripheral	central	[%]	$[km^3]$	$[m^3/m^2]$
Europe	8.3	1.7	2.5	0.3	6.3	133	0.013
Asia	31.4	12.7	12.5	-0.3	31.4	666	0.015
Africa	17.6	12.2	3.4	n/a	8.5	181	0.0061
Australia	4.7	4.2	2.4	n/a	6.0	128	0.014
North America	23.2	0.9	5.9	n/a	14.8	314	0.013
South America	16.4	1.5	11.1	n/a	27.9	591	0.033
Antarctica	14.1	n/a	2.0	n/a	5.0	107	0.0076
Sum	115.7	33.2	39.8	0.0	n/a	n/a	n/a

$$Weight_{\text{volume of zone i in catchment c}} = \frac{A_{\text{drainage area of zone i}} \cdot \frac{A_{\text{area of zone i}}}{A_{\text{area of catchment c}}}}{\sum_{n}^{\text{zones of catchment c}} A_{\text{drainage area of zone n}} \cdot \frac{A_{\text{area of zone n}}}{A_{\text{area of catchment c}}}} \tag{B-2}$$

One sees that the total catchment area cancels down. The freshwater volume of streams in each zone is computed accordingly as:

$$V_{\text{water compartment in zone i}} = Weight_{\text{volume of zone i in catchment c}} \cdot V_{\text{total freshwater volume of catchment c}} \tag{B-3}$$

Furthermore, one needs to define the area of the water compartments as it constitutes the interface between the atmosphere and the water bodies (e.g., for atmospheric deposition). Assuming that the total area of river water bodies constitutes 0.5 % of the total land areas showing discharge would yield an average depth of 2.7 m for Europe according to the world water balance given in Table B-1. A value of 0.5 % of a zone's area is, therefore, assumed as a default. In small zones through which a large river flows, however, the water compartment's depth might become unrealistically large following this rule. A further rule is, therefore, set into place: If the stream water's depth is larger than the sum of the incoming streams' depths, a larger zone area share of between 0.5 % and up to 100 % is adopted assuming at least a depth that is as big as the mentioned sum of the incoming streams' depths.

B.4.3 Dimensions of the freshwater compartment

In the water volume derivation for streams in the previous section, the volumes and areas given for lakes (section B.4.1) are not considered. These are finally added if applicable to yield the ultimate values for the freshwater compartment. Their average depth is yielded by dividing the volume by the respective area covered. Note that this way it is assumed that all of the water entering a zone flows through all lakes contained therein.

B.4.4 Mass transfer coefficient at the water-sediment interface

In order to define the diffusion from water body to sediment and vice versa, the overall mass transfer coefficient needs to be known (cf. sections A.3.14 and

Table B-5: Organic carbon content and pH values for compartments other than permeable soils as used by WATSON

Compartment	pH	Organic carbon content $[kg_{Corg} / kg_{solid}]$
Glaciers	not applicable	not applicable
Impervious surfaces	5.5[a]	0.1[b]
Freshwater bodies	7.0[c]	variable[d]
Freshwater sediment	7.0[e]	variable[d]

a.pH of 'pristine' rain water at 25°C (Stumm and Morgan, 1996, p. 161) adjusted to 0.5 pH units.
b.Analogy assumption to freshwater bodies.
c.Huijbregts (1999).
d.Refer to Table B-11.
e.According to Huijbregts (1999) and Devillers et al. (1995) noting that the pH value may be higher than in freshwater due to less oxidizing conditions.

A.3.15). Reported values range from about $2.8 \cdot 10^{-8}$ (Mackay et al., 1992; 1996a; Wania and Mackay, 1995; Brandes et al., 1996; Severinsen et al., 1996) to $2 \cdot 10^{-6}$ metres per second at the shore line of a lake (Wania, 1996). The values tend to be smaller for (the deeper parts of) lakes (Mackay and Diamond, 1989; Wania, 1996) than for generic freshwater bodies. This tendency may be explained by the on average lower temperatures and, thus, slower Brownian motion (Schwarzenbach et al., 1993) in deep water environments. In any case, it is not plausible to assume a quicker transport of substances in rivers with a lot of water currents and eddies due to diffusive processes than due to water advection or resuspension (cf. section 6.1). Thus, an overall applicable value of $2.8 \cdot 10^{-8}$ metres per second is adopted.

B.5 Computation of spatially-resolved compartment properties and process rates

There is only little information on variable soil and water properties readily available in a GIS format without substantial payments. An example for a relatively expensive data source for soils is the European Soil Data Base (European Commission, 1998).[44] Nevertheless, information on soil pH and organic carbon content (C_{org}) could be found from the International Soil Reference and Information Centre (ISRIC, Batjes, 1996) which are given on a half-degree grid. These datasets only provide information on the respective properties of those soils that are classified as pervious in this study. For the other compartments, the default pH and C_{org} values are given in Table B-5.

Spatially-resolved data on the hydrological cycle were also found. Their description and processing are presented in section B.5.2.

In contrast to these environmental parameters, there are other parameters whose values are not allowed to vary between zones and which were adopted from the literature. These are given in the sections which describe the respective processes or in the following sub-sections.

B.5.1 Spatially variable properties of soils

Values for pH and organic carbon content have been assigned to the different soil compartments after intersecting the land use coverage (cf. section B.3) with the respective geo-datasets. The ISRIC datasets distinguish classes of pH and organic carbon reservoir values that are not assigned single numbers but span ranges (cf. Fig. B-2). Single values have been assigned to the given ranges according to Table B-6 and Table B-7.

Calculation of soil-related pH values

The pH of a permeable soil compartment has generally been derived from the original data (Batjes, 1996) according to the following formula:

$$pH_{\text{compartment}} = -\log \frac{\Sigma(A_{\text{compartment with same pH}} \cdot 10^{-pH})}{A_{\text{compartment total}}} \qquad \text{(B-4)}$$

where

A : area of the compartment [m]

pH : soil reaction, i.e., pH value [-].

The values have been rounded according to 0.5 pH units.

For arable land and pastures, however, the minimally allowed (and default) pH values have been set to 6.0 and 5.5, respectively, due to land management practices taking place ('optimal pH'). If no data had been available for certain zones, the default values of 6.5 and 6.0 have been used for semi-natural ecosystems and non-vegetated land, respectively.

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[44] Note that an aggregated version has become publicly available via the internet only recently.

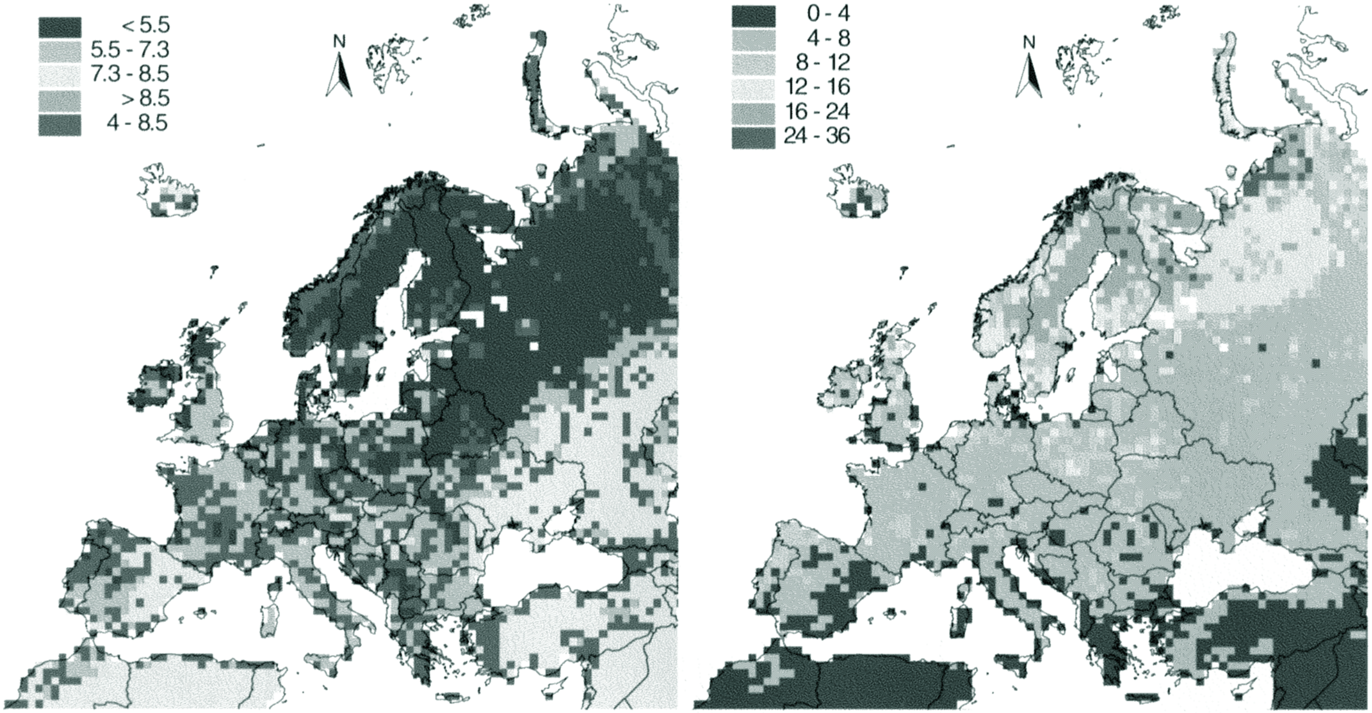

Fig. B-2: Properties of top soil in terms of soil reaction (pH, left) and organic carbon reservoir (right, [kg_{carbon}/m^2]; taken from Batjes, 1996)

Table B-6: Classes of pH values as given by Batjes (1996) and assigned representative single pH values

Range class	Assigned pH value
$pH \leq 5.5$	5.0
$5.5 < pH \leq 7.3$	6.5
$7.3 < pH \leq 8.5$	8.0
$8.5 < pH$	9.0 [a]
$4.0 < pH \leq 8.5$ (complex unit)	6.0

[a] Soil types rich in soda can have pH values up to 11.

Table B-7: Organic carbon classes as given by Batjes (1996) and assigned organic carbon reservoir values [kg_{carbon}/m^2]

Range class	Assigned value
0-4	2.0
4-8[a]	6.0
8-12	10.0
12-16	14.0
16-24	20.0
24-36	30.0
36-48	42.0
>48	60.0 [b]

[a] Mode value in the area covered.

[b] Explanation: bogs have up to 200 kg_{carbon}/m^2 in the first metre which is exactly 60 kg_{carbon}/m^2 in the first 0.3 m (Gisi, 1990).

Calculation of soil-related organic carbon content values

The organic carbon contents of soils are given in mass per square metres for a given soil depth, i.e., 0-30 and 30-100 cm (Batjes, 1996). In order to arrive at the organic carbon concentration for a given compartment in one zone, the original data are multiplied by the area to which they apply. These are then summed over all patches of the same compartment and finally divided by the overall respective compartment area in a respective zone. Division by the appropriate depth yields the organic carbon concentration according to:

$$C\_w/v_{\mathrm{Corg}}(i, z) = \frac{1}{d} \cdot \frac{\Sigma(A_{i,\ \text{with same Corg content}}(z) \cdot Corg)}{A_i(z)} \tag{B-5}$$

where

A : area of the compartment *i* in zone *z*; either as total or for which the same organic carbon content is given [m^2]

C_w/v : concentration of organic carbon in the bulk volume of compartment *i* in zone *z* [kg C_{org} per m^3]

C_{org} : reservoir or inventory of organic carbon in soil [kg C_{org} per m^2] according to Batjes (1996)

d : depth for which the reservoir data are provided [m]; here: 0.3 m.

The mass fraction of organic carbon related to total solid matter in permeable soils, i.e., arable land (*i*: ag), pastures (*i*: p), semi-natural ecosystems (*i*: n) and non-vegetated land (*i*: b), is computed according to:

$$fr\_w_{\text{organic carbon/solid phase}}(i, z) = \frac{M_{\mathrm{Corg}}(i, z)}{M_{\text{total solids}}(i, z)} = \frac{M_{\mathrm{Corg}}(i, z)}{M_{\mathrm{OM}}(i, z) + M_{\mathrm{MM}}(i, z)} \tag{B-6}$$

where

fr_w : mass fraction of organic carbon in overall solid matter of compartment *i* in zone *z* [kg C_{org} per kg_{solid}]

M_{Corg} : mass of organic carbon of compartment *i* in zone *z* [kg C_{org}]

M_{MM} : mass of mineral matter (MM) of compartment *i* in zone *z* [kg_{MM}]

M_{OM} : mass of organic matter (OM) of compartment *i* in zone *z* [kg_{OM}].

In the following, the computation of the different parameters on the right hand side of Eq. (B-6) will be presented. Note that the dependency on the compartment and the zone will not be denoted although existing.

The organic carbon mass is simply calculated by multiplying the organic carbon concentration by the total volume:

$$M_{\mathrm{Corg}} = C\_w/v_{\mathrm{Corg,\,c}} \cdot V_{\mathrm{compartment\ total}} \tag{B-7}$$

where

C_w/v : concentration of organic carbon in the bulk volume of a compartment [kg C_{org} per m^3]

M_{Corg} : mass of organic carbon [kg C_{org}]

V : volume of the bulk compartment [m^3].

The organic matter mass (M_{OM}) consists of compounds containing carbon as well as other elements. Thus:

$$\begin{aligned} M_{\mathrm{OM}} &= M_{\mathrm{Corg}} + M_{\mathrm{non\text{-}Corg}} \\ &= \frac{M_{\mathrm{Corg}}}{fr\_w_{\mathrm{Corg\ mass\ fraction\ of\ total\ organic\ solids}}} \end{aligned} \tag{B-8}$$

where

fr_w : mass fraction of organic carbon in organic matter [kg C_{org} per kg_{OM}]

M_{Corg} : mass of organic carbon [kg C_{org}]

$M_{non\text{-}Corg}$: mass in organic matter not consisting of organic carbon [kg non-C_{org} elements]

M_{OM} : mass of organic matter [kg_{OM}].

The mass fraction of organic carbon in organic matter generally assumes values of 0.5 according to 'model' humic and fulvic acids as given by Schnitzer (1978). For impervious land uses, the value is set to 0.7 based on the consideration that the organic matter on roads mostly consists of soot which is richer in organic carbon (e.g., Gustafsson et al., 1997).

The mineral matter mass (M_{MM}) is yielded by subtracting the organic matter volume from the overall (constant) solid matter volume and multiplying this difference by the mineral matter density:

$$\begin{aligned} M_{\mathrm{MM}} &= \rho_{\mathrm{MM}} \cdot V_{\mathrm{MM}} \\ &= \rho_{\mathrm{MM}} \cdot (V_{\mathrm{solids}} - V_{\mathrm{OM}}) \\ &= \rho_{\mathrm{MM}} \cdot \left(fr\_V_{\mathrm{solids}} \cdot V_{\mathrm{bulk}} - \frac{M_{\mathrm{OM}}}{\rho_{\mathrm{OM}}}\right) \end{aligned} \tag{B-9}$$

where

fr_V	: volume fraction of solids in bulk compartment [m^3_{solids} per m^3_{bulk}]; defined as described in section 5.1.3
M_{MM}	: mass of mineral matter [kg_{MM}]
M_{OM}	: mass of organic matter [kg_{OM}]
ρ_{MM}	: density of mineral matter [kg_{MM} per m^3_{MM}]
ρ_{OM}	: density of organic matter [kg_{OM} per m^3_{OM}]
V	: volume of mineral matter (MM), organic matter (OM), solids, or the bulk compartment [m^3].

The density of mineral and organic matter is not allowed to vary in space and set to 2650 and 1400 kg/m^3 (Scheffer and Schachtschabel, 1989), respectively. Note that the mineral matter density was set equal to that of quartz which makes up the most part of the mineral phase. The volume fraction of soils consisting of solids is invariantly set to 0.5 according to Mackay et al. (1992) and McKone and Bennett (2003) corresponding to a loamy soil, i.e., a soil that is neither rather sandy nor rather clayey.

In the case that the mass of mineral matter (M_{MM}) would become negative, i.e., the term in parenthesis of Eq. (B-9) is negative due to the fact that the soil is very rich in organic carbon, M_{OM} is adjusted so that the total solid matter in a compartment consists of 10 vol.-% mineral solids as a default. Exceptions to this default value apply to freshwater bodies with a value for suspended matter of 5 vol.-% and to the solids in the urban environment and in aquifers (ground water compartment if distinguished) with 10 vol.-% and 50 vol.-%, respectively.

The solid phase density is computed according to:

$$\rho_{\mathrm{solids}} = \frac{M_{\mathrm{OM}} + M_{\mathrm{MM}}}{fr\_V_{\mathrm{solids}} \cdot V_{\mathrm{bulk}}} \tag{B-10}$$

where

fr_V	:	volume fraction of solids in bulk compartment [m^3_{solids} per m^3_{bulk}]; defined as described in section 5.1.3
M_{MM}	:	mass of mineral matter [kg_{MM}]
M_{OM}	:	mass of organic matter [kg_{OM}]
ρ_{solids}	:	density of solid matter [kg_{solids} per m^3_{solids}]
V	:	volume of the bulk compartment [m^3].

In case no organic carbon contents could be assigned to a compartment, default values have been assumed. Arable land, pastures and semi-natural ecosystems were assigned to the category containing 4-8 kg C_{org}/m^2 and non-vegetated land to category with 0-4 kg C_{org}/m^2 corresponding to the mode value and the lowest value in the area covered, respectively (cf. Table B-7).

B.5.2 Hydrological data

In search of a consistent dataset on all components of the hydrological cycle, i.e., at least two of the list of precipitation, evaporation and runoff when disregarding storage changes, the dataset by the Center for Environmental Systems Research at Kassel university, Germany could be found (Döll and Lehner, 2002; Döll et al., 2002, 2003) which builds on precipitation data by New et al. (1999). These provide consolidated 30 year (1961-90) long-term average estimates on precipitation, runoff and ground water recharge. In addition to these data, global GIS data on lakes, wetlands and reservoirs have also been made available (Lehner and Döll, 2001) which have been used for the derivation of a GIS dataset on lakes (cf. section B.2.1).

One problem has occurred when computing the derived figures described below. There are cases in which precipitation is smaller than runoff. This problem had already been identified and reported in Döll et al. (2003). It is due to a calibration exercise performed on measured runoff data which overrules the information on precipitation that are considered to be too small also in parts of Europe. This calibration is owing to the generally recognised fact in hydrology that runoff measurements provide more reliable data than those of precipitation (e.g., Shuttleworth, 1993). The respective values for evapotranspiration have been set to zero in the present study although not fulfilling the water mass balance. However, the measure evapotranspiration is presently not used in the assessment.

Consideration of evaporation

In the geo-datasets used, evaporation is considered to occur from canopies, soils and so-called global lakes and wetlands (Döll et al., 2003). While the evaporation from canopies and soils is included in the runoff values employed, those for lakes and wetlands could not be considered. In order to account for lake water evaporation, the watershed-based distinction of zones in WATSON would need to be allocated to the respective lakes. This, however, has not been possible due to the way how a lake's water balance is considered in the global hydrological model. It is only the most downstream grid cell in which the whole water balance of the global lakes and wetlands is performed. This may even be a grid cell in which two lake water balances happen to be computed. The same problem exists for the consideration of the consumptive use of water by man. Although information on both lake evaporation and water abstraction are principally provided by the hydrological data sources, these have not been considered partly leading to an overestimation of runoff and, thus, discharge.

Computation of runoff and groundwater recharge

Runoff is defined as "(t)hat part of precipitation that appears as streamflow" (Deutsches Nationalkomitee für das internationale Hydrologische Programm (IHP) der UNESCO und das Operationelle Hydrologische Programm (OHP) der WMO, 1998, p. 130). The information provided by Döll and co-workers (Döll et al., 2002, 2003) is given on a grid cell base (cf. Fig. B-3). The environmental fate model of WATSON, in turn, is spatially differentiated according to catchment delineations (see section B.2). In order to transform the original data to match catchments, these are intersected using the GIS tool ArcInfo 7.0. The runoff of a particular zone in WATSON is then computed by multiplying the specified runoff by the area for which it is applicable first. These are summed for all areas contained in a zone. Finally, the resulting value is divided by the overall area. Unfortunately not all grid cells contain valid runoff data. Therefore, also the area by which it is divided is equal to that area for which valid entries are given.

Groundwater recharge, recharge, or accretion is defined as the "process by which water is added from outside to the zone of saturation of an aquifer, either directly into a formation, or indirectly by way of another formation" (Deutsches Nationalkomitee für das internationale Hydrologische Programm (IHP) der UNESCO und das Operationelle Hydrologische Programm (OHP) der WMO, 1998, p. 123). The same computational procedure as for runoff applies to ground water recharge. Groundwater recharge is not used within WATSON as such. Rather the share of the precipitation that reaches the rivers via the so-called quickflow is computed. This is done by first computing the baseflow or base runoff

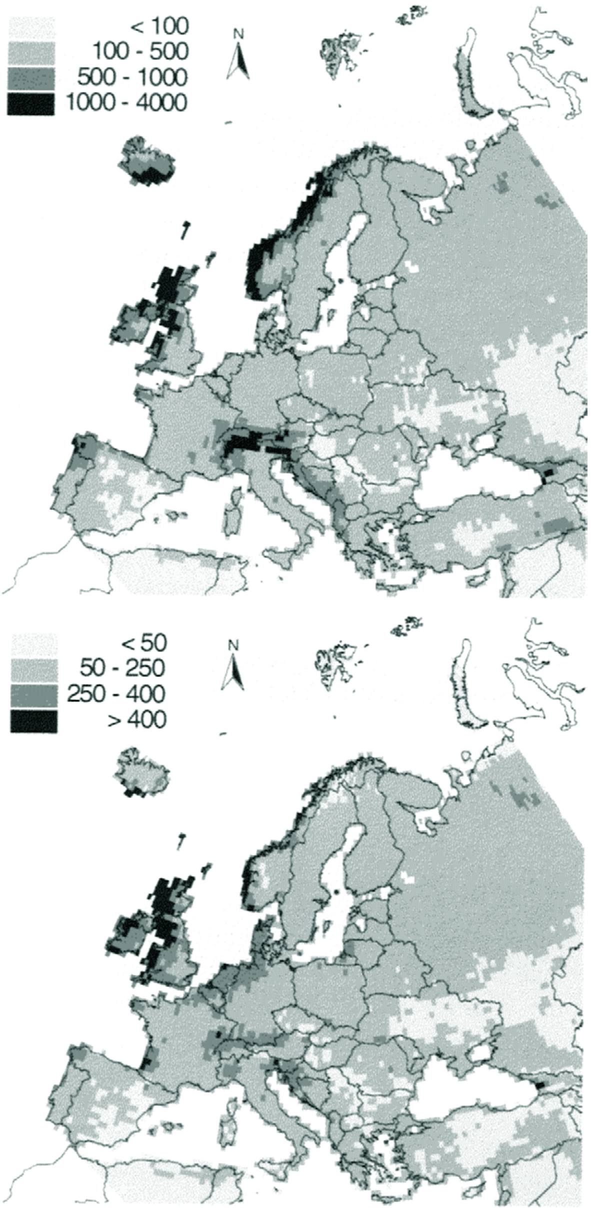

Fig. B-3: Long-term values for runoff from land (top) and ground water recharge (bottom) in the area of interest according to Döll and co-workers (Döll and Lehner, 2002; Döll et al., 2002, 2003) [mm/yr] which is defined as "part of the discharge which enters a stream channel mainly from groundwater, but also from lakes and glaciers during long periods when no precipitation or snowmelt occurs" (ibid., p. 18) relating the groundwater recharge to the runoff. The complement is considered the share of quickflow.

Computation of discharge

Discharge or rate of flow is defined as the "volume of water flowing through a river (or channel) cross section in unit time" (Deutsches Nationalkomitee für das internationale Hydrologische Programm (IHP) der UNESCO und das Operationelle Hydrologische Programm (OHP) der WMO, 1998, p. 45). Based on the runoff information (see above), discharge is simply computed by multiplying the runoff (in metre per second) and the area of a zone (in square metres). In case there are several interconnected zones distinguished in a catchment, the discharge of an upstream zone adds to all downstream zones. Note that evaporation and anthropogenic water abstraction from larger water body surfaces such as lakes is not taken into account in WATSON at present (see above).

Preferential flow

Preferential flow is a non-equilibrium process in soils that rapidly transfers waters and substances entrained towards the subsurface (cf. section A.3.7). It may, therefore, constitute an important removal process of substances from the modelled system unless the subsurface and/or groundwater is considered.

In order to account for this process, it must be known which portion of the vertical water balance, i.e., runoff equals precipitation minus evaporation plus/minus storage (Becker, 1995; Döll et al., 2003), undergoes this rapid flow through the soil. Since preferential flow is known to also occur in arid climates with little to no runoff formation, the amount of water preferentially flowing through soils is assessed based on precipitation rather than on runoff.

Preferential flow was chosen to be 1 % of the rain rate. When applying this value it occurred at times that this amount of the rain rate exceeded the total groundwater recharge. In such instances, it has, therefore, been assumed that 50 % of groundwater recharge happens as preferential flow if there is groundwater recharge at all. If a zone does not show groundwater recharge, the volumetric share of precipitation undergoing preferential flow was set to zero.

B.5.3 Modelling erosion for different soil compartments

The proposed methodology distinguishes between compartments in the terrestrial environment as given in Table 5-1. One criterion for their distinction is water soil

Table B-8: Reported erosion rates in multimedia models

Erosion rate	Reference	Comment
0.03 mm/yr	Brandes et al. (1996)	for any soil
0.04 mm/yr	Hertwich et al. (1999)	Erosion of surface soil 0.0003 $kg/m^2/d$ divided by solid phase density of 2600 kg/m^3

erosion for which the erosion rate shall be derived in the following. It is noted here that only a differentiation of erosion rates according to compartments is implemented at present. A possible improvement of this situation is also described below.

Selection of a representative erosion rate for European conditions

There are only few reported values on erosion rates used in multimedia models (Table B-8). Their appropriateness shall be evaluated against assessed numbers of the measure 'sediment yield'. Sediment yield is defined as "(t)otal sediment outflow from a watershed ... in a specified period of time ... Usually expressed in weight per unit of time" (Deutsches Nationalkomitee für das internationale Hydrologische Programm (IHP) der UNESCO und das Operationelle Hydrologische Programm (OHP) der WMO, 1998, p. 134). It provides a rather reliable assessment of water soil erosion (Morgan, 1999). Although also containing eroded material originating from the rivers, these might serve as a rough estimate of what is transported from soil to water in a spatially-resolved way assuming that in-bed erosion equals the amount deposited within a catchment and no other long-term storage of suspended particulates within the catchment occurs.

The value of 0.04 mm/yr given in Table B-8 is used in CalTOX (Hertwich et al., 1999), a model developed for Californian conditions (McKone, 1993a). This value is substantially lower than the sediment yields given by Walling and Webb (1983) for California, ranging from 250 to more than 1000 $t/km^2/yr$ corresponding to 0.10 to above 0.38 mm/yr. This may be explained by the fact that the non-coastal areas in California are mountainous. CalTOX was designed in the first place to assist risk assessments of hazardous waste sites (in California, McKone, 1993a) which are most likely not located on steep slopes. For Europe, more than 50 % of the area show sediment yields below 50 $t/km^2/yr$ (= 0.02 mm/yr) whereas the rest ranges predominantly between 50 and 750 $t/km^2/yr$ (< 0.29 mm/yr) showing some peaks in the Mediterranean area with values above 1000 $t/km^2/yr$ (> 0.38 mm/yr). Thus, the erosion rate in SimpleBox 2.0 (Brandes et al., 1996) can be considered representative for rather large parts of Europe although heavily underestimating the more Mediterranean areas and overestimating erosion rates on about 50 % of the European area. This value which is also assumed by EUSES (European Commission, 1996a) is adopted here. It is also used when no further differentiation of the water soil erosion process in terms of compartments and/or zones is performed.

Distribution of the overall erosion rate to soil compartments

In order to allow for different erosion intensities on different soil compartments, the crop management factor (C-factor) of the Universal Soil Loss Equation (USLE; Wischmeier and Smith, 1978; Renard et al., 1997) is made use of according to what is presented in the main text (section 5.1.5). The resulting values are given in Table 5-7 on page 103.

Improvement of the water soil erosion process description

Due to the various factors influencing the soil erosion process (Wischmeier and Smith, 1978; Renard et al., 1997; Morgan, 1999), it is clear that erosion rates that only vary by compartment/land cover will fail to represent the real erosion rate occurring at a given site. On the other hand, there exist no quantitative models for the assessment of erosion rates at the regional scale to the knowledge of the author which is due to several problems as noted, for instance, by van der Knijff et al. (2000) and Wickenkamp et al. (2000). For a modelling approach that does not take into account temporally variable conditions in the environment (only 'quasi-dynamic', cf. section 2.3), there exists a possible improvement by making use of estimated sediment yields. Two groups have published global estimates on sediment yields (Milliman and Meade, 1983; Walling and Webb, 1983). The interaction of meteorological, soil-related and management-related parameters which are needed in order to model erosion (e.g., Wischmeier and Smith, 1978; Renard et al., 1997; Morgan, 1999) can be considered integrated in the sediment yield. Considering sediment yield would allow especially for differences between the south and the north of Europe in terms of rainfall erosivity factors (van der Knijff et al., 2000) and with respect to the grazing of different animals[45] which contribute to the explanation why soils of semi-arid and semi-humid areas to which the Mediterranean areas belong tend to have the highest observable erosion rates

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[45] Small ruminants such as sheep and goats that are predominantly kept in Mediterranean areas bite off blades of grass closer to the soil surface than large ruminants leading to enhanced water soil erosion.

(Morgan, 1999). Estimated values for Europe range from below 50 to values around a few hundred (Milliman and Meade, 1983) to even above 1000 t/km^2/yr (Walling and Webb, 1983) corresponding to less than 0.02 and above 0.38 mm/yr assuming an average sediment density of 2600 kg/m^3.

In order to become even more sophisticated, a weighting scheme within the different catchments could allow for different land uses (variable C-factors as reported amongst other in Morgan, 1999 and Umweltbundesamt, 1999) similar to the compartment-specific erosion velocities as described above. Furthermore, it appears that former estimates have been either over- or underestimating sediment yields (Milliman and Syvitski, 1992) which should also be corrected accordingly. Additionally, there exist more advanced GIS-based techniques in order to describe for example the slope with respect to the USLE in a spatially-resolved context (e.g., Moore et al., 1993; Desmet and Govers, 1996). However, such attempts will not solve the general poor quantitative prediction of erosion in spatially-resolved applications (de Roo, 1993).

The use of the sediment yield is, however, left to future developments.

B.5.4 Components of the particle mass balance in surface freshwater bodies

Three processes are covered by the assessment methodology that are involved in the particle mass balance in the aquatic environment (cf. section 6.1.4):

- sediment deposition,
- resuspension, and
- sediment burial.

These will be presented in the following together with the derivation of values needed for their mathematical description (cf. sections A.3.11, A.3.12 and A.3.13) after exploring some general considerations.

Sediment particle inventory and general properties

Different sources of particles may be considered in the mass balance. Examples are soil erosion, sewer effluents and primary production in the water column (Brandes et al., 1996; Wania et al., 2000). All of the multimedia models reviewed provide constant values for the volume fraction of particles in the water column. These range from $2 \cdot 10^{-5}$ vol.-% (Mackay and Diamond, 1989; Wania et al., 2000) to $1 \cdot 10^{-3}$ vol.-% (Brandes et al., 1996, at the continental scale; Severinsen et al., 1996). The bulk of the reported values is in the order of 10^{-4} vol.-% (Mackay et al., 1992, 1996a; Wania and Mackay, 1995; Rantio and Paasivirta, 1996; Mackay and Hickie, 2000). One has to note, however, that suspended mat-

Table B-9: Characteristics of suspended matter as reported for some multimedia models and implications

Models	Stated values		Resulting values	
	Mass fraction of organic carbon [weight-%]	Density of suspended matter [kg per m^3]	Mass fraction of mineral matter[a] [weight-%]	Density of mineral matter[b] [kg per m^3]
Mackay et al. (1992), Mackay et al. (1996a), Devillers et al. (1995)	20	1500	60	1575
Rantio and Paasivirta (1996)	22	1800	56	2321

[a] Assuming that half of the organic matter mass consists of organic carbon (Schnitzer, 1978) and taking the complement as mineral matter.

[b] Assuming an organic matter density of 1400 kg/m^3 (Scheffer and Schachtschabel, 1989).

ter contents in natural channels varies substantially with time and place due to factors such as magnitude of the flood, seasonal conditions, the source of the water and the sediment, and altitudinal location (Milliman and Syvitski, 1992; Shen and Julien, 1993).

As is argued in the main text (section 6.1.4), a simple mass balance for particles is followed which will only employ such constant inventories. As the present particle mass balance does not only cover organic suspended matter, the values on volume fractions of suspended particulates shall be compared to reported values. Before proceeding with this, the properties of suspended as well as sediment particles shall be defined.

The composition of the suspended matter as well as that of particles in the sediment varies considerably according to the information provided by several multimedia models (Tables B-9 and B-10). Assuming that the organic carbon mass makes up 50 % of the organic matter mass (Schnitzer, 1978) with an organic matter density of 1400 kg/m^3 (Scheffer and Schachtschabel, 1989) the respective mineral matter mass fractions as well as their densities are obtained. As can be seen from both Tables, the resulting mineral matter densities tend to be lower than

Table B-10: Characteristics of sediment solids as reported for some multimedia models and implications

Models	Stated values		Resulting values	
	Mass fraction of organic carbon [weight-%]	Density of sediment solids [kg per m^3]	Mass fraction of mineral matter[a] [weight-%]	Density of mineral matter[b] [kg per m^3]
Mackay et al. (1992), Mackay et al. (1996a), Devillers et al. (1995)	4	2400	92	2559
Rantio and Paasivirta (1996)	20	2000	60	2800
Mackay (1991)	5	1500	90	1512
Mackay and Hickie (2000)	2.7-4.6	2000	94.6 - 90.8	2050 - 2091

a. Assuming that half of the organic matter mass consists of organic carbon (Schnitzer, 1978) and taking the complement as mineral matter.

b. Assuming an organic matter density of 1400 kg/m^3 (Scheffer and Schachtschabel, 1989).

that of clay minerals (2200 - 2900 kg/m^3) and of quartz (2650 kg/m^3, Scheffer and Schachtschabel, 1989) ranging from 1500 to 2800 kg/m^3. While the organic carbon content of the sediment particles as given in Table B-10 spans the value range found in other publications (from 3 to 20 vol.-%, Mackay and Diamond, 1989; Mackay and Southwood, 1992; Wania and Mackay, 1995; Brandes et al., 1996; Severinsen et al., 1996; Wania, 1996), the values for the organic carbon content of suspended matter as shown in Table B-9 are located at the higher end of the range from 0.04 (Wania et al., 2000) to 0.4 in the deep water zone of a lake (Wania, 1996) or in the tropic zone (Wania and Mackay, 1995). Like for other characteristics of the freshwater environment, a distinction of suspended solids in stream water and lakes is made. Generally, the organic matter content of suspended and deposited solids in streams is much smaller than that found in lakes. For this reason, the reported lower bound and upper bound values are used as an ori-

Table B-11: Characteristics of solids in the freshwater environment as used in the presented methodology

Property	Particle type	Stream	Lake
Mass fraction of organic carbon in ...	suspended matter	0.02[a]	0.4[b]
	sediment solids	0.005[c]	0.3[b]
Density of solids [kg per m^3][d] of ...	suspended matter	2469	1539
	sediment solids	2627	1726

a.Half the value as used in Wania et al. (2000) assumed for 'pure' stream conditions.

b.In the deep water zone of a lake (Wania, 1996).

c.Although the smallest value found is 0.02 for the northern-boreal and the polar zones in Wania and Mackay (1995) an even smaller value is adopted for 'pure' stream sediments which usually have an organic matter content below 1 % (Scheffer and Schachtschabel, 1989) due to water erosion and oxic conditions.

d.Assumptions: half of the organic matter mass consists of organic carbon (Schnitzer, 1978) and taking the complement as mineral matter; densities: 1400 kg_{OM}/m^3, 2550 $kg_{clay\ minerals}/m^3$ (for suspended solids) and 2650 kg_{MM}/m^3 (for sediment solids, Scheffer and Schachtschabel, 1989).

entation for the characterisation of stream and lake solids, respectively (Table B-11).

If no distinction was made, a value of 0.2 and 0.05 should be used for the mass fraction of organic carbon in suspended solids and sediment solids, respectively.

Based on the information on the respective organic carbon contents and the densities for organic and mineral matter, the respective densities of solids in the water column as well as in the sediment can be defined. The densities of suspended particles and sediment solids in streams and lakes are used as given in Table B-11 which were calculated according to:

$$\rho_{solids} = \frac{1}{\frac{fr\_w_{OM/solids}}{\rho_{OM}} + \frac{fr\_w_{MM/solids}}{\rho_{OM}}} \qquad \text{(B-11)}$$

where

ρ : density of bulk solids and their organic matter (OM) or mineral matter phases (MM) [kg per m^3]

fr_w : organic (OM) or mineral matter (MM) mass fraction of bulk solids [-].

Note that the mass fraction of organic carbon needs to be multiplied by a factor of two (Schnitzer, 1978) to arrive at the overall organic matter mass fraction. The remainder mass fraction consists of mineral matter. The assumed density of organic matter is 1400 kg/m^3 (Scheffer and Schachtschabel, 1989). Two different mineral matter densities are used for the computation of suspended solid and sediment solid densities. For suspended matter, the mineral phase's density is set to that of clay minerals, i.e., 2550 kg/m^3 (Scheffer and Schachtschabel, 1989), whereas for sediment solids it is set to that of quartz, i.e., 2650 kg/m^3 (Scheffer and Schachtschabel, 1989).

Comparing the densities in Tables B-9 and B-10 to those given in Table B-11, it is obvious that the reported values correspond more to the lake situation of the present study while the stream densities are higher than those given in the multimedia modelling literature.[46]

In Table B-12, the sediment delivered to the world's oceans and seas is given per river. The rivers are selected according to whether they are located in the geographical scope of WATSON and whether there is sufficient information available in Milliman and Syvitski (1992) for the derivation of a volume fraction of suspended matter in water. In order to arrive at volume fractions, the sediment discharge was divided by the product of the water discharge and the area. After unit adjustments and division by an assumed suspended particle density of 2469 kg/m^3 in streams (Table B-11), the respective volume fractions were obtained.

The derived volume fractions of suspended matter range from an exceptionally low value of $4 \cdot 10^{-5}$ vol.-% for a lowland river to $4 \cdot 10^{-2}$ vol.-% for mountainous rivers (Table B-12). These values, thus, tend to be larger than those adopted by the multimedia models cited above. Due to the fact that the values given in Table B-12 comprise fine particles active in chemical sorption as well as coarser ones, a value of $1 \cdot 10^{-3}$ vol.-% is adopted in the present study for stream waters which appears to be applicable to non-Alpine mountainous, upland and lowland European rivers. As a result, the concentration of suspended matter in freshwater streams is set to 0.02469 kg/m^3. In the absence of more specific data,

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[46] In terms of its settling behaviour, the effective suspended particle density in water bodies is usually smaller due to water contained in the associations of the single particles (Shen and Julien, 1993). However, this is not taken account of by multimedia models. Rather, these only distinguish between phases (for values on volume fractions of suspended particles as assumed in multimedia models see above) and sub-phases such as organic carbon contents.

Table B-12: Water discharge, area, sediment discharge and volume fractions of transported sediment for several rivers in the geographical scope of WATSON as compiled in Milliman and Syvitski (1992)

River (country)	Water discharge [mm/yr]	Area [10^6 km^2]	Sediment discharge [10^6 t/yr]	Volume fraction[a] [vol.-%]
Mountain (1000-3000 m) - Alpine Europe				
Ebro (Italy, lower estimate)	220	0.085	1.5	0.003
Danube (Romania)	250	0.81	67	0.013
Po (Italy)	670	0.054	13	0.015
Rhone (France)	530	0.09	31	0.026
Arno (Italy)	400	0.0081	2.2	0.028
Tiber (Italy)	450	0.016	6.8	0.038
Ebro (Italy, higher estimate)	220	0.085	18	0.039
Mountain (1000-3000 m) - non-Alpine Europe				
Ardour (France)	670	0.016	0.24	0.001
Loire (France)	245	0.115	1.5	0.002
Garonne (France)	320	0.055	2.2	0.005
Upland (500-1000 m)				
Oder (Germany)	150	0.11	0.13	0.0003
Muonio Alv (Sweden)	500	0.024	0.36	0.001
Volga (Russia, Ukraine)	400	1.4	19	0.001
Elbe (Germany)	160	0.13	0.84	0.002
Pechora (former USSR)	425	0.25	6.1	0.002
Vistula (Poland)	165	0.2	2.5	0.003
Dnester (former USSR)	135	0.062	2.5	0.012

Table B-12: Water discharge, area, sediment discharge and volume fractions of transported sediment for several rivers in the geographical scope of WATSON as compiled in Milliman and Syvitski (1992)

River (country)	Water discharge [mm/yr]	Area [10^6 km^2]	Sediment discharge [10^6 t/yr]	Volume fraction[a] [vol.-%]
Lowland (100-500 m)				
Kalkkinen (Finland)	250	0.025	0.006	0.00004
Exe (UK)	860	0.0006	0.01	0.001
Weser (Germany)	230	0.038	0.33	0.002
Nene (UK)	160	0.0015	0.01	0.002
Kymijoki (Finland)	80	0.037	0.15	0.002
Dnieper (former USSR)	86	0.38	2.1	0.003
Wye (UK)	630	0.004	0.2	0.003
Creedy (UK)	500	0.00026	0.01	0.003
Bristol Avon (UK)	400	0.00067	0.02	0.003
Tyne (UK)	680	0.0022	0.13	0.004
Welland (UK)	200	0.00053	0.01	0.004
Seine (France)	130	0.065	1.1	0.005
Clyde (UK)	430	0.0019	0.11	0.005
Ystwyth (UK)	1100	0.00017	0.028[b]	0.006
Severn (UK)	380	0.0068	0.44	0.007

a. Volume fractions derived by assuming a suspended matter density of 2090 kg/m^3 which consists of 40 weight-% of organic matter with a density of 1400 kg/m^3 (Scheffer and Schachtschabel, 1989) and of 60 weight-% of mineral matter with a density of 2550 kg/m^3 which is the average of the range given for clay minerals by (Scheffer and Schachtschabel, 1989).

b. Value derived by multiplying the sediment yield of 164 t/km^2/year by the respective area.

a value for the volume fraction of suspended matter of $1 \cdot 10^{-4}$ vol.-% is assumed for lakes which complies with the bulk of the reported values in the multimedia literature (see above).

The corresponding value for the volume fraction of solids in sediments also needs to be specified. Reported values range from 0.1 (Mackay and Hickie, 2000) to 0.4 (Mackay, 1991; Rantio and Paasivirta, 1996).[47] Based on this information and using the respectively provided solid phase densities, the corresponding bulk densities range from about 1100 kg/m^3 (Rantio and Paasivirta, 1996; Mackay and Hickie, 2000) over 1185 kg/m^3 (Mackay, 1991) and 1280 kg/m^3 (Mackay et al., 1992, 1996a) to 1420 kg/m^3 (Devillers et al., 1995).

Shen and Julien (1993) report porosities or volume fractions of void spaces in sediments of between 44 and 17 % for fine sand to coarse gravel and boulder sediments, respectively. Thus, the pore volumes assumed by the multimedia models represent sediments which are made up of finer solids than fine sand which is most likely due to the fact that these represent lakes rather than streams. Additionally, the sediment compartments only comprise the active part of the overall sediments which is not as consolidated as the parts below. The median and the average of the reported volume fractions of sediments that consist of solids is 20 % which is adopted here.

Except for the sediment's volume fraction that consists of solids, a distinction between sediments and suspended matter in streams and in lakes has been made. Within WATSON, freshwater compartments may consist also of mixtures of lakes and streams. The respective property values, therefore, need to be determined taking into account both types of aquatic ecosystems. A weighting according to water and sediment volumes is, therefore, employed.

Sedimentation

Sedimentation is defined as the "(p)rocess of settling and depositing by gravity of suspended matter in water" (Deutsches Nationalkomitee für das internationale Hydrologische Programm (IHP) der UNESCO und das Operationelle Hydrologische Programm (OHP) der WMO, 1998, p. 133). It, thus, leads to a transfer of substances from the freshwater compartment to the sediment compartment. If sedimentation prevails over resuspension, this may lead to the ultimate removal of substances from the modelled system especially due to the 'sediment burial'

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[47] Note that two values are used by Rantio and Paasivirta (1996): a value of 0.6 for sediment porosity corresponding to 40 vol.-% solids and a value of 0.05 for all segments concerning 'volume fraction of sediment solids'. It is unclear to the author how these match.

process assumed to occur (cf. section A.3.13) while degradation being usually largely reduced in sediments. Thus, modelling this process appropriately is rather important also in light of the availability of substances towards aquatic organisms (Håkanson, 1984).

Sedimentation together with erosion is an unresolved research area according to Shen and Julien (1993): "Despite extensive research effort, knowledge of erosion and sediment transport still remains incomplete, and there is no generally accepted formula to be used for an accurate solution of the sediment transport rate and watershed sediment yield" (p. 12.1). Sediment transport characteristics are determined by the size, shape, concentration, fall velocity, bulk density of sediment particles and properties such as coatings (Shen and Julien, 1993; Nicholas and Walling, 1996; Droppo et al., 1998; Aboul-Kassim and Simoneit, 2001a; Lick and McNeil, 2001). In the context of in-water chemical transport models, basically only those particles are of interest to which chemicals may be sorbed. These are mostly fine particles and colloids (although frequently measured as dissolved organic carbon) whose surfaces are especially efficient in sorbing metals and organic chemicals (Walling, 1983; McCutcheon et al., 1993; Aboul-Kassim and Simoneit, 2001a).

There have been only few attempts to represent still water areas unlike those with flowing waters in multimedia (-type) modelling exercises. This was done either by distinguishing different parts of lakes (Wania, 1996; Mackay and Hickie, 2000) or by explicitly accounting for stagnant water compartments (Beck et al., 2000; Scheringer et al., 2000a).

The first approach requires measured or estimated data on the different water bodies included in the assessment which is rather data-intensive and may be considered when further developing the model. At the same time it shall be noted that this will be a more process-based approach in agreement with the hydrological literature. The second approach would further extend the amount of compartments distinguished, leading to higher requirements in terms of resources (computation time, data storage). A more pragmatic approach has, therefore, been adopted.

Due to their small size and, thus, their fairly reduced settling velocity, those particles or suspended matter to which most of the assessed substances are attached are only allowed to settle in lakes and stagnant waters which is in line with Scheringer et al. (2000a) and Beck et al. (2000). In the absence of more specific information, it is assumed that sedimentation occurs in all lakes at a specified rate. In contrast, only 5 % of the in-stream water volumes are assumed to allow for sedimentation due to their low amount of stagnant waters. This volume fraction is substantially lower than the 25 % that were assumed by Scheringer et al. (2000a). However, these authors did not distinguish lakes explicitly. Also, their value appears to be rather high.

The overall volume fraction of stagnant waters in a given zone is calculated according to the following equation:

$$fr\_V_{\text{stagnant}}(w, z) = \frac{V_{\text{lake}}(w, z) + V_{\text{stream}}(w, z) \cdot 0.05}{V(w, z)} \qquad \text{(B-12)}$$

where

$$V_{\text{lake}}(w, z) = A_{\text{lake}}(w, z) \cdot d_{\text{lake}}(w) \qquad \text{(B-13)}$$

$$V_{\text{stream}}(w, z) = (A(w, z) - A_{\text{lake}}(w, z)) \cdot d_{\text{stream}}(w) \qquad \text{(B-14)}$$

$$V(w, z) = V_{\text{lake}}(w, z) + V_{\text{stream}}(w, z) \qquad \text{(B-15)}$$

where

A	: area of the freshwater compartment as a whole or the lake present in zone z [m^2] (information available as described in sections B.2, B.3 and B.4)
d	: depth of streams or lakes [m] (defined in section B.4)
fr_V	: volume fraction of stagnant waters [-]
V	: volume of the bulk freshwater compartment, its lake portion or its stream portion in zone z [m^3].

Another distinction is made in that sedimentation in freshwater bodies of zones that pour directly into the sea ('river mouth') is increased due to slower flow velocities, also called aggradation zone or "area of deposition" in an idealised fluvial system (Schumm, 1977). By default, $fr\_V_{\text{stagnant}}(w,z)$ is set to 21 % in these zones provided they are part of a larger drainage basin. This is guided by the idea that a smaller percentage of the deposition rate is resuspended in these areas than in other 'pure' stream zones (see footnote a. of Table B-13).

Reported values for sedimentation rates are given in Tables B-14 and B-15 for generic or evaluative and site-specific multimedia models, respectively. The values span six orders of magnitude when also considering the values in the order of $2 \cdot 10^{-5}$ metres per second (cf. Brandes et al., 1996; Scheringer et al., 2000a). Assuming that no inter-annual accumulation of suspended particulates occurs even in the large lakes which are assumed to are 74 metres deep (cf. section B.4.1), the net removal of these particles must be set accordingly. By 'net removal' from the water column the following three processes may principally be considered to be active for both organic and mineral particles: (a) sedimentation, (b) resuspension and (c) water advection out of the water body noting that organic particles may additionally undergo mineralization (see below). Due to the potentially long residence times of waters in large lakes, water advection is not further considered for this one year balance. Thus, the lower bound of the net sedimentation rate results by subtracting the resuspension velocity from the sediment deposition velocity:

$$v_{\text{net sedimentation}} = v_{\text{sedimentation}} - v_{\text{resuspension}} \tag{B-16}$$

where

v : velocity of particles while undergoing net sedimentation, sedimentation or resuspension [m^3 per m^2 per s] or [m per s].

In order for 74 metres to be cleared in a one year (balancing) period, a net sediment deposition rate of $2.35 \cdot 10^{-6}$ metres per second would be necessary. Following Stokes' law, this value is in the range of velocities obtained for temperatures between 5 and 10°C for a spheric particle with a radius of 1 µm (i.e., of the clay fraction) and a density of 1539 kg/m^3 (assumed for suspended particles in lakes, cf. Table B-11). The settling velocities range between $2.21 \cdot 10^{-6}$ and $2.56 \cdot 10^{-6}$ metres per second for a temperature of 5 and 10°C and a corresponding (absolute) water viscosity of $1.518 \cdot 10^{-3}$ and $1.307 \cdot 10^{-3}$ kg/m/s (McCutcheon et al., 1993), respectively. Thus, the value appears to be reasonable.

Within the presented methodology, it is not suggested to include the lumped process of net sedimentation but to rather address both sedimentation and resuspension separately. One, therefore, needs to set both of the single-process velocities on the right hand side of Eq. (B-16) accordingly. The ratios between the velocity of resuspension, burial and mineralization on the one hand and the sedimentation velocity on the other shall be used in order to derive the different velocities for large lakes and rivers separately. These are also provided in Tables B-14 and B-15. One can see that several authors do not take into account the mineralization of organic matter in the sediment while others consider them to amount between 5 % in lakes (Mackay and Hickie, 2000) to up to 30 % in rivers (Rantio and Paasivirta, 1996). In principle, one would need to distinguish between the mineral and organic phases of the respective sediment and suspended particles when taking account of mineralization. This is not done at present in WATSON. The relationships used in this study are given in Table B-13.

Table B-13: Relationships between the different process rates active in the particle mass balance for surface freshwater as assumed in this study

Relationships	Pure river	River mouth[a]	Pure lake
Ratio resuspension / sedimentation	95 %[b]	45 %	33 %
Ratio burial / sedimentation	5 %	55 %	67 %[c]
Ratio remainder / sedimentation	0 %[d]	0 %	0 %[e]

a. In order to obtain the ratios for river mouth situations while following the computations described below, a stagnant volume fraction of 21 % needs to be specified.

b. The highest reported value is 85 % for the shore line of a lake (Wania, 1996); due to the even higher flow rate in streams a higher value has been adopted; note that the 'effective' sedimentation is higher in lake and river mouth situations of larger rivers.

c. Value selection guided by the burial at the deep water zone of a lake (Wania, 1996).

d. In case mineralization was to be considered the value of 14 % as used in the POPCYCLING-Baltic model would be suggested to be used for organic matter in rivers (Wania et al., 2000).

e. In case mineralization was to be considered the value of 7 % as used for the southern segment of Lac Saint Louis would be suggested to be used for organic matter in lakes (Mackay and Hickie, 2000), owing to the smaller biological activity and lower temperatures throughout the course of a year.

The overall sedimentation rate in a freshwater compartment is calculated according to:

$$\begin{aligned} v_{\text{sedimentation, total}} = {} & fr\_V_{\text{stagnant water}} \cdot v_{\text{sedimentation, lake}} + \\ & (1 - fr\_V_{\text{stagnant water}}) \cdot v_{\text{sedimentation, stream}} \end{aligned} \tag{B-17}$$

where

v : velocity of particles while undergoing sedimentation or resuspension in pure streams, pure lakes or the mixture of the freshwater bodies present in a given zone ('total') [m^3 per m^2 per s] or [m per s]

fr_V : volume fraction of stagnant waters [-].

For a 'pure' lake situation, Eq. (B-17) reduces to:

$$v_{\text{sedimentation, total}} = 1 \cdot v_{\text{sedimentation, lake}} \tag{B-18}$$

so that the overall sedimentation rate is equal to that of a lake or still water body. Based on the relationships as given in Table B-13 and assuming a net sedimentation rate of $2.35 \cdot 10^{-6}$ metres per second for lakes, the respective sediment deposition velocity amounts to:

$$\begin{aligned} v_{\text{net sedimentation, lake}} &= v_{\text{sedimentation, lake}} - v_{\text{resuspension, lake}} \\ 2.35 \cdot 10^{-6} &= v_{\text{sedimentation, lake}} - 0.33 \cdot v_{\text{sedimentation, lake}} \\ \Rightarrow v_{\text{sedimentation, lake}} &= \frac{2.35 \cdot 10^{-6}}{1 - 0.33} = 3.50 \cdot 10^{-6} \end{aligned} \tag{B-19}$$

where

v : velocity of particles while undergoing net sedimentation, sedimentation or resuspension [m^3 per m^2 per s] or [m per s].

For still-water areas within streams, the same net sedimentation rate of $2.35 \cdot 10^{-6}$ metres per second as for lakes is adopted due to the compliance with Stokes' law. In contrast to lakes, streams only consist in parts of more or less still water portions. While in the present methodology the water flows are allowed to vary between zones (cf. section B.5.2), a more generic approach is taken for illustration purposes. Assuming a water flow velocity similar to that used by Scheringer et al. (2000a) which is 1 metre per second and which complies to the upper typical flow velocity as stated in Schwarzenbach et al. (1993) one can see that there is a difference of about five orders of magnitude between the net sedimentation rate and the flow velocity. Thus, sedimentation is negligible. In order to follow the computation of the overall sedimentation rate of a compartment as given in Eq. (B-17), however, an explicit value for the sedimentation rate under still-water conditions is needed.

Allowing the total resuspension rate to be 95 % of that of the total sedimentation rate (cf. Table B-13) and employing the formula for the overall sedimentation rate (Eq. (B-17)), one can derive the gross sedimentation rate according to:

$$\begin{aligned} 0.05 \cdot v_{\text{sedimentation, lake}} &= fr\_V_{\text{stagnant water}} \cdot v_{\text{sedimentation, lake}} + \\ &\quad (1 - fr\_V_{\text{stagnant water}}) \cdot v_{\text{sedimentation, stream}} \\ \Rightarrow v_{\text{sedimentation, stream}} &= 0 \end{aligned} \tag{B-20}$$

where

v : velocity of particles while undergoing sedimentation or resuspension in streams or lakes [m^3 per m^2 per s] or [m per s]

fr_V : volume fraction of stagnant waters [-].

As a result, the overall sediment deposition rates as computed according to Eq. (B-17) are $3.50 \cdot 10^{-6}$ and $1.75 \cdot 10^{-7}$ metres per second for lakes and streams, respectively. Both values for the (gross) sedimentation rate are in the range found in the literature although closer to the higher end (cf. Tables B-14 and B-15). Note that the net sedimentation rate in streams is significantly reduced due to the higher resuspension rate in streams.

Resuspension

Although different processes are involved in the resuspension and the sedimentation process, it is assumed here that when sedimentation is large resuspension is small mostly depending on the flow velocities of the water body. Resuspension affects the sediment compartment which is assumed to have a uniform depth (cf. section 6.1) irrespective of whether it is situated below waters of a stream or a lake. In order for resuspension to become active, first the so-called incipient motion needs to take place (Shen and Julien, 1993): "(s)ediment particles are moved by the flow whenever the magnitude of instantaneous fluid force acting on the sediment particle exceeds the resistance force for this particle to be moved" (p. 12.16). For turbulent flows which predominate in natural waters, this fluid force fluctuates rather substantially in time and may, therefore, require a similar approach as for intermittent rain in multimedia models (e.g., Hertwich et al., 2000; MacLeod et al., 2001; Hertwich, 2001) that are based on constant environmental conditions.

In any case, the degree of resuspension is considered to be a function of the magnitude of the water-sediment interface. Thus, a corresponding area fraction of sediments located below stagnant waters is defined:

$$fr\_A_{\text{stagnant}}(ws, z) = \frac{A_{\text{lake}}(ws, z) + A_{\text{stream}}(ws, z) \cdot 0.05}{A(ws, z)} . \qquad \text{(B-21)}$$

The respective terms are defined analogously to Eq. (B-12), replacing volumes by areas.

Reported values for resuspension rates are given in Tables B-14 and B-15 for generic or evaluative and site-specific multimedia models, respectively. Like for the sedimentation rate, the values span six orders of magnitude. For the site-specific models in Table B-15, resuspension rates in lake waters are in the order of 10^{-11} to 10^{-10} (Wania, 1996; Mackay and Hickie, 2000) whereas those for rivers are about 10^{-7} (Rantio and Paasivirta, 1996).

Table B-14: Reported invariant (organic) particle mass balances in surface freshwater bodies of non-site-specific multimedia models

Sedimentation rate [m/s]	Resuspension rate [m/s]	Sediment burial rate [m/s]	Ratio resuspension / sedimentation	Ratio burial / sedimentation	Ratio mineralization / sedimentation[a]	Reference and remarks
$1.27 \cdot 10^{-11}$	$3.17 \cdot 10^{-12}$	$9.51 \cdot 10^{-12}$	25 %	75 %	0 %	Devillers et al. (1995)
$1.39 \cdot 10^{-10}$	$5.56 \cdot 10^{-11}$	$5.56 \cdot 10^{-11}$	40 %	40 %	20 %	Mackay et al. (1992), Mackay et al. (1996a)
$1.39 \cdot 10^{-10}$	$5.56 \cdot 10^{-11}$	$5.56 \cdot 10^{-11}$	40 %	40 %	20 %	Wania and Mackay (1995); invariant for all non-polar zones
$2.09 \cdot 10^{-10}$	$1.46 \cdot 10^{-10}$	$6.34 \cdot 10^{-11}$	70 %	30 %	0 %	Severinsen et al. (1996); freshwater (burial termed 'netto sedimentation rate')
$6.11 \cdot 10^{-6}$	$3.42 \cdot 10^{-6}$	$1.83 \cdot 10^{-6}$	56 %	30 %	14 %	Wania et al. (2000); upper bound for freshwater
$8.73 \cdot 10^{-6}$	$4.89 \cdot 10^{-6}$	$2.61 \cdot 10^{-6}$	56 %	30 %	14 %	Wania et al. (2000); lower bound for freshwater

[a] The remainder of 100 % minus what is resuspended and buried is considered to be the fraction which is mineralized.

Table B-15: Reported invariant (organic) particle mass balances in surface freshwater bodies of site-specific multimedia models

Sedimentation rate [m/s]	Resuspension rate [m/s]	Sediment burial rate [m/s]	Ratio resuspension / sedimentation	Ratio burial / sedimentation	Ratio mineralization / sedimentation[a]	Reference
$1.74 \cdot 10^{-11}$	$1.16 \cdot 10^{-11}$	$4.86 \cdot 10^{-12}$	67 %	28 %	5 %	Mackay and Hickie (2000); northern and eastern segment of Lac Saint Louis
$3.47 \cdot 10^{-11}$	$2.31 \cdot 10^{-11}$	$9.26 \cdot 10^{-12}$	67 %	27 %	7 %	Mackay and Hickie (2000); southern segment of Lac Saint Louis
$4.17 \cdot 10^{-10}$	$2.78 \cdot 10^{-10}$	$1.39 \cdot 10^{-10}$	67 %	33 %	0 %	Wania (1996); intermediate zone of a lake
$4.17 \cdot 10^{-10}$	$1.39 \cdot 10^{-10}$	$2.78 \cdot 10^{-10}$	33 %	67 %	0 %	Wania (1996); deep water zone of a lake
$5.56 \cdot 10^{-10}$	$4.72 \cdot 10^{-10}$	$8.33 \cdot 10^{-11}$	85 %	15 %	0 %	Wania (1996); shore line of a lake
$1.39 \cdot 10^{-9}$	$5.56 \cdot 10^{-10}$	$8.33 \cdot 10^{-10}$	40 %	60 %	0 %	Wania (1996); river delta in a lake
$3.17 \cdot 10^{-7}$	$1.90 \cdot 10^{-7}$	$3.17 \cdot 10^{-8}$	60 %	10 %	30 %	Rantio and Paasivirta (1996); River Kymijoki, invariant for all segments

a. The remainder of 100 % minus what is resuspended and buried is considered to be the fraction which is mineralized.

The overall resuspension rate in the present study is calculated according to the following equation taking into account one 'pure' resuspension rate for streams and one for lakes (or rather stagnant waters, cf. section A.3.12):

$$\begin{aligned} v_{\text{resuspension, total}} &= fr\_A_{\text{stagnant water}} \cdot v_{\text{resuspension, lake}} + \\ &\quad (1 - fr\_A_{\text{stagnant water}}) \cdot v_{\text{resuspension, stream}} \end{aligned} \quad . \tag{B-22}$$

For a situation in which the freshwater body entirely consists of a lake, Eq. (B-22) reduces to:

$$v_{\text{resuspension, total}} = 1 \cdot v_{\text{resuspension, lake}} \ . \tag{B-23}$$

According to the relationship between the resuspension rate and the sedimentation rate in lakes (cf. Table B-13), the overall resuspension rate for a 'pure' lake situation in the present study are, thus, given as:

$$\begin{aligned} v_{\text{resuspension, lake}} &= 0.33 \cdot v_{\text{sedimentation, lake}} \\ &= 0.33 \cdot 3.51 \cdot 10^{6} = 1.156 \cdot 10^{-6} \end{aligned} \quad . \tag{B-24}$$

If the freshwater body consists purely of a river, Eq. (B-22) becomes:

$$\begin{aligned} v_{\text{resuspension, total}} &= fr\_A_{\text{stagnant water}} \cdot v_{\text{resuspension, lake}} + \\ &\quad (1 - fr\_A_{\text{stagnant water}}) \cdot v_{\text{resuspension, stream}} \\ &= 0,05 \cdot v_{\text{resuspension, lake}} + (1 - 0,05) \cdot v_{\text{resuspension, stream}} \end{aligned} \quad . \tag{B-25}$$

Substituting for the lake resuspension rate as calculated by Eq. (B-24) and allowing the overall in-stream resuspension rate to equal 95 % of the (actual) in-stream sedimentation rate (cf. Table B-13), one obtains Eq. (B-26).

The overall resuspension rate for lakes and streams as computed according to Eq. (B-22) using the values obtained by Eqs. (B-24) and (B-26) are $1.156 \cdot 10^{-6}$ and $1.66 \cdot 10^{-7}$ metres per second for lakes and streams, respectively. Both values for the (gross) resuspension rate are in the range found in the literature although closer to the higher end (cf. Tables B-14 and B-15).

$$
\begin{aligned}
v_{\text{resuspension, total}} &= 0.95 \cdot (0.05 \cdot v_{\text{sedimentation, lake}} + \\
&\quad (1 - 0.05) \cdot v_{\text{sedimentation, stream}}) \\
&= 0.05 \cdot v_{\text{resuspension, lake}} + (1 - 0,05) \cdot v_{\text{resuspension, stream}} \\
\Rightarrow v_{\text{resuspension, stream}} &= \frac{[0.95 \cdot (0.05 \cdot 3.50 \cdot 10^{6} + 0.95 \cdot 0)] - (0.05 \cdot 1.156 \cdot 10^{-6})}{1 - 0.05} \\
&= 1.143 \cdot 10^{-7}
\end{aligned}
\tag{B-26}
$$

Sediment burial

'Sediment burial' means a process that leads to the translocation of substances from the active layer to the inactive layer further down the sediment. It constitutes an ultimate loss process from the modelled system.

Several authors of multimedia fate models report rates or rather velocities for the sediment burial process which span six orders of magnitude (cf. Tables B-14 and B-15).

The overall burial rate in the present study is calculated analogously to Eq. (B-22) by taking into account one 'pure' burial rate for streams and one for lakes (or rather stagnant waters, cf. section A.3.13):

$$
v_{\text{burial, total}} = fr\_A_{\text{stagnant water}} \cdot v_{\text{burial, lake}} + (1 - fr\_A_{\text{stagnant water}}) \cdot v_{\text{burial, stream}} \,. \tag{B-27}
$$

For a situation in which the freshwater body entirely consists of a lake, Eq. (B-27) reduces to:

$$
v_{\text{burial, total}} = 1 \cdot v_{\text{burial, lake}} \,. \tag{B-28}
$$

According to the relationship between the burial rate and the sedimentation rate in lakes (cf. Table B-13), the overall burial rate for a 'pure' lake situation in the present study are, thus, given as:

$$
\begin{aligned}
v_{\text{burial, lake}} &= 0.67 \cdot v_{\text{sedimentation, lake}} \\
&= 0.67 \cdot 3.51 \cdot 10^{-6} = 2.35 \cdot 10^{6} \,.
\end{aligned}
\tag{B-29}
$$

If the freshwater body consists purely of a river, Eq. (B-27) becomes:

$$\begin{aligned} v_{\text{burial, total}} &= fr\_A_{\text{stagnant water}} \cdot v_{\text{burial, lake}} + (1 - fr\_A_{\text{stagnant water}}) \cdot v_{\text{burial, stream}} \\ &= 0.05 \cdot v_{\text{burial, lake}} + (1 - 0.05) \cdot v_{\text{burial, stream}} \end{aligned} \qquad \text{(B-30)}$$

Substituting for the lake burial rate as calculated by Eq. (B-29) and allowing the overall in-stream burial rate to equal 5 % of the (actual) in-stream sedimentation rate (cf. Table B-13), one obtains:

$$\begin{aligned} v_{\text{burial, total}} &= 0.05 \cdot (0.05 \cdot v_{\text{sedimentation, lake}} + \\ &\quad (1 - 0.05) \cdot v_{\text{sedimentation, stream}}) \\ &= 0.05 \cdot v_{\text{burial, lake}} + (1 - 0.05) \cdot v_{\text{burial, stream}} \\ \Rightarrow v_{\text{burial, stream}} &= \frac{[0.05 \cdot (0.05 \cdot 3.50 \cdot 10^{-6} + 0.95 \cdot 0)] - 0.05 \cdot 2.35 \cdot 10^{-6}}{1 - 0.05} \\ &= -1.143 \cdot 10^{7} \end{aligned} \qquad \text{(B-31)}$$

The overall sediment burial rate for lakes and streams as computed according to Eq. (B-27) using the values obtained by Eqs. (B-29) and (B-31) are $2.35 \cdot 10^{-6}$ and $8.76 \cdot 10^{-9}$ metres per second for lakes and streams, respectively. These correspond to the net sedimentation rates. Both values for the overall burial rate are in the range found in the multimedia modelling literature, the one for lakes being closer to the higher end (cf. Tables B-14 and B-15). The rather high sediment burial rate in lakes may also be due to the fact that in this study no mineralization of sediment particles is assumed to occur. In order to compare these values to values found in the literature, the burial velocities are converted into annual volumetric additions to sediments. The velocities are multiplied by the volume fractions of solids in the respective water column, i.e., $1 \cdot 10^{-4}$ and $1 \cdot 10^{-3}$ vol.-% for lakes and streams, respectively. The resulting values are 0.074 mm/yr, 0.003 mm/yr and 0.13 mm/yr for lakes, streams and river mouth locations, respectively. These are mostly within the range found for geologic aggradation rates (0.01 mm/yr to 3 mm/yr in the non-marine environment, Hohl, 1985) noting that under pure stream conditions a very small aggradation takes place. In particular the higher values found for deltas, i.e., 3 mm/yr, exceed those adopted for river mouths by one order of magnitude.

Note that the value obtained for the in-stream burial rate by Eq. (B-31) is negative. All of the velocities derived for streams (not only the velocity for burial, but also for sedimentation and resuspension (Eqs. (B-31), (B-20) and (B-26), respectively)) should, however, be regarded as hypothetical as these are not directly used in the process formulations (section A.3). These values are obtained in order to fulfil the following requirements:

- in order to provide a generally applicable computation of the overall process rates, the approach as given by Eq. (6-9) is followed which distinguishes between stagnant and non-stagnant domains within any freshwater compartment. Due to the heterogeneity of freshwater compartments ranging from pure streams over mixtures of streams and lakes to pure lakes, this methodological approach is adopted, and
- the overall in-stream net sedimentation rate, i.e., resulting sediment deposition rate minus resuspension rate, shall amount to 5 % of the lake net sedimentation rate (cf. Eq. (B-20)).

As a result, especially the negative value for the burial rate is hypothetical and is only used in order to yield a (non-negative) total process velocity. The hypothetic values for pure moving water conditions are, therefore, considered justified and scientifically defendable as long as they are consistently derived and used. As stated above, any water body is assumed to at least contain 5 % of still waters which assures that no negative end-values result.

B.5.5 Average surface temperature

The volatility of substances with non-negligible vapour pressures depends on the ambient temperature. Furthermore, exposure response functions may depend on temperature, such as for damages to materials (Tidblad et al. (1998) quoted in Friedrich and Bickel, 2001a). Therefore, the ambient temperature at the surface is needed.

Annual average temperature data for ground level air were taken from the EcoSense multi-source version for Europe on the EMEP 50 x 50 km grid. Although the heat contained in a volume of air consists of the sensitive as well as the latent heat, i.e., that is contained in the entrained humidity, the temperature was taken as the indicator for both components. This data processing, thus, assumes that the latent heat in air volumes of adjacent grid cells are so close that its influence on the total heat can be disregarded.

The temperature was distributed to the respective zones by area weighting. By doing so it was revealed that temperature data for the most southern EMEP 50 y row are missing (mostly Africa). This data gap was filled by assuming equal temperatures as in the next more northern EMEP 50 y row.

B.6 Spatial differentiation for the exposure and impact assessment

In contrast to the environmental fate model, the exposure and the impact assessments follow a spatial differentiation based on administrative units mostly according to the Nomenclature of Territorial Units for Statistics (Nomenclature des Unités Territoriales Statistiques, NUTS) used by the Statistical Office of the European Communities (EUROSTAT).[48] Thus, the information that is available in a spatially-resolved way is attributed to the different administrative levels distinguished. The highest resolution is available for the larger member states of the European Union for which NUTS level 3 is distinguished corresponding to municipalities (Fig. B-4). For countries that are not (yet) part of the European Union as of the beginning of 2004, usually only the countries themselves are distinguished. Exceptions which have one subdivision below country-level are Albania, Azerbaidjan, Bulgaria, the Czech Republic, Georgia, Hungary, Norway, Poland, Romania, Slovenia, Switzerland and the former Yugoslavia. Non-European Union countries with a threefold subdivision are Russia and the Ukraine (Fig. B-4).

B.6.1 Production-related data

There are presently two types of production-related data included in the assessment: the production and the yield.

Production data

In order to consider trade and to introduce a production-based human exposure assessment, one needs to know the actual amounts of food produced. These are taken from the EcoSense multi-source version database to the extent possible (e.g., wheat, barley, potatoes, rye, oats). Missing data on animal produce such as beef, pork, milk, poultry, eggs and pork as well as spinach are taken from the Food and Agriculture Organization of the United Nations' (FAO) statistical database (Food and Agriculture Organization of the United Nations - Statistics Division, 2002b, 2002a; Food and Agriculture Organization of the United Nations - Statistics Division, 2003) for the year 2000. Information on the production of cereals in Russia have been taken from the same source. The amounts of the respective food groups produced are shown in Table B-16.

The original data utilized are given for different levels of aggregation. Whereas the FAO data are given at country level (NUTS0 or equivalent), the in-

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[48] Note that also the direct releases into water and soil are specified according to these administrative units.

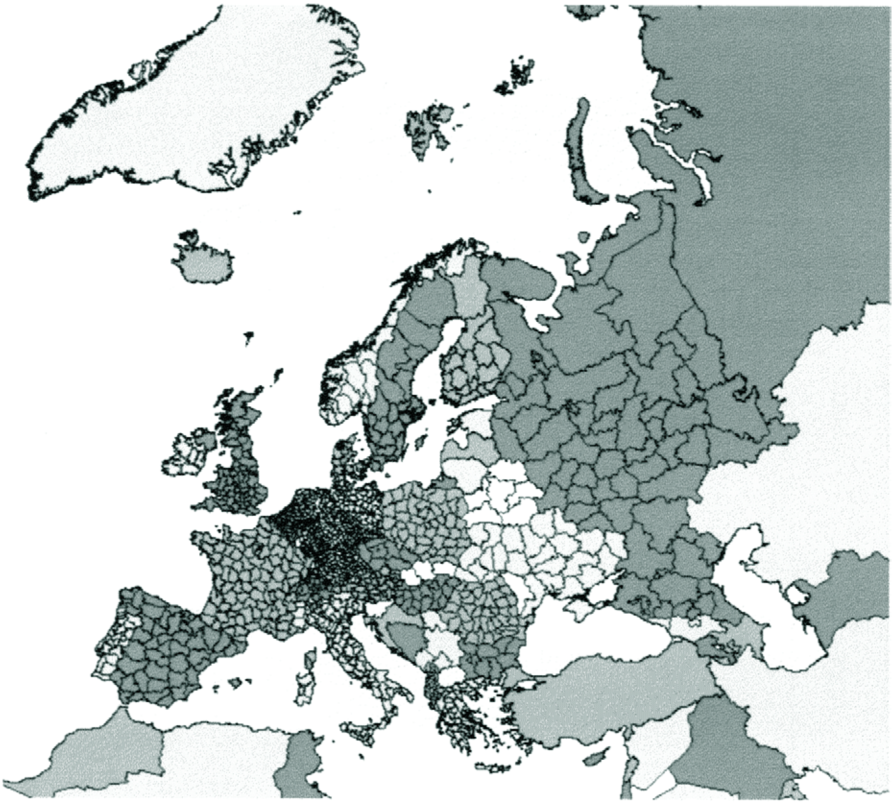

Fig. B-4: Subdivision of the geographical scope of the model into administrative units. Countries are distinguished by different shades of grey (see Fig. B-1 for the model's boundaries).

formation stored in the EcoSense database may be as detailed as at the municipality level. Apart from the FAO, information on agricultural production data contained in the EcoSense database were mostly extracted from the country-specific editions of the series by Statistisches Bundesamt (various volumes) which were issued in different years from 1991-1995 providing data at country level. Agricultural production data below the country level were to a large extent taken from the respective national statistical agencies (e.g., Statistisches Bundesamt in Germany, Istituto Nazionale di Statistica in Italy) or from the Statistical Office of the European Communities. All data are valid for the early nineties.

Table B-16: Annual national production of different produce [kt/yr]

Country	Beef and veal[a]	Cereals[b, c]	Cow milk, whole fresh[a]	Eggs[d]	Freshwater fish[d]	Spinach[e]	Pork[a]	Potatoes[b]	Poultry meat[d]
Albania	36	49	807	21	0.0008	0	6.8	65	4.0
Armenia	13	121	177	8.2	0.0002	0	2.4	163	0.46
Austria	203	2439	3340	86	0.0035	7.3	624	594	111
Azerbaijan, Republic of	10	170	196	5.8	0.0009	0	0.30	63	3.3
Belarus	269	3727	4490	182	0.0058	0	256	10000	76
Belgium	253	1908	3398	194	0.0013	75	981	1906	407
Bosnia and Herzegovina	13	1573	540	15	0.0025	0	5.0	0	8.4
Bulgaria	67	3762	1390	82	0.010	3.0	243	478	104
Croatia	27	1773	607	46	0.0037	0	114	507	33
Czech Republic	107	6631	2789	188	0.023	3.5	417	1460	215
Denmark	154	7669	4720	74	0.044	0	1624	1359	202
Estonia	15	462	629	16	0.0042	0	30	340	7.3
Faroe islands	0.077	0	0	0	0	0	0	0	0

Table B-16: Annual national production of different produce [kt/yr]

Country	Beef and veal[a]	Cereals[b, c]	Cow milk, whole fresh[a]	Eggs[d]	Freshwater fish[d]	Spinach[e]	Pork[a]	Potatoes[b]	Poultry meat[d]
Finland	91	3298	2450	59	0.072	0	173	798	64
France	1514	39318	24898	1038	0.064	109	2312	5464	2221
Georgia	48	168	619	20	0.0002	0	37	350	14
Germany	1301	36934	28300	901	0.060	60	3981	26170	801
Greece	66	2606	789	117	0.026	37	143	946	154
Hungary	49	3934	2145	176	0.019	7.0	622	1042	470
Iceland	3.6	0	107	0	0.0043	0	0	0	0
Ireland	577	1447	5160	32	0.024	0	226	584	123
Italy	1154	11739	11740	686	0.056	91	1478	2308	1089
Kazakhstan	63	2846	770	19	0.0056	0	28	289	6.9
Latvia	22	726	823	24	0.0017	0	32	701	7.2
Liechtenstein	0	0	12	0	0.0032	0	0	0	0
Lithuania	75	2706	1725	39	0.0036	0	84	1849	25
Luxembourg	22	107	291	0	0.0001	0	84	20	15
Macedonia	7.0	537	200	26	0.0018	0	9.0	180	4.8

Table B-16: Annual national production of different produce [kt/yr]

Country	Beef and veal[a]	Cereals[b, c]	Cow milk, whole fresh[a]	Eggs[d]	Freshwater fish[d]	Spinach[e]	Pork[a]	Potatoes[b]	Poultry meat[d]
Malta	1.6	9	48	6.0	0	0	9.1	13	5.3
Moldova, Republic of	21	926	555	32	0.0016	0	60	400	16
Netherlands	471	1338	11135	668	0.0071	49	1623	7699	754
Norway	91	1177	1699	48	0.466	0	103	455	43
Poland	349	19728	11889	424	0.052	0	1923	36270	626
Portugal	83	1749	1442	117	0.0012	14	317	1242	268
Romania	162	5692	4301	263	0.014	0	502	4143	259
Russian Federation	385	12163	6490	384	0.116	0	318	7671	153
Serbia and Montenegro	98	2821	1830	72	0.010	0	655	0	89
Slovakia	48	2378	1067	61	0.0023	1.1	164	483	104
Slovenia	42	221	649	23	0.0013	0.39	59	185	67
Spain	629	15536	5997	658	0.038	62	2904	5000	987
Sweden	150	3830	3297	102	0.0086	0	277	738	92

Table B-16: Annual national production of different produce [kt/yr]

Country	Beef and veal[a]	Cereals[b, c]	Cow milk, whole fresh[a]	Eggs[d]	Freshwater fish[d]	Spinach[e]	Pork[a]	Potatoes[b]	Poultry meat[d]
Switzerland	128	1064	3871	36	0.0030	17	225	908	49
Turkey	236	17158	5800	449	0.043	136	0.18	0	439
Ukraine	754	22300	12436	497	0.048	0	676	15000	193
United Kingdom	708	19841	14489	589	0.15	0	923	6445	1513

a. Year 2000 taken from Food and Agriculture Organization of the United Nations - Statistics Division (2002b).

b. Different years and sources.

c. Comprising wheat, barley, rye and oats.

d. Year 2000 taken from Food and Agriculture Organization of the United Nations - Statistics Division (2002a).

e. Year 2000 taken from Food and Agriculture Organization of the United Nations - Statistics Division (2003).

The exposure assessment is performed at the lowest administrative level distinguished (see Fig. B-4, 1355 administrative units in total) unless aggregation takes place. Different distribution schemes have been followed in order to distribute the food production and also population data from for instance the country level to the lowest administrative level distinguished. These schemes may be based on the total area (e.g., for human population), water volume (fish), or the land uses pastures (cattle) and arable land (all other agricultural produce). From the degree to which farm animals are kept outside (cf. section 7.1.1), it is clear that especially the distribution of farm animals other than cattle is difficult according to a particular land use. Rather than using a purely (total) area-weighted distribution scheme, the distribution scheme according to arable land is adopted in order to follow agricultural activity. Prior to distributing the animal produce eggs, poultry, beef and pork according to one of these schemes, however, the stock and production information available from the REGIO database (European Commission, 2003e) is used to distribute the FAO data to below country level to the extent possible.

Some countries shown in Fig. B-4 are not entirely covered by the models WATSON and EcoSense (cf. Fig. B-1). In case receptor data for example on production but also on population are only provided at the country level, this may lead to overestimates of the affected amounts of food produced and/or population living in the assessed area. For instance, Russia is only covered to 20 % in terms of space by both models. Adopting the country total for food production for instance is, therefore, misleading. Affected countries are Russia, Kazakhstan, Armenia, Azerbaijan, Turkey, Libya, Algeria and Morocco. The receptor data provided at the country level (NUTS0) are, therefore, corrected according to the area share of the respective countries in the geographical scope of the model. Total land areas were taken from Central Intelligence Agency (CIA) (2003) while the areas covered were derived from the WATSON database (Table B-17).

Data on yield

The second type of production-related data is the respective yield. This is needed for the assessment of the removal from the environmental fate model due to harvest of agricultural produce when exposed via atmospheric deposition (cf. section A.6.5). Note that in contrast to agricultural practice, this parameter needs to reflect the total mass produced on a given area over a one year period, accounting for potentially several harvests of the same crop. The values for spinach in the different countries were taken from Food and Agriculture Organization of the United Nations - Statistics Division (2003) for the year 2000.

Table B-17: Correction of country total receptor values according to area covered by WATSON

Country	Total area[a] [km^2]	Area covered [km^2]	Share [%]
Algeria	2381740	641750	27
Armenia	28400	10871	38
Azerbaijan	86100	16384	19
Kazakhstan	2669800	551390	21
Libya	1759540	517360	29
Morocco	2381740	21500	1
Russia	16995800	3449200	20
Turkey	770760	511960	66

a.Total land area taken from Central Intelligence Agency (CIA) (2003).

B.6.2 Human consumption data

According to the official report on nutrition for Germany (Deutsche Gesellschaft für Ernährung e.V., 2000), there are different types of data for the assessment of food uptake by a population. It is distinguished between use data ('Verbrauchsdaten') based on agricultural statistics and consumption data ('Verzehrsdaten') which are inquired at the end user level. The latter are not readily available for all countries covered by the present assessment (cf. the Euromonitor (1992) dataset discussed below). If consumption data are available, these are often only representative for a small sub-population of a country (e.g., a municipality; cf. consumption data for Catalans (Buckley-Golder et al., 1999) and the whole of Spain (Euromonitor, 1992 given in European Centre for Ecotoxicology and Toxicology of Chemicals, 1994)).

It was, therefore, explored to what degree the per capita food supply data of the FAO Food Balance Sheets (FBSs, Food and Agriculture Organization of the United Nations - Statistics Division, 2002a) which give the "quantities of food reaching the consumer" (ibid.) can be taken as a proxy for the real intake. The consumption data for several EU countries published by Euromonitor (1992) reproduced in European Centre for Ecotoxicology and Toxicology of Chemicals (1994) and European Commission (2003a) were compared to those provided by

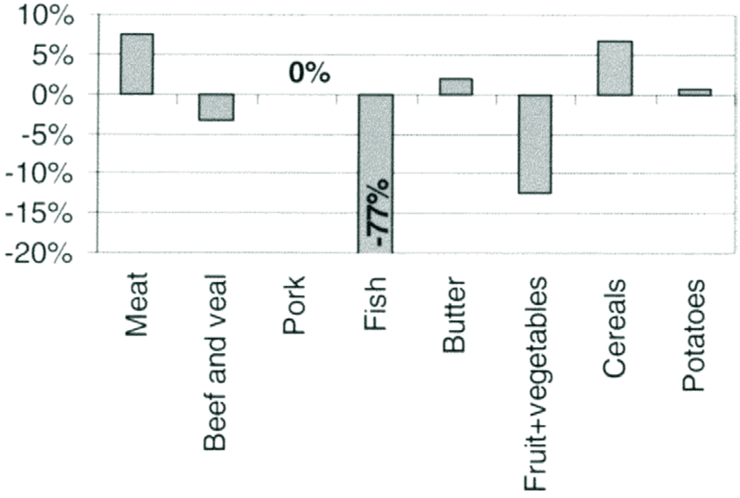

Fig. B-5: Example on the deviation of the food supply data (Food and Agriculture Organization of the United Nations - Statistics Division, 2002a) from the consumption data by Euromonitor (1992): EU15 countries in 1990

the FBSs. No reference year was stated which is why the comparison was done for the years 1990 through 1992. As an example, the result of the comparison for the European Union 15 (EU15) countries in 1990 is given in Fig. B-5. The following conclusions can be drawn:

- the most severe deviations occur for aggregated food items (e.g., meat, fish, fruit/vegetables),
- fish as well as fruit and vegetable supply as estimated by the FBS tend to overestimate the consumption given by Euromonitor (1992), and
- a simple derivation of a loss fraction of edible food in the households is not apparent.

However, one would expect that the supply is usually larger than the consumption. This can be explained by the fact that not all food that is assessed to be available for consumption is finally eaten (e.g., due to loss, plate-waste). Additionally, there are many gaps in deriving the FBSs particularly in the statistics of utilization for non-food purposes which might lead to a reduction of the estimated per capita food supply.[49] Within the assessment, use is made of the food supply data that are corrected by assuming that 5 % of the retailed food is lost in order to arrive at a more representative, country-dependent proxy of real consumption. In the equations, this is considered through the inclusion of the parameter $fr\_w_{\text{not consumed/food supply}}$.

It occurs that the agricultural production data for 'cow milk, whole, fresh' (Food and Agriculture Organization of the United Nations - Statistics Division, 2002b) are smaller than those given for 'milk - excluding butter' in the Food Balance Sheets (Food and Agriculture Organization of the United Nations - Statistics Division, 2002a) based on which the milk supply shall be determined. While both apparently exclude butter and cream, the difference is explicable by production of milk from animals other than cows (i.e., buffalos, goats and sheep). It is assumed that the per capita supply has the same milk composition as the domestic production. Based on this assumption, the 'milk - excl. butter' is converted into 'cow milk, whole, fresh' by a country-specific conversion factor ('share' in Table B-18) in order to yield the cow milk supply available for intake by humans.

The predicted substance concentrations in food are only valid for those food items that are produced within the geographical scope of the model. In order to know to what degree the European[50] food supply relies on imports or formulated inversely to what degree the European food production can sustain its food demand, the self-supply is derived from trade statistics at the border of Europe for the year 2000 (Food and Agriculture Organization of the United Nations - Statistics Division, 2002a; Food and Agriculture Organization of the United Nations - Statistics Division, 2003). In general, the amounts produced in Europe can at least sustain consumption as regards the food groups considered in the assessment (Table B-19). These self-supply figures only consider net trade effects. Import of food (and feed) produced outside the geographical area considered (also taking place to varying degrees), however, leads to a 'dilution' of the predicted pollutant concentrations due to the fact that the exposure assessment is confined to a certain portion of the world and all produce imported except for re-imports is, thus, considered unexposed. Nevertheless, it is assumed that people only take in food items produced within the area modelled. This applies to all food groups listed in Table B-19 except spinach. Although the case of spinach may be regarded is in-

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[49] See comment to the FBS data found at http://www.fao.org/waicent/faostat/agricult/fbs-e.htm.

[50] By 'Europe', the following countries are meant: Albania, Austria, Belarus, Belgium, Bosnia and Herzegovina, Bulgaria, Croatia, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Ireland, Italy, Latvia, Lithuania, Luxembourg, Macedonia, Malta, Republic of Moldova, Netherlands, Norway, Poland, Portugal, Romania, Russian Federation, Serbia and Montenegro, Slovakia, Slovenia, Spain, Sweden, Switzerland, Ukraine, United Kingdom.

Table B-18: Difference between cow milk production and overall milk production and assumed share of cow milk production with respect to the overall milk production

Country	Cow milk, whole, fresh production[a] [t/yr]	Milk - excluding butter (total inland production)[b] [t/yr]	Difference [t/yr]	Share [-]
Albania	807000	948007	141007	85%
Armenia	462000	473760	11760	98%
Austria	3340126	3364290	24164	99%
Azerbaijan, Republic of	1031110	1031110	0	100%
Belarus	4489600	4489600	0	100%
Belgium	3398296	3398296	0	100%
Bosnia and Herzegovina	540000	547100	7100	99%
Bulgaria	1389800	1706300	316500	81%
Croatia	2145000	2188740	43740	98%
Cyprus	146600	180200	33600	81%
Czech Republic	2789364	2805120	15756	99%
Denmark	4719800	4719800	0	100%
Estonia	628911	628911	0	100%
Finland	2450100	2450100	0	100%
France	24898000	25630100	732100	97%
Georgia	618900	618900	0	100%
Germany	28331216	28354410	23194	100%
Greece	789000	1958740	1169740	40%
Hungary	606816	615470	8654	99%

Table B-18: Difference between cow milk production and overall milk production and assumed share of cow milk production with respect to the overall milk production

Country	Cow milk, whole, fresh production[a] [t/yr]	Milk - excluding butter (total inland production)[b] [t/yr]	Difference [t/yr]	Share [-]
Iceland	107353	107353	0	100%
Ireland	5159788	5159790	2	100%
Italy	11741000	12891000	1150000	91%
Kazakhstan	3730200	3774690	44490	99%
Latvia	822983	824970	1987	100%
Liechtenstein	12000	12000	0	100%
Lithuania	1724700	1724700	0	100%
Luxembourg	290704	290704	0	100%
Macedonia	200000	240000	40000	83%
Malta	47969	49642	1673	97%
Moldova, Republic of	554800	571000	16200	97%
Netherlands	11135000	11135000	0	100%
Norway	1699000	1720500	21500	99%
Poland	11889300	11901860	12560	100%
Portugal	1994788	2132860	138072	94%
Romania	4301259	4622760	321501	93%
Russian Federation	31977000	32300000	323000	99%
Serbia and Montenegro	1830000	1862000	32000	98%

Table B-18: Difference between cow milk production and overall milk production and assumed share of cow milk production with respect to the overall milk production

Country	Cow milk, whole, fresh production[a] [t/yr]	Milk - excluding butter (total inland production)[b] [t/yr]	Difference [t/yr]	Share [-]
Slovakia	1067000	1123090	56090	95%
Slovenia	649300	649300	0	100%
Spain	6047000	6673000	626000	91%
Sweden	3297000	3300000	3000	100%
Switzerland	3871300	3887800	16500	100%
Turkey	8732041	9807500	1075459	89%
Ukraine	12436000	12710000	274000	98%
United Kingdom	14488000	14489000	1000	100%

a. According to Food and Agriculture Organization of the United Nations - Statistics Division (2002b).

b. According to Food and Agriculture Organization of the United Nations - Statistics Division (2002a).

significant, a correction factor is introduced in order for the exposure assessment to be applicable for any type of produce, regardless of the degree of self-supply. This correction factor is equal to the values given in Table B-19 ('degree of self-supply') setting values larger than 100 % to unity ('value adopted').

B.6.3 Further substance-independent data used in the exposure assessment

In the following, some of the variable parameter values are given that neither fall into the groups presented above nor are substance-dependent.

Farm animals take in different feed at varying rates. These are given for two exposure assessment frameworks separately (Tables B-21 and B-20).

Some of the bioconcentration factors are given as a ratio of dry weight concentrations in soil and produce, respectively (cf. section C.2). However, the food consumption information is given on a fresh weight basis. One, therefore, needs

Table B-19: Degree of self-supply in Europe[a] with respect to the food groups considered in the exposure assessment; derived based on (Food and Agriculture Organization of the United Nations - Statistics Division, 2002a; Food and Agriculture Organization of the United Nations - Statistics Division, 2003)

Food group	Degree of self-supply [%]	Value adopted [%]
Barley	112	100
Bovine Meat	100	100
Eggs	101	100
Freshwater Fish	101	100
Milk - Excluding Butter	108	100
Oats	106	100
Pork	103	100
Potatoes	102	100
Poultry Meat	101	100
Rye	104	100
Spinach	97	97
Wheat	107	100

a.See also footnote 50.

to perform a unit conversion correspondingly. The respective values used are given in Table B-22.

At present only wheat is considered as the main source of grains fed to farm animals. Its mass fraction of the total amount of grains eaten by farm animals as assumed in the assessment is given in Table B-23.

Table B-20: Ingestion of feed and soil particles by farm animals ($ING_{feed\ or\ soil}$) [kg DW/capita/s] according to United States - Environmental Protection Agency (1998)

Farm animal	Feed or soil	$ING_{feed\ or\ soil}$	Remark
Beef	Forage	$4.40 \cdot 10^{-5}$	forage consumption of typical beef cattle (Table in section 5.4.4.2, United States - Environmental Protection Agency, 1998)
	Grains	$4.40 \cdot 10^{-5}$	grain consumption of typical beef cattle (Table in section 5.4.4.2, United States - Environmental Protection Agency, 1998)
	Silage	$1.16 \cdot 10^{-5}$	silage consumption of typical beef cattle (Table in section 5.4.4.2, United States - Environmental Protection Agency, 1998)
	Soil particles	$3.47 \cdot 10^{-6}$	section 5.4.4.4 (United States - Environmental Protection Agency, 1998); the recommended value of 0.5 kg/day is for subsistence farmer beef cattle; thus, the quoted value by US-EPA 1990 of 0.3 kg/day which is representative for typical beef farmers' cattle is used
Cow milk and products	Forage	$7.18 \cdot 10^{-5}$	forage consumption of typical dairy farmer cattle (Table in section 5.4.5.2, United States - Environmental Protection Agency, 1998)
	Grains	$1.41 \cdot 10^{-4}$	grain consumption of typical dairy farmer cattle (Table in section 5.4.5.2, United States - Environmental Protection Agency, 1998)
	Silage	$2.20 \cdot 10^{-5}$	silage consumption of typical dairy farmer cattle (Table in section 5.4.5.2, United States - Environmental Protection Agency, 1998)

Table B-20: Ingestion of feed and soil particles by farm animals ($ING_{\text{feed or soil}}$) [kg DW/capita/s] according to United States - Environmental Protection Agency (1998)

Farm animal	Feed or soil	$ING_{\text{feed or soil}}$	Remark
Cow milk and products (continued)	Soil particles	$2.31 \cdot 10^{-6}$	section 5.4.5.4 (United States - Environmental Protection Agency, 1998); the recommended value of 0.4 kg/day is for subsistence farmer dairy cattle; thus, the quoted value by NC DEHNR of 0.2 kg/day is used which is representative for typical dairy farmers' cattle
Laying hens (eggs)	Grains	$2.31 \cdot 10^{-6}$	value for hens (section 5.6.1.2, United States - Environmental Protection Agency, 1998)
	Soil particles	$2.31 \cdot 10^{-6}$	value for hens (section 5.6.1.2, United States - Environmental Protection Agency, 1998)
Pork	Grains	$3.82 \cdot 10^{-5}$	section 5.5.1.2 (United States - Environmental Protection Agency, 1998)
	Soil particles	$4.28 \cdot 10^{-6}$	section 5.5.1.4 (United States - Environmental Protection Agency, 1998)
Poultry	Grains	$2.31 \cdot 10^{-6}$	section 5.6.1.2 (United States - Environmental Protection Agency, 1998)
	Soil particles	$2.31 \cdot 10^{-6}$	section 5.6.1.2 (United States - Environmental Protection Agency, 1998)

Table B-21: Ingestion of forage by farm animals (ING_{forage}) [kg DW/capita/s] according to International Atomic Energy Agency (2001)

Farm animal	ING_{forage}	Remark
Beef	$1.39 \cdot 10^{-4}$	Table XII (value for large animal, diet consists of fresh forage only, International Atomic Energy Agency, 2001)
Cow milk and products	$1.85 \cdot 10^{-4}$	Table XII (value for large animal, diet consists of fresh forage only, International Atomic Energy Agency, 2001)

Table B-22: Mass fraction of food dry matter ($fr\_w_{solid\ phase/bulk}$) [kg_{food} DW per kg_{food} FW]

Produce	$fr\_w_{solid\ phase/bulk}$	Remark
Cereals	0.9	on average 10 % moisture content for cereals assumed (Table 9-19, United States - Environmental Protection Agency, 1997a)
Fish	0.2468	average of carp, drum (fw), perch, pike and trout (all in raw status; Table 10-48, United States - Environmental Protection Agency, 1997a)
Meat	0.284	moisture content of beef (71.6%) taken as representative although varying from 68.3% for goose to 75.5% for wild duck (Table 11-21, United States - Environmental Protection Agency, 1997a)
Potatoes	0.1671	moisture content of 'potatoes (white) - whole' is 83.29% according to Table 9-19 in United States - Environmental Protection Agency (1997a)
Spinach	0.0842	moisture content of spinach is 91.58% according to Table 9-19 in United States - Environmental Protection Agency (1997a)

Table B-23: Mass fraction of grains fed to farm animals consisting of wheat ($fr\_w_{wheat/total\ grain}$) [-]

Farm animal	$fr\_w_{wheat/total\ grain}$	Remark
Beef and milk cattle	0.013	0.03 of cereals in fodder for cattle (rule of thumb), overall fodder consumption 11095100 t of which 4861700 t are cereals and 2153000 t are wheat in Germany from July 2003 through January 2004 (Menz, 2004)
Pork, poultry and laying hens	0.29	0.65 of cereals in fodder for non-cattle, overall fodder consumption 11095100 t of which 4861700 t are cereals and 2153000 t are wheat in Germany from July 2003 through January 2004 (Menz, 2004)