Generic Estuary Model for Contaminants (GEMCO)

Final Report :

Conceptual background and User Manual

October, 2003
Z2725

Contents

Appendices

A.   Clustering of European estuaries

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1 Introduction

1.1 Background

The model presented in this report is the result of research conducted under the Long-range Research Initiative (LRI); a research program that is initiated by the chemical associations American Chemistry Council (US), JCIA (Japan) and the European Chemical Industry Council (CEFIC). The LRI addresses emerging and existing health and environmental issues. It provides financial support for research to focus on developing sound scientific understanding of the impact of chemicals on people and the environment.

The fate of contaminants in the environment is an important issue within the LRI. CEFIC sponsors a number of research programs, including the fate of contaminants in the atmosphere and in riverine and marine environments. WL | Delft Hydraulics (lead-contractor) in co-operation with IFREMER[1] and IVM[2] (sub-contractor), was contracted to conduct the research that deals with the fate of contaminants in estuaries. The original objectives of the project were:

To improve understanding and forecasting techniques of the fate, distribution and impact of contaminants in estuaries in order to develop and implement a generic model framework to be applicable for any 'virtual' European estuary.

At a later stage in the project, additional attention was given to include the marine environment in the model. This was in response to the publication of the Technical Guidance Document (TGD) on Risk Assessment of Chemical Substances following European Regulations and Directives (ECB, 2003), which gives specific attention to risk assessment in the marine systems rather than for estuaries.

The 'Generic Estuary Model for Contaminants' (GEMCO), is the final product of this research project. It was designed as an easy-to-use tool to determine the sediment and water concentrations as well as the concentrations and fluxes of contaminants through the different trophic levels in a schematic food web. WL | Delft Hydraulics focused on the sediment and water concentrations of contaminants and the definition of a 'generic' estuary, while IFREMER focused on the food chain module. The resulting model can be applied to any European estuary and its adjacent marine waters.

This study was conducted during the period October 2000 – September 2003.

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[1] *l'Institut Français de Recherche pour l'Exploitation de Mer*
[2] *Institute for Environmental Studies, Vrije Universiteit, Amsterdam*

1.2   Study framework

In order to accomplish the established objectives, the project was divided into two integrated parts:

1. Modelling of transport and fate of contaminants through the *abiotic* system (water, suspended particles and sediment), conducted by WL | Delft Hydraulics, the Netherlands;
2. Modelling of transport of contaminants through the *biotic* system (foodweb), conducted by IFREMER, France and supported by IVM, the Netherlands.

This report presents a summary of the model including a User's Manual for the model (Appendix B). More complete information can be found in the following references:

- An overview and description of the abiotic estuarine processes (WL | Delft Hydraulics, 2001);
- A description of the abiotic model including conceptual background and Scheldt case study (WL | Delft Hydraulics, 2003a);
- An overview of biological systems in European estuaries (Ifremer, 2001), and
- A description of the biotic model for contaminant fate in estuarine trophic food chains (Ifremer, 2003).

1.3   Overview of report

In chapter 2 the conceptual background of the model is described. It includes a summary of the main processes of the abiotic and biotic components of the generic estuary model. In chapter 3 the model use with its applicability is outlined.

2   Conceptual background of GEMCO

2.1   General approach to modelling

Current risk assessment methods within the EC are based on the EUSES model. This basically is an emission estimation and exposure assessment model. The model uses a one box approach to estimate environmental concentrations. In order to allow for the uncertainty and dilution introduced by this approach, safety factors of 100 - 1000 are used.

The GEMCO Generic Estuary Model for Contaminants has a different approach, it calculates spatial variation in concentrations within an estuary.
The model developed is considered to be a 'Generic Estuary model' and therefore has two important characteristics:
1. In principle it is applicable to any European estuary and its bordering marine waters for the purpose of an environmental risk assessment;
2. The model is easy to use, i.e. the user interface is simple and the user required input is limited, as the model is designed for non-specialists.

The overall set-up of the modelling work is illustrated in Figure 2.1. (PEC = Predicted Environmental Concentration).
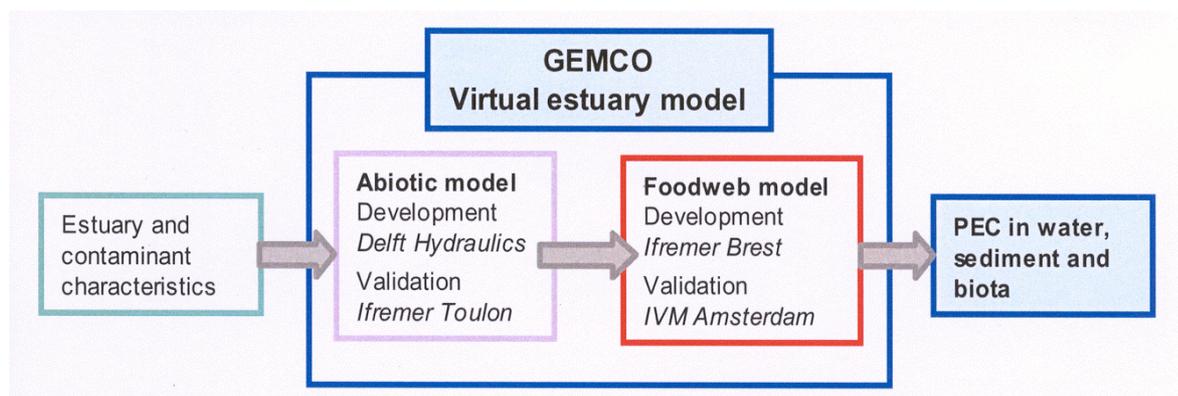

Figure 2.1 Overview of the GEMCO project

As input the GEMCO model requires three types of information:
1. Estuary characteristics and environmental conditions (e.g. river discharge, estuary dimensions, tidal amplitude at estuary mouth, water temperature);
2. Chemical properties of the contaminants (e.g. molecular mass, organic carbon partition coefficient, Henry coefficient);
3. Emission of the contaminants (e.g. concentration in the river, atmospheric load, direct loads to the estuary).

The model has an associated database in which various default input values are stored. As shown in Figure 2.1, the GEMCO model comprises an abiotic and a biotic module. Based on the user input, the GEMCO abiotic module firstly calculates the contaminant concentration in the estuary and marine area in terms of: Total concentration, dissolved concentration, concentration adsorbed to suspended particulate matter and concentration in the bed sediment. The biotic module uses these environmental concentrations as the starting point and calculates the concentrations in different food web compartments.

The abiotic and biotic model components are fully coupled in the GEMCO model. The final output of a model calculation consists of 'predicted environmental concentrations' (PEC) in water, sediment and biota.

For developing an easy to use generic estuary model, the following requirements are specified:
- fast computing time (in the order of seconds);
- applicable for a wide range of European estuaries;
- limited data-storage;
- limited input by the end-users;
- predicted concentration levels must be in reasonable agreement with measurements.

Estuaries are generally known to be very diverse and complex water systems, where tidal motions and density currents induced by change from fresh to salt water, are both of particular importance in determining the transport and behaviour of contaminants. Considering the high complexity of estuaries, a number of assumptions and simplifications regarding geometry, hydrodynamics and water quality processes are made in setting up the generic model.

2.2   Classification of estuaries

Considering the broad range of conditions and characteristics of European estuaries, one single model application representing all estuaries is simply not possible. It was therefore decided to define a limited number of estuary classes and to develop a model for each estuary class. This approach led to a classification study with the objective of grouping European estuaries in clusters of estuaries with more or less similar properties.

Estuary classification is not a new subject, and the scientific literature includes many different estuary classification schemes, the most important of which have previously been reported in the literature review for this project (WL | Delft Hydraulics, 2001). Most of these classification schemes are based on:

1. Flow (hydraulic) and circulation characteristics (e.g. well-mixed, partially mixed, stratified due to co-occurrence of fresh and salt water) or
2. Horizontal and vertical shape (e.g. coastal plain estuary or fjord).

Initial attempts to apply one or more of these existing schemes in the present project identified two difficulties:

1. The characteristics or parameters necessary to classify a specific estuary in one of the schemes were not readily available in the literature (this is especially true for the classification systems based on hydraulic and circulation characteristics, requiring e.g. Froude number, Reynolds number, skewness coefficient of flow discharge, etc.); and

2. Even if some estuaries could be placed in a specific class, this information did not directly link with a method for a developing a 'generic' model for that class.

To develop a classification system for European estuaries for application in the GEMCO model, it had to be based on a number of easily available transport and mixing characteristics (also called '*indicators*') that would be useful as input to the generic model for that class. The neural network (ANN = Artificial Neural Network) method was selected as the best approach for defining estuary classes based on available indicators of European estuaries (WL, 2003a). An additional condition was that clearly *distinct* classes could be identified, i.e.:

- averaged values of indicators would be different between different classes
- the range per indicator within one class would not be 'too big'

The procedure for developing the classification followed the main steps below:

1. Identify ideal estuary 'indicators' for classification,
2. Collect data of more than 50 European estuaries (from literature and nautical charts), and assess availability of ideal indicators,
3. Select set of available indicators for estuary classification,
4. Apply neural network software,
5. Identify estuary clustering and classes based on neural network results, and
6. Assess if clustering is satisfactory.

In practice, steps 3-6 formed an iterative loop as shown in Figure 2.2.
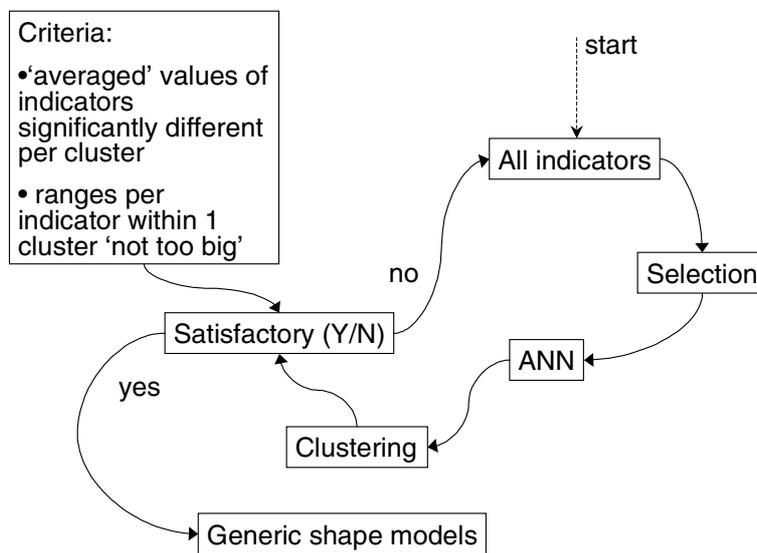
Figure 2.2   Classification methodology (ANN = Artificial Neural Network)

After performing many iterations, a final set of indicators for the estuary classification was identified, as presented in Table 2.1.

Table 2.1:   Final selection of estuary indicators used for neural network classification

Indicator	Unit	Name
Q_{mean}	m^3/s	Mean annual river discharge
H_0	M	Tidal range
B_0	M	Width at estuary mouth
h	M	Depth at estuary mouth
b	M	Convergence width
N	-	Estuarine flood number
D_0	m^2/s	Dispersion coefficient at mouth

From the results of the neural network analysis, four main classes of estuaries can be distinguished, together with characteristic values of the indicators used to identify each class (in terms of high, medium or low values for different indicators, see Table 2.2).

Table 2.2   The four main classes of estuaries and characteristic values of key indicators

Estuary class (cluster)	high values	Medium values	low values
1. River dominated (stratified) estuaries, channel type	Q_{mean}, D_0, b, N	H_0, L_s	H_0, B_0
2. Small, high dispersive estuaries, funnel shape	D_0	H_0, N	$h, B_0, L_s,$ Q_{mean}, b
3. Shallow, low dispersive estuaries		b, B_0, H_0	D_0, Q_{mean}, h_0, L_s
4. Deep, large estuaries	L_s, B_0, h_0, b	H_0, Q_{mean}, D_0	N

L_s: salt intrusion length

In appendix A, a comprehensive list of more than 50 European estuaries and their characteristics is presented.

2.3   Abiotic model component

The abiotic model consists of linked hydrodynamics and water quality processes, from which the concentration of a chemical contaminant in the water column and in the seabed of an estuary is computed. The model is adapted from the Delft3D modelling framework (WL | Delft Hydraulics, 2003b).

Schematization

The first step in the hydrodynamic and water quality modelling was to develop a generic 'schematisation' for European estuaries, i.e. the definition of the shape (geometry) and correlating model grid to be used as the basis for the calculations. In order to derive a generic description of estuary shapes, the work of Savenije (1992 & 1993) on salt intrusion in alluvial estuaries was applied. This work showed that the estuary shape is to a large extent determined by the relation between the tidal range and the fresh water input.

Savenije developed a set of simple generalised (generic) expressions for relating the estuary cross-sectional area (A), width (B), and depth (h) as a function of distance from the estuary

mouth. These equations were shown to fit a wide range of estuaries, and therefore were considered ideal as the basis of the generic estuary model for GEMCO (see Figure 2.3).
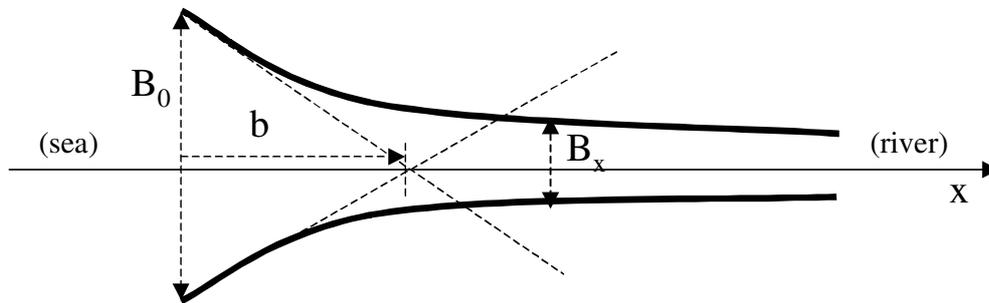

Figure 2.3:   Relation between estuary width at mouth (B_o) and width convergence length (b)

The generic estuary ("trumpet") shape can be defined on the basis of 6 estuary parameters, as shown in Table 2.3 for the three European estuaries included in Savenije's study.

Table 2.3   Parameters for 3 European estuaries (from Savenije, 1992)

Estuary parameter		unit	Scheldt	Ems	Thames
Ao	Area	m^2	150000	61000	58500
A	x-sectional area conv. Length	km	26	19	23
B	width conv. Length	km	28	19	23
h	Depth	m	10	3.9	7.1
L	Length	km	105	40	100
Bo	Width	km	15.0	15.64	8.24

With the above method for defining the generic shape for any European estuary, the next step to developing a generic model was to create a computational model grid for each estuary. For the purpose of this study, a two-dimensional model grid is defined containing 50 grid elements in the longitudinal direction and 10 grid cells in lateral direction. This results in a total of 500 computational elements to simulate a 2 dimensional depth-averaged distribution of contaminants by using appropriate dispersion coefficients for both x and y directions, as shown in figure 2.4, as an example.
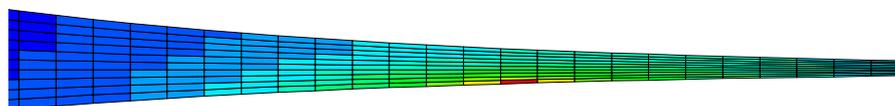
Figure 2.4:   Example of 2-dimensional concentration distribution of a site discharge in a generic estuary

In a latter stage of the project, a marine compartment was included in the generic schematisation in response to the publication of the Technical Guidance Document on risk assessment of chemical substances (ECB, 2003). This coastal region is applied to assess the potential impacts of multiple point and diffuse sources of substances originating from the estuary. The fixed size of the coastal compartment is defined as 40 km long, 10 km wide

and 10 m deep. In addition to the input from the estuary, the TGD proposes a direct emission into the marine compartment being 1% of the direct emissions from the inland sources which is supposed to represent a relevant fraction of sources that are located near the sea. Figure 2.5 shows a schematic overview of the generic estuary geometry and adjacent marine compartment including the emission sources.
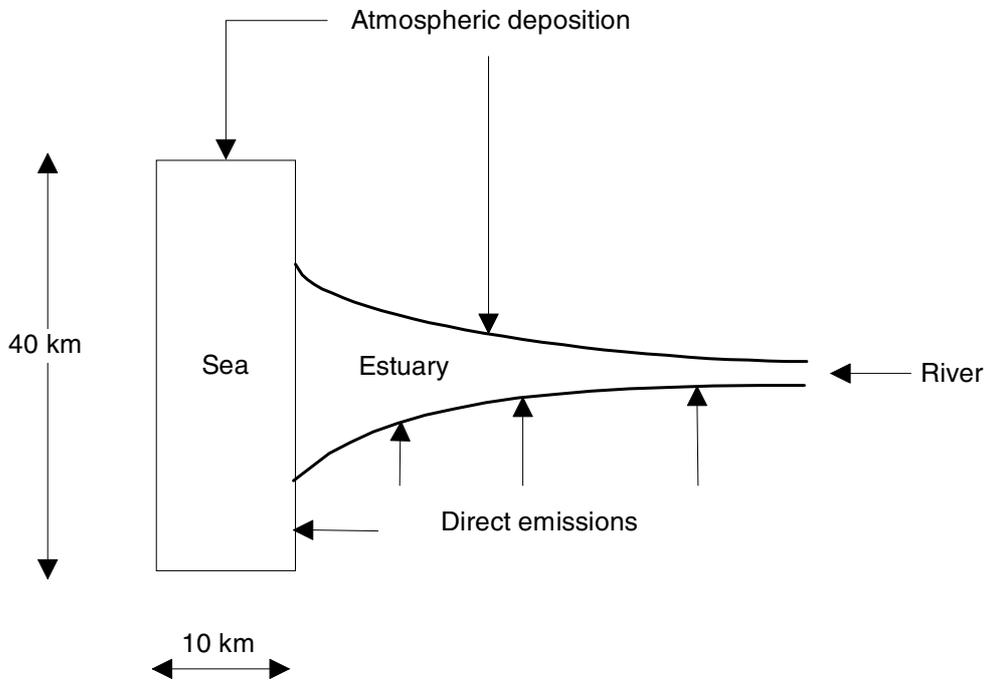
Figure 2.5:   Schematic overview of generic model system and emissions

Transport and mixing

It is commonly known that the transport and mixing (hydrodynamic) processes in estuaries are highly complex mechanisms and require detailed description of the processes involved. However, considering the requirements of the GEMCO model (see section 2.1) a simplified approach was needed. It was thus decided to use a '*tidal-averaged*' approach for describing the advective transport. This means that there is no detailed computation of the incoming and outgoing tidal movement, but rather the average flow over a tidal cycle is calculated. Computationally, this is a much simpler approach and is more appropriate for the simplified geometry and schematization being addressed.

In the tidal-averaged generic approach, the effective tidal average longitudinal dispersion is a bulk parameter that expresses the results of all mixing processes that occur within a tidal cycle and that are neglected in the simplified hydrodynamic description. The use of a dispersion coefficient (D) enables a description of the longitudinal (and transverse) distribution of steadily released substances without the detailed knowledge of the current behaviour. However, the great difficulty is to derive an appropriate value of the dispersion coefficient. No general analytical expression exists for this coefficient.

In the GEMCO model there are two possibilities for estimating the overall dispersion coefficient (D) for an estuary:

1. The value can be determined from salinity measurements, if these are available (preferred method), or
2. The value can be determined based on empirical equations of geometric and hydraulic characteristics of the estuary.

The first method is based on the use of estuarine salinity as a tracer of the tidal mixing. The tidal-averaged dispersion coefficient (D) can be calculated if the salinity at different locations in the estuary is known, together with the river flow and cross-sectional area. Furthermore, this method allows the calculation of a spatially varying dispersion coefficient, e.g. for the lower and upper regions of the estuary.

If salinity measurements are not available, an estimate of the overall dispersion coefficient can be made based on geometric and hydraulic characteristics of an estuary, such as: The freshwater discharge, the cross-sectional area at the estuary mouth, the width of the estuary mouth, the tidal range, the tidal excursion and the tidal period. In this method, the overall dispersion at the mouth of the estuary is calculated (D_o), as well as the dispersion at different distances along the estuary (D_x), given the known "trumpet" geometry of the estuary.

Water quality

The calculation of the contaminant concentration in the estuary and the marine coastal box is based on the conservation of mass. The mass balance equation for a chemical in the water column of a compartment under a steady state condition, is described with:

load + inflow - outflow - settling - volatilisation - decomposition = 0

Furthermore, partitioning among the dissolved and particulate phases affects the loss and distribution of a chemical as well as the exposure of organisms to this substance. Partitioning is formulated according to the equilibrium concept of partition coefficients, based on K_{oc} and K_d partition coefficients. The total concentration of a micro-pollutant is the sum of four fraction components:

$$C_t \quad = (f_{poc} + f_{doc} + f_{in} + f_{df}) \,.\, C_t$$

in which:

C_t	= total concentration	$(g.m^{-3})$
f_{df}	= freely dissolved fraction	(-)
f_{doc}	= fraction adsorbed to dissolved organic matter	(-)
f_{poc}	= fraction adsorbed to the organic part of (suspended) matter	(-)
f_{in}	= fraction adsorbed to the inorganic part of (suspended) matter	(-)

Combining the fractions with the total concentration yields the individual predicted environmental concentrations (PEC) in water and particulate matter.

In summary the water quality component of the GEMCO model includes the following processes which can affect the total concentration available in the water:

- Adsorption of organic chemicals to organic particulates, as a function of a Koc partition coefficient;
- Adsorption of heavy metals to inorganic and organic particulates, as a function of a Kd partition coefficient;
- Settling of adsorbed chemicals as a function of net settling velocity of suspended particulate matter and the concentration of suspended particulates;
- Loss of (organic) chemical due to volatilisation, as a function of Henry's constant;
- Loss of (organic) chemical due to decomposition (e.g. biodegradation, hydrolysis), as a function of an overall first order decomposition rate in water

In the GEMCO model, default values of the overall decomposition rate and other process parameters and coefficients are provided for a number of substances.

The spatial and temporal behaviour of suspended matter in estuaries are predominantly determined by a complex interaction between various forces and processes such as, tide- and wind-driven currents, density-driven gravitational circulation, storm events and sedimentation and erosion processes. In addition, the organic part of suspended matter (POC) highly depends on the primary production and algae kinetics, which in turn depends on the nutrients cycles of N, P, C and Si. Considering the necessarily applied simplifications in the generic model approach, it is not feasible to simulate the suspended matter processes in a physically sound, legitimate manner. Therefore, both inorganic and organic suspended matter are supplied as 'forcing functions' to the GEMCO model. This means that the concentrations are not modelled, but that they may be defined by the model user or taken from the default values available. Since these parameters often vary over the estuarine area, the concentration values can be specified for three different salinity zones: fresh water zone (salinity 0-8 ppt), intermediate zone (salinity 8-20 ppt) and saline zone (salinity > 20 ppt).

Within the GEMCO model the estuarine filtering capacity is estimated. This filtering capacity is a measure to what extend estuaries and coastal areas are able to trap significant quantities of material (both solid and dissolved), and thus act as filters between land and ocean. The contaminant specific estuarine filtering efficiency is calculated by the ratio between the chemical removal rates within the estuary (sedimentation, biodegradation, volatilisation etc) and the total input of the chemical by the river.

The sediment layer

The GEMCO model also calculates the chemical concentration in the upper layer of the seabed in the estuary. In order to calculate this concentration, a fully (homogeneous) mixed upper sediment layer is defined with a fixed density (ρ) and thickness (δ). In a similar fashion to the water column, the calculation of chemical concentration in sediment is based on the conservation of mass. Assuming that the sediment influx towards the sediment layer equals the outgoing flux of the sediment layer, the mass balance equation for the homogeneous mixed upper sediment layer can be described by:

Mass influx – mass outflux – chemical decomposition in sediment = change in chemical mass in sediment

In case of steady-state, and a decomposition rate of zero, the concentration adsorbed to suspended matter equals the contaminant concentration in the seabed. In case of decomposition this results in:

$$C_s = \frac{1}{1 + \dfrac{k \cdot \rho_s \cdot \delta}{F}} \cdot C_p$$

In which:
F	= sedimentation flux of suspended matter	(g. m^{-2} d^{-1})
F	= v$_s$.S$_s$	
v$_s$	= net sedimentation rate	(m. d^{-1})
S$_s$	= suspended matter concentration	(g. m^{-3})
C$_s$	= contaminant concentration in upper sediment layer	(mg. kg^{-1})
C$_p$	= contaminant concentration in suspended matter	(mg. kg^{-1})
ρ_s	= dry density of sea bed	(g.m^{-3})
k	= decomposition rate of contaminant in sediment	(1.d^{-1})
δ	= thickness of homogeneous mixed upper layer	(m)

The density of the seabed depends on the characteristic of the sediment layer. For sandy sediment layer a value of 1500 kg/m^3 and for a muddy layer a value of 500 kg/m^3 is appropriate. The sedimentation flux F is determined based on the net sedimentation velocity and the suspended matter concentration in the water phase. The net sedimentation velocity is a model parameter that is defined by the model user in the input (or a default value can be used). The thickness of the homogeneous mixed upper sediment layer depends on the local physical conditions, human activities (i.e. dredging) and the biological activity. Appropriate values in estuarine systems are in the range of 0.1 to 0.5 meter. The sediment thickness used in the model should be a yearly averaged value, as the time-scale of the sediment processes is in the order of decades.

2.4   Biotic model component[3]

The biotic model component uses the environmental concentrations calculated by the abiotic model component as the starting point and calculates chemical concentrations in different food web compartments. This model relies upon biological processes and is an extension of previous PCB bioaccumulation models validated in the case of the dab food web in the Baie de Seine and that of the seabass in the Seine estuary. The biotic model includes two typical food webs:
1. a pelagic (round fish) food web, in which the top predator is the sea bass,
2. a benthic (flat fish) food web, in which the top predator is the flounder or dab.

Both food webs are representative of main food chains in estuarine ecosystems.

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[3] *This section is compiled from the final report of Ifremer on the trophic model (Ifremer, 2003)*

The simplified food webs

For purposes of the generic modelling in GEMCO, the round fish and the flat fish food webs needed to be simplified in a manner that each trophic level in the full food web would be represented, but no specific organisms would be designated (only 'generic' species). The two food webs and their simplified versions are shown in Figure 2.6 and Figure 2.7.
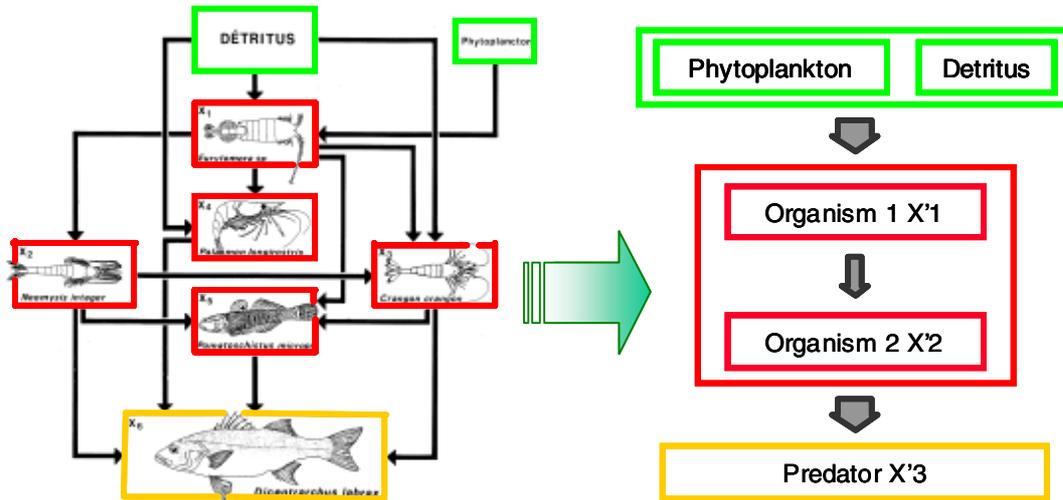
Figure 2.6   The sea bass model food web and its simplified version for the generic round fish food web in GEMCO. Colours are used to represent different trophic levels: Green: detritus and primary producers. Red: secondary producers. Orange: predators. X1= Eurytemora affinis, X2= Neomysis integer, X3= Crangon crangon, X4= Palaemon longirostris, X5= Pomatochistus microps, X6= Dicentrarchus labrax.
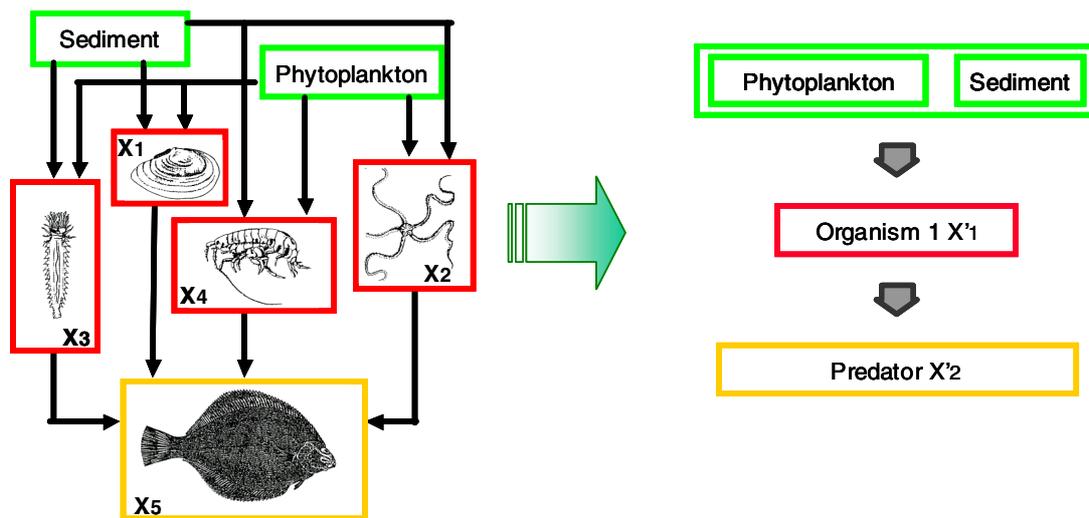

Figure 2.7   The dab model food web and its simplified version for the generic flat fish generic foodweb in GEMCO. Colours code is the same as for Figure IV 1. X1 = Tellina fabula, X2 = Acrocnida brachiata, X3 = Pectinaria koreni, X4 = Bathyporeia pelagica, X5 = Limanda limanda.

In the generic model, as well as in the specific ones, each biomagnification step had to be preserved so that the overall contaminant bioaccumulation was correctly evaluated. This implied that the dab food web could be simplified into a two link food chain (the flat fish and its prey) whereas the sea bass food web had to contain 3 links: zooplankton, one suprabenthic organism and the top predator. By doing so, the number of trophic links in the generic models was kept equal to the number of trophic links in the original specific models.

Structure of the generic food web model

In the generic food web model of GEMCO, it is assumed that the contaminant concentration in an organism varies as the result of uptake and loss processes. The transfer of contaminants from water, through the food web to a predator fish follows a number of different pathways schematised in Figure 2.8.

Direct uptake from water occurs during respiration. Feeding is the other main pathway through which contaminants adsorbed on particles (e.g. living phytoplankton cells, bacteria, detritus or sediment) enter the food chain. In the present models, bacteria are assimilated to their substrate (detritus or sediment) and are not modelled as explicit variable. The three loss processes taken into account are excretion, growth (which acts as dilution in enlarging body) and biotransformation. Contaminant losses during reproduction are not considered to be a relevant process for the GEMCO model, which is built to represent a steady state situation.
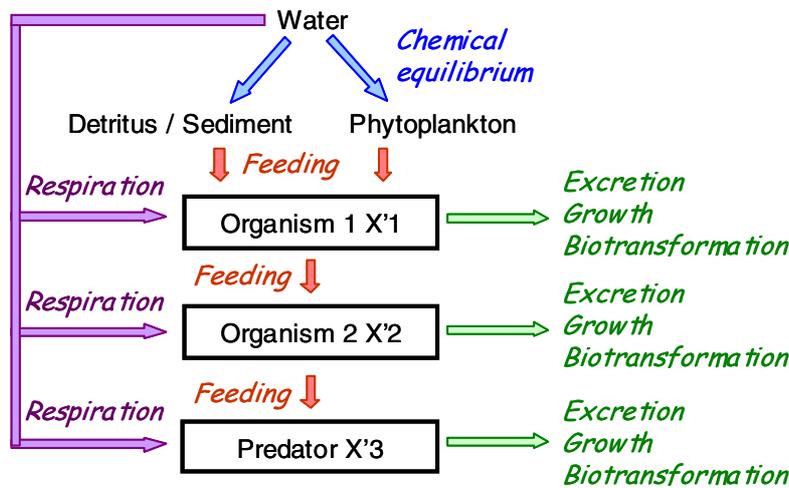
Figure 2.8 Schematisation of the bioaccumulation model within GEMCO. Normal characters symbolise the compartments in which the contaminant concentrations are known or calculated. Italics are used to show processes that affect these concentrations. The round fish food chain is represented here. The flat fish food chain contains only one species intermediate between particles and predator.

The variation of contaminant concentration in organism i (X_i) with time can be expressed as:

dX_i/dt = (uptake through respiration + uptake though nutrition) –
   (loss through excretion + dilution during growth + reproduction +biotransformation)

This balance equation represents the basic equation of bioaccumulation and is valid for each individual species in the trophic web. It shows that bioaccumulation relies upon the supply

of food and energy through respiration and feeding and most physiological functions such as excretion, growth, reproduction and metabolism act to decrease the contamination levels (see Figure 2.8).

Biotransformation is not represented in the generic food web model, thus in this respect the model leads to an overestimation of the predicted concentration in biota. Since the environmental abiotic conditions in which the flat fish or round fish food webs exist are in equilibrium, there is no evolution of the contaminant concentration in an organism over time, hence:

Xi = (uptake through respiration + uptake though nutrition) / (loss though excretion + dilution during growth)

Many physiological processes are dependent on animal age and size. In the formulations for the biological processes, organism weight is used as a proxy for age or size. Each organism used in the GEMCO model therefore has a default weight.

Biological processes

The biological processes included in the model are:

- *Respiration*: During respiration, marine organisms exchange chemicals with the surrounding water. The respiration rate is dependent on organism weight, water temperature, oxygen concentration in water and, for zooplankton, on food (chlorophyll) availability. The respiration rate 'R' describes the contribution of biology to contaminant uptake during respiration but this uptake is also related to contaminant concentration in water and to the contaminant properties (e.g. Kow).
- *Feeding*: Feeding has been shown to be the main route of contamination for hydrophobic persistent compounds. Contaminants are ingested with the prey and the predator contamination is therefore proportional to its nutrition rate. Assimilation is the process through which food and contaminant pass through the organism guts into its tissues. Contaminant assimilation efficiency through feeding is related to the contaminant hydrophobicity. The contamination through feeding is also dependent on the amount and the contamination of the prey.
- *Excretion*: Excretion in the context of the GEMCO model is considered to be loss of contaminant after it has been assimilated. Contaminant is then evacuated from the organism without chemical modification. The contaminant concentration in faeces is assumed to be the same as in the body.
- *Growth*: Growth can be regarded as a loss process because if there were no contaminant uptake during growth, the amount of contaminant in the body would be diluted as the organism increases its weight, and concentration would decrease. Contaminant losses are proportional to growth rates.
- *Biotransformation*: Biotransformation is the process through which contaminant assimilated in the organism is transformed via enzymatic reactions into chemicals that are *usually* less hydrophobic than the parent compound and that are more easily eliminated. Biotransformation is therefore a process of elimination that is exerted on contaminant incorporated in the organism flesh. In GEMCO, a simple formulation to simulate the effect of biotransformation on chemicals has been established (based on a biotransformation coefficient). Given the large uncertainties in the biotransformation

coefficients, it is recommended to calculate the concentrations in biota without including biotransformation (coefficient value = 1) unless appropriate values can be obtained.

Forcing variables

Forcing variables in the model are mainly the variables that depend on and define each estuary and the period of the year for which the simulation is carried out. In Table 2.4 an overview is given of the forcing variables within GEMCO and its default values.

Table 2.4:   Forcing variables of the food web model and their default values within GEMCO

Forcing variable	Definition	Default value in GEMCO	Unit
Chla	Chlorophyll a concentration in water column	18	μg/l
Lip	Phytoplankton lipid concentration	.045	g/g
O2	Dissolved oxygen concentration in water	5.8	mg/l
SPM*	Particle concentration in water column	120	mg/l
T*	Water Temperature	14.5	°C
f_{oc}*	Organic carbon fraction in SPM (flat fish model)	0.02	-
Zoo	Zooplankton density (round fish model)	1.17	mg/l
secprod	Secondary producer density (found fish model)	0.016	mg/l

* These forcing variables are also used in the abiotic model component of GEMCO

2.5   Validation of the GEMCO model

Several different calibration and validation steps have been performed within the GEMCO project, as summarised below.

Validation of the transport and mixing approach

In order to validate the method of applying an overall dispersion coefficient obtained from estuarine geometric and hydraulic characteristics, WL | Delft Hydraulics conducted several simulations using the generic shapes of the Scheldt, Seine and Guadalquiver. In these validation calculations, salinity in each estuary was calculated and compared with salinity measurements. This comparison is made based on 'salt intrusion curves', i.e. salinity as a function of distance along the estuary. Sensitivity tests in which the dispersion coefficient was varied were also conducted.

From these calculations, it was concluded that the use of the overall dispersion coefficient results in reasonable agreement between calculated and annual averaged measured salinity values. From the model sensitivity tests, it was clear that the salt intrusion curves are highly sensitive to the overall dispersion coefficient. As a bulk parameter, it represents all hydraulic and mixing processes, which are neglected in the tidal average approach of the GEMCO model. Further details of this validation study are provided in (WL | Delft Hydraulics, 2003a).

Validation of the abiotic model: application to the Scheldt estuary

A validation of the abiotic component of the generic GEMCO model was conducted by WL | Delft Hydraulics for the Scheldt estuary by analysing to what extent the generic estuary model with simple inputs can reproduce the results of a detailed numerical Scheldt model. For the validation, simulations of Cd, Cu, BaP, Atrazine, Lindane and PCB were performed using both the generic as well as the detailed Scheldt model. The calculated contaminant concentration from the GEMCO and the detailed model, were compared with each other as well as with field measurements. In general, it was concluded that the model results are in good agreement with the measurement, especially for BaP. Furthermore, it was observed that the GEMCO model results were comparable with those of the detailed Scheldt model. In view of the computational time (seconds versus hours) this is indeed a very satisfactory result. For a complete description of the validation study including information on the detailed Western Scheldt model, the reader is referred to (WL | Delft Hydraulics, 2003a).

Validation of the abiotic model: application to the Seine estuary

Ifremer also conducted a further validation of the abiotic component of the GEMCO model for the Seine estuary. The study evaluated model results for several different types of compounds: some organics and some metals, with affinity for the dissolved or particulate phase. The different model options were investigated and the sensitivity of results to the dispersion coefficients, to contributions and to boundary conditions was analyzed. The concentrations calculated by GEMCO model were compared with numerous measurements available in this estuary, measurements carried out by the Seine anti-pollution Unit (autonomous Port of Rouen) and by the laboratories taking part to the "Seine Aval" project (Chiffoleau and Tronczynski). The results were compared with information coming from SiAM-3D model for dissolved and particulate transport developed by Ifremer and applied to the Seine estuary (Cugier and Le Hir, 2000).

The Seine estuary is a man-altered macro-tidal estuary. At its mouth, a navigation channel is bordered by two flooded submersible dykes and two less deep channels that extend to the lateral banks. Inter-tidal muddy sand flats settled there sheltered by the dykes, therefore the depths vary a lot. Because of the dominant role of tidal pumping, turbidity maximum in the Seine estuary is usually situated around the salinity front. Depending on river flow and tidal cycle, the turbidity maximum moves along the estuary and suspended solids concentrations are very unsteady, varying between 0.5 to several g/l.

The basic concept of the GEMCO model does not describe or simulate the turbidity maximum area which is perceived as a trap or a filter for the contaminants. The model validation in an estuary like the Seine estuary reveals several limits for evaluation of chemical risk assessment. This aspect is in progress and a report will be issued in the near future.

Validation of the food web model

Both Ifremer and IVM conducted several different validation studies of the food web model:
- Validation of the round fish food web on PCB (congener) concentrations in the Ebro estuary show that the model is in good agreement with the field measurements, in this case within an order of magnitude.

- Validation of both food web models was conducted using the Dutch data from the Scheldt and Ems estuaries for PCBs (7 congeners) and HCB. In both cases the model predictions can be considered acceptable; in the sense that they are around (PCBs) or within (HCB) one order of magnitude lower than measured values. Predictions of pyrene and benzo(a)pyrene for molluscs were a factor of 1-7 higher than measured values in both estuaries in *Mytilus edulis*. In relation to the results for PCB153, the under prediction of the model for PAHs seems in line with the known biotransformation of PAHs in many aquatic organisms.
- Validation of both food web models for PCB congeners in the Seine estuary and Bay showed very good agreement between modelled results and measurements

Based on the conducted validation studies, it is concluded that given the generic nature of the food web model, the performance of the model for compounds tested in the log(Kow) range 5-8 were considered quite acceptable especially given the difficulty in obtaining some important estuary-specific input data and the lack of measurement data for comparison (both of which required many assumptions to convert available data to the required data). A complete description of the food web validation studies is given in the Ifremer- GEMCO Final Report (Ifremer, 2003).

3   Model use, applicability and way forward

A first version of the Generic Estuary Model for COntaminants (GEMCO) has been developed and includes both abiotic and biotic model components. The model has been developed to be user-friendly and is in principle applicable to all estuaries in Europe. It calculates chemical concentrations in water, sediment and biota in the estuary and the bordering coastal marine compartment.

3.1   Model use

Within the GEMCO model, each run is defined as an unique combination of three main components: "Compound" + "Emission" + "Estuary". For each component the user can either select or edit its default values, or create new properties.

The model can be applied for the 4 clusters of estuaries as obtained from the estuary classification as well as for specific real estuaries. For this, GEMCO contains a database with default values of the hydraulics characteristic and environmental conditions of more than 50 European estuaries. However, it should be noted that these values are obtained from a global literature screening and therefore have to be considered as preliminary. For more detailed site-specific information, the user is strongly invited to verify (and modify) these values for the selected estuary. Furthermore, to use GEMCO in real estuaries, it is strongly advised to apply salinity measurements for estimating the overall bulk mixing dispersion parameter.

Further detailed model instructions in the form of a User's Guide are given in Appendix B.

3.2   Applicability – abiotic component

As a direct consequence of the project objective, i.e. development of an easy-to-use generic estuary model, various assumptions and simplifications has been built into the model. The model assumptions and simplifications ultimately determine the applicability and use of the model. Based on the currently performed validation of the model, the following issues are addressed towards the applicability of the model.

1. The model has a standard and simplified geometric shape for a *generic* estuary, and incorporates simplified processes under long-term average conditions. Obviously, there are no real estuaries, which will exactly match the shape and characteristics of such a generic estuary. For detailed fate and transport analysis of a specific estuary under particular conditions, the use of a detailed site-specific model is recommended.

2. The model has a standard and simplified "trumpet" shaped estuary and assumes that the estuary is vertically well mixed (2DH model). For application of the model to specific estuaries that are known to be strongly stratified or have significant density currents, results have to be carefully analysed and interpreted. Results of these analyses should be

used as guidelines for including additional functionality's and descriptions in the model concept.

3. The model does not taken into account the impact of man-made structures in the estuary (like channel and dykes) or activities influencing the sediment behaviour like dredging and dumping of contaminated sediments.

4. The generic model cannot take into account the complex behaviour of hydrodynamics and the fine sediment dynamics in inter-tidal areas. As such the modelling of suspended matter is not included, but rather a default (or user specified) suspended solids concentration is imposed on the estuary as a model forcing function. As a result, the turbidity maximum and its filtering capacity caused by tidal asymmetry and density induced currents is not included. In case of trapping of material, this is considered as a conservative approach in the risk assessment since the particulate contaminant concentrations will be overestimated.

5. The same holds for modelling of primary production based on nutrient concentrations and algae growth. Default (or user specified) chlorophyll concentrations are imposed on the estuary as a model forcing function (in a similar manner to suspended solids).

6. GEMCO is a steady state model, calculating an equilibrium concentration of a contaminant based on a continuous discharge from upstream of the estuary or from one of the estuary banks. As such, the model calculates seasonal changes only in terms of a 'winter average' and a 'summer average'. Furthermore, at present the model is not suitable to evaluate temporary discharges or accidental spills.

3.3   Applicability – biotic component

1. The biotic model component has been calibrated for neutral organic substances (PCBs and several other persistent compounds). Its applicability is recommended for substances having values of Log(Kow) in the range of 5-7.

2. The model calculates concentration data for PCBs or for compounds that are persistent and behave like PCBs within one order of magnitude of measured concentrations. In the case of less persistent compounds, the model is expected to over-estimate concentration in biota, as biotransformation is not considered. in default mode.

3. A simple formulation for biotransformation is included by means of an empirical biotransformation factor. However, uncertainty remains as to the accuracy of this method. Therefore, a two step approach is proposed for calculating the concentration in biota. First the model should be run without considering biotransformation,- assuming that the substance is persistent and behaves like PCBs. This calculated concentration could be considered as the worst case scenario. In a second step, the model can be run with biotransformation, and the two calculated concentrations can be compared.

4. The models provide the predicted concentration in a generic target fish. There are no real fish which perfectly match with the virtual fish and with which they could be directly compared. In the case of lower organisms, there are no real intermediary species

that could be compared with intermediary species simulated by the generic models. Mussels have been extensively used as sentinel species in pollution monitoring programmes and much information can be found in the literature on contaminants in these organisms. However, mussels do not exactly correspond to the intermediary species of the models.

5. Predicted concentrations in biota are expressed in terms of dry weight concentrations in a whole organism (e.g. fish species). This usually differs from contaminant concentrations as reported in literature: Contaminants are measured in specific types of organs (tissues) and concentrations are often expressed in a different manner, either dry weight, fresh weight or lipid basis. Thus, in comparing model results with actual data, the predicted dry weight concentrations could not be compared directly with actual measurements.

3.4   Way forward

With the present developed generic GEMCO model, it is emphasised that a major step forward has been achieved for risk assessment of contaminants in estuaries and coastal marine areas. The model allows for a far more spatial resolution than the currently applied one box exposure approaches that necessarily include large safety factors.

Inherent to the objective, i.e. development of an easy-to-use generic estuary model, various assumptions and simplifications have been built into the model. In order to quantify the impact of the model simplifications and its related range of applicability, a further sensitivity analysis as part of an extended validation is proposed.

Within the present study, GEMCO has been validated for both the Scheldt and the Seine estuary. However, for an improved understanding of the range of applicability, the validation has to be extended to various other estuaries with different system behaviour.

As such, the objectives of an extended application/validation study can be formulated as follows:

- *Achieve a broadly accepted and supported risk assessment model for estuaries and adjacent coastal compartment by application and validation of the GEMCO model for a wide range of estuaries, chemicals and environmental conditions.*
- *Identify and quantify the applicability of GEMCO (e.g. for certain types of systems or chemicals).*

At the end this might result in:
1. A broadly supported risk assessment model within industry and the EC;
2. More accurate predictions and descriptions of the fate of contaminants in estuaries (i.e. lower and more scientifically sound safety factors or confidence intervals);
3. Recommendations and guidelines for additional monitoring campaigns.

Within an extended application/validation study, the required model parameters and their ranges can be quantified with respect to a certain accuracy level of the model outcome. In other words, several validation levels can be distinguished each having a list of required input parameters and ranges and associated level of accuracy. By comparison of the required

model input with the available data, guidelines for further field measurements can be addressed.

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A   List of European estuaries

Table A   Results of literature search on estuary indicators (Class 1)

Cluster	ID	Name	Q_{mean}	h_0	B_0	A_0	H_0	b	b / h	P	N	F_d	N_r	D_0	K	L_s
			[m³/s]	[m]	[m]	[m²]	[m]	[km]	[-]	[m³]	[-]	[-]	[-]	[m²/s]	[-]	[km]
1	85	Douro	544.0	6.0	800	4800	2.8	29	4833	66240000	0.37	0.6	0.7	2350	0.5	30.3
1	7	Ebro	430.0	6.8	1500	10200	0.6	29	4265	140760000	0.14	0.5	0.3	1729.3	0.4	46.6
1	33	Firth of Tay	175.0	30.0	3000	90000	3.7	44	1467	1242000000	0.01	0.1	0.1	2268.3	0.6	176
1	87	Minho	320.0	7.0	1900	13300	2.9	17	2429	183540000	0.08	0.5	0.2	2327.6	0.5	47.6
1	80	Nieuwe Waterweg	1648.0	24.0	2000	48000	1.9	90	3750	662400000	0.11	0.1	0.8	3334.2	0.6	110
1	83	Odra Estuary	640.0	6.0	1500	9000	0.1	25	4167	124200000	0.23	0.6	0.4	2159.3	0.4	37.6
1	79	Po	1550.0	2.0	2100	4200	0.8	26	13000	57960000	1.20	1.7	0.7	910.29	0.3	9.46
1	20	Rhone	1687.0	7.0	1000	7000	0.3	36	5143	96600000	0.78	0.5	1.7	3478.7	0.5	26
1	55	Tees Estuary	20.0	18.0	700	12600	4.4	17	944	173880000	0.01	0.2	0.0	2465.2	0.8	84.5
1	78	Tiber	250.0	4.0	400	1600	0.8	19	4750	22080000	0.51	0.8	0.6	2292.5	0.5	20.1
1	59	Tweed Estuary	78.0	3.0	150	450	4.1	14	4667	6210000	0.56	1.1	0.5	2128.4	0.6	14.6
1	84	Wisla Estuary	1055.0	4.0	2000	8000	0.1	23	5750	110400000	0.43	0.8	0.5	1739.8	0.4	25.3

1.   Indicators shaded in grey are those used in the final classification

Table A   Results of literature search on estuary indicators (Class 2)

Cluster	ID	Name	Q_{mean}	h_0	B_0	A_0	H_0	b	b / h	P	N	F_d	N_r	D_0	K	L_s
			[m³/s]	[m]	[m]	[m²]	[m]	[km]	[-]	[m³]	[-]	[-]	[-]	[m²/s]	[-]	[km]
2	17	Aulne	24.0	5.0	3000	15000	7.4	5	1000	207000000	0.01	0.7	0.0	1232	0.4	30.4
2	68	Blackwater	77.0	7.0	1500	10500	3.8	11	1571	144900000	0.02	0.5	0.1	1986	0.5	45.2
2	73	Corrib	110.0	4.0	700	2800	4.5	14	3500	38640000	0.13	0.8	0.2	1560.1	0.5	29.9
2	25	Dart Estuary	11.0	9.0	2025	18225	4.0	6	667	251505000	0.00	0.4	0.0	1522.8	0.6	40.9
2	72	Erne	85.0	3.0	1500	4500	3.9	6	2000	62100000	0.06	1.1	0.1	1639.5	0.4	22.8
2	30	Exe Estuary	41.0	2.0	600	1200	4.1	6	3000	16560000	0.11	1.7	0.1	1200.2	0.4	17.3
2	31	Falmouth	8.0	5.5	1600	8800	5.3	5	909	121440000	0.00	0.6	0.0	1071.4	0.5	31.7
2	34	Fowey Estuary	19.0	6.0	600	3600	4.8	8	1333	49680000	0.02	0.6	0.0	1838.3	0.6	35.9
2	35	Helford Estuary	6.0	6.0	2600	15600	4.7	4	667	215280000	0.00	0.6	0.0	992.54	0.5	29.6
2	71	Liffey (Dublin)	34.0	2.0	700	1400	3.3	3	1500	19320000	0.08	1.7	0.0	2023.8	0.5	13
2	38	Loch Crinan	16.0	5.0	1000	5000	3.7	4	800	69000000	0.01	0.7	0.0	2177.9	0.6	23.7
2	39	Loch Gilp	8.0	4.0	2000	8000	3.1	2	500	110400000	0.00	0.8	0.0	1742.3	0.5	15.4
2	82	Lupawa Estuary	12.0	2.0	200	400	0.1	4	2000	5520000	0.10	1.7	0.1	1687	0.6	13.8
2	41	Lyne	30.0	4.0	3000	12000	6.8	3	750	165600000	0.01	0.8	0.0	1836.6	0.4	19.7
2	42	Medway Estuary	34.0	8.0	2000	16000	4.1	7	875	220800000	0.01	0.4	0.0	2052.5	0.5	40.4
2	45	Neath Estuary	37.0	2.0	1500	3000	8.6	4	2000	41400000	0.04	1.7	0.0	1081.7	0.4	17.2
2	46	Nith Estuary	44.5	3.0	1000	3000	6.6	3	1000	41400000	0.05	1.1	0.0	2905.7	0.5	15.3
2	47	Ouse Estuary (Newhaven Estuary)	5.0	2.0	50	100	6.1	4	2000	1380000	0.16	1.7	0.1	2177.9	0.8	11.7
2	11	Ria A Coruna	6.0	16.0	3100	49600	3.0	5	313	684480000	0.00	0.2	0.0	1939.1	0.7	43.5
2	9	Ria de Arosa	49.0	4.0	3000	12000	3.1	6	1500	165600000	0.01	0.8	0.0	1173.6	0.4	30.2
2	10	Ria de Camarinas	7.0	6.0	600	3600	2.9	5	833	49680000	0.01	0.6	0.0	1785.3	0.7	29.3
2	12	Ria de Murosy Noya (Ria de Muros)	34.0	14.0	2200	30800	3.1	12	857	425040000	0.00	0.2	0.0	1997.7	0.6	69
2	14	Ria de Vigo	13.0	20.0	4600	92000	3.1	8	400	1269600000	0.00	0.2	0.0	1830.6	0.6	64.7
2	49	Salcombe & Kingsbridge Estuary	5.0	10.0	2200	22000	4.6	3	300	303600000	0.00	0.3	0.0	2188.9	0.6	26.2
2	77	Sligo Bay	90.0	6.0	4000	24000	3.9	8	1333	331200000	0.01	0.6	0.0	1549.6	0.4	40.5
2	52	Spey Bay	64.0	5.0	400	2000	3.4	16	3200	27600000	0.10	0.7	0.2	1721.8	0.6	34

2	54	Tamar Estuary	44.0	10.0	4800	48000	4.7	7	700	662400000	0.00	0.3	0.0	1884	0.5	46.4
2	56	Teifi Estuary	28.0	3.0	1800	5400	4.1	3	1000	74520000	0.02	1.1	0.0	1717.9	0.4	17.3
2	91	Tejo	380.0	7.0	5800	40600	3.4	11	1571	560280000	0.03	0.5	0.1	2243.6	0.4	47
2	16	Tinto Estuary	35.0	5.0	1450	7250	3.2	9	1800	100050000	0.02	0.7	0.0	1188.9	0.5	38.7
2	61	Yealm Estuary	5.0	4.0	525	2100	4.7	4	1000	28980000	0.01	0.8	0.0	1344.2	0.6	22.7

Table A   Results of literature search on estuary indicators (Class 3)

Cluster	ID	Name	Q_{mean}	h_0	B_0	A_0	H_0	b	b / h	P	N	F_d	N_r	D_0	K	L_s
			[m³/s]	[m]	[m]	[m²]	[m]	[km]	[-]	[m³]	[-]	[-]	[-]	[m²/s]	[-]	[km]
3	62	Barthe River	2.0	2.0	800	1600	0.1	3	1500	22080000	0.00	1.7	0.0	459.14	0.5	17.5
3	69	Boyne	35.0	1.0	700	700	3.1	5	5000	9660000	0.16	3.3	0.0	616	0.3	11.6
3	70	Carlingford Lough	3.0	6.0	2900	17400	4.5	5	833	240120000	0.00	0.6	0.0	531.63	0.5	37
3	24	Cree Estuary (Wigtown Estuary)	16.0	2.5	6000	15000	6.7	11	4400	207000000	0.00	1.3	0.0	161.66	0.3	46.1
3	27	Dee Estuary (Dumfriess & Galloway) -	47.0	2.0	2500	5000	6.7	4	2000	69000000	0.03	1.7	0.0	944.31	0.3	18.2
3	28	Dee Estuary (Grampian) - Aberdeen	42.0	1.0	800	800	3.7	10	10000	11040000	0.17	3.3	0.1	315.61	0.3	12.7
3	26	Dee Estuary (North Wirral) - Wales	31.0	2.0	6600	13200	7.6	25	12500	182160000	0.01	1.7	0.0	75.52	0.2	53.6
3	29	Duddon Estuary	23.0	1.0	5000	5000	8.1	10	10000	69000000	0.01	3.3	0.0	93.421	0.2	26.1
3	15	Guadalquivir	101.0	2.0	6750	13500	3.2	16	8000	186300000	0.02	1.7	0.0	210.61	0.2	37.9
3	86	Guadiana	166.0	1.5	1450	2175	3.2	9	6000	30015000	0.25	2.2	0.1	776.76	0.3	15.5
3	8	Jucar	42.0	3.0	400	1200	0.6	13	4333	16560000	0.11	1.1	0.1	1030	0.5	24.9
3	2	Kolding Fjord	19.0	4.5	3000	13500	0.3	8	1667	186300000	0.00	0.7	0.0	657.71	0.4	39.6
3	40	Lune	31.0	2.0	1700	3400	8.4	4	2000	46920000	0.03	1.7	0.0	930.02	0.4	17.9
3	4	Mariager Fjord	18.0	2.5	1000	2500	0.4	25	10000	34500000	0.02	1.3	0.0	184.8	0.3	38.8
3	43	Mersey Estuary	84.0	5.0	1600	8000	8.9	30	6000	110400000	0.03	0.7	0.1	526.01	0.4	55.4
3	88	Mondego	126.0	1.0	800	800	2.7	10	10000	11040000	0.51	3.3	0.2	546.65	0.3	9.05
3	89	Odelouca	4.0	6.0	700	4200	3.3	10	1667	57960000	0.00	0.6	0.0	624.74	0.6	49.6
3	5	Randers Fjord	28.0	1.6	2600	4160	0.4	20	12500	57408000	0.02	2.1	0.0	114.35	0.2	33.3
3	65	Rechnitz River	4.0	2.0	3000	6000	0.1	2	1000	82800000	0.00	1.7	0.0	502.96	0.4	14.4
3	13	Ria de Pontreveda	15.0	7.0	1800	12600	2.9	9	1286	173880000	0.00	0.5	0.0	977.98	0.5	48.8
3	48	Ribble Estuary	33.0	2.0	8000	16000	7.9	5	2500	220800000	0.01	1.7	0.0	353.87	0.3	25.6
3	90	Sado	55.0	1.0	2600	2600	2.9	20	20000	35880000	0.07	3.3	0.0	100.17	0.2	17.6
3	22	Somme	34.0	1.0	4500	4500	10.0	10	10000	62100000	0.02	3.3	0.0	119.73	0.2	23.7
3	51	Southampton Water	41.0	8.0	3000	24000	4.0	23	2875	331200000	0.01	0.4	0.0	560.09	0.4	86.7
3	53	Stour Estuary	7.0	4.0	2200	8800	3.6	20	5000	121440000	0.00	0.8	0.0	155.39	0.4	71.2
3	60	Tyne Estuary	3.0	12.0	1200	14400	4.3	19	1583	198720000	0.00	0.3	0.0	434.97	0.6	103
3	6	Vejle Fjord	38.0	8.3	6000	49800	0.3	18	2169	687240000	0.00	0.4	0.0	505.46	0.4	86.4
3	66	Warnow River	18.0	2.0	800	1600	0.1	5	2500	22080000	0.04	1.7	0.0	826.45	0.4	19

Table A   Results of literature search on estuary indicators (Class 4)

Cluster	ID	Name	Q_{mean}	h_0	B_0	A_0	H_0	b	b / h	P	N	F_d	N_r	D_0	K	L_s
			[m^3/s]	[m]	[m]	[m^2]	[m]	[km]	[-]	[m^3]	[-]	[-]	[-]	[m^2/s]	[-]	[km]
4	23	Clyde Estuary	169.0	31.0	8000	248000	3.0	43	1387	3422400000	0.00	0.1	0.0	1443.3	0.5	206
4	63	Elbe	726.0	13.5	17250	232875	3.3	20	1481	3213675000	0.01	0.2	0.0	1907.4	0.4	93.6
4	64	Ems	125.0	3.9	12000	46800	3.6	17	4359	645840000	0.01	0.8	0.0	322.51	0.3	61
4	32	Firth of Forth	44.0	45.0	15000	675000	4.8	33	733	9315000000	0.00	0.1	0.0	1017.3	0.5	232
4	1	Flensborg Fjord	12.0	12.0	5000	60000	0.2	25	2083	828000000	0.00	0.3	0.0	323.9	0.4	131
4	18	Gironde	900.0	10.0	14000	140000	4.5	33	3300	1932000000	0.02	0.3	0.1	1058.3	0.3	100
4	36	Humber Estuary	294.0	19.0	12000	228000	8.0	20	1053	3146400000	0.00	0.2	0.0	2048.2	0.4	109
4	37	Inverness Firth	91.0	35.0	6000	210000	3.7	38	1086	2898000000	0.00	0.1	0.0	1562.4	0.6	203
4	74	Lee	39.0	8.0	8000	64000	3.7	12	1500	883200000	0.00	0.4	0.0	641.15	0.4	68.2
4	19	Loire	835.0	13.0	12750	165750	5.1	27	2077	2287350000	0.02	0.3	0.1	1697.2	0.4	102
4	44	Morecambe Bay	51.0	10.0	16000	160000	8.4	33	3300	2208000000	0.00	0.3	0.0	235.66	0.3	150
4	75	Moy	51.0	15.0	11000	165000	3.9	14	933	2277000000	0.00	0.2	0.0	1004.9	0.4	91.2
4	81	Schelde	110.0	10.0	15000	150000	3.7	28	2800	2070000000	0.00	0.3	0.0	421.27	0.3	123
4	21	Seine	435.0	6.0	13500	81000	7.0	9	1500	1117800000	0.02	0.6	0.0	1648.4	0.3	44.2
4	50	Severn Estuary	131.0	10.0	19500	195000	12.3	25	2500	2691000000	0.00	0.3	0.0	451.59	0.3	118
4	76	Shannon River	176.0	10.0	3500	35000	4.5	30	3000	483000000	0.02	0.3	0.0	1029.6	0.4	91.4
4	57	Thames Estuary	150.0	8.0	7500	60000	6.5	23	2875	828000000	0.01	0.4	0.0	677.55	0.3	86.8
4	58	The Wash	48.0	10.0	5500	55000	6.5	30	3000	759000000	0.00	0.3	0.0	428.93	0.4	120
4	67	Weser	326.0	10.0	12000	120000	3.6	17	1700	1656000000	0.01	0.3	0.0	1335.5	0.4	78.8
4	67	Weser	326.0	10.0	12000	120000	3.6	17	1700	1656000000	0.01	0.3	0.0	1335.5	0.4	78.8

Table B   Summary results

Average values	Qmean	h0	B0	A0	H0	b	b / h	P	N	Fd	Nr	D0	Ksav	Ls
cluster 1, river dominated estuaries	646	9	1312	16088	2	28	4243	240522500	0.34	1	1	2091	1	48
cluster 2, small high disperive estuaries	44	6	1937	15112	4	6	1319	208546935	0.03	1	0	1719	1	31
cluster 3, small low disperive estuaries	38	3	2800	9016	4	12	5618	124414393	0.06	2	0	476	0	37
cluster 4, large estuaries	252	14	11275	160571	5	25	2118	2215883250	0.01	0	0	1030	0	114

B   Gemco User Manual

1   Installation

The program needs about 30 Mb disk space, 128 MB memory and a Pentium III processor or better. It runs on Windows 95, 98, 2000, XP and NT.
GEMCO is provided as either a downloadable set-up program or is provided on CD.

From CD:
Insert the CD in your CD-ROM player. Run D:\setup.exe Where D stands for you CD-ROM drive letter.

From download:
Download the files :

- setup.exe

- gemco.cab

- setup.lst

to a temporary directory. Run "setup.exe".

2   Introduction

This manual provides a step by step instruction to installing and running the GEMCO model. The program calculates concentrations in water sediment and biota in a generic or user defined estuary. The user interface provides access to the main functions:

- select a chemical compound

- select an estuary

- select an emission of a compound in the estuary

- calculate concentrations

- view results

and provide access to the database:

- add/edit/delete chemical compounds

- add/edit/delete estuaries

- add/edit/delete emissions

The program comes provided with an existing database, containing several compounds and dimensions of over 50 European estuaries.

3   Main menu

When you start the GEMCO program you'll see the main menu on the left, which provides access to starting a calculation (run) or viewing previous results. The main menu bar on top gives access to adding, changing and deleting compounds, estuaries and emissions.
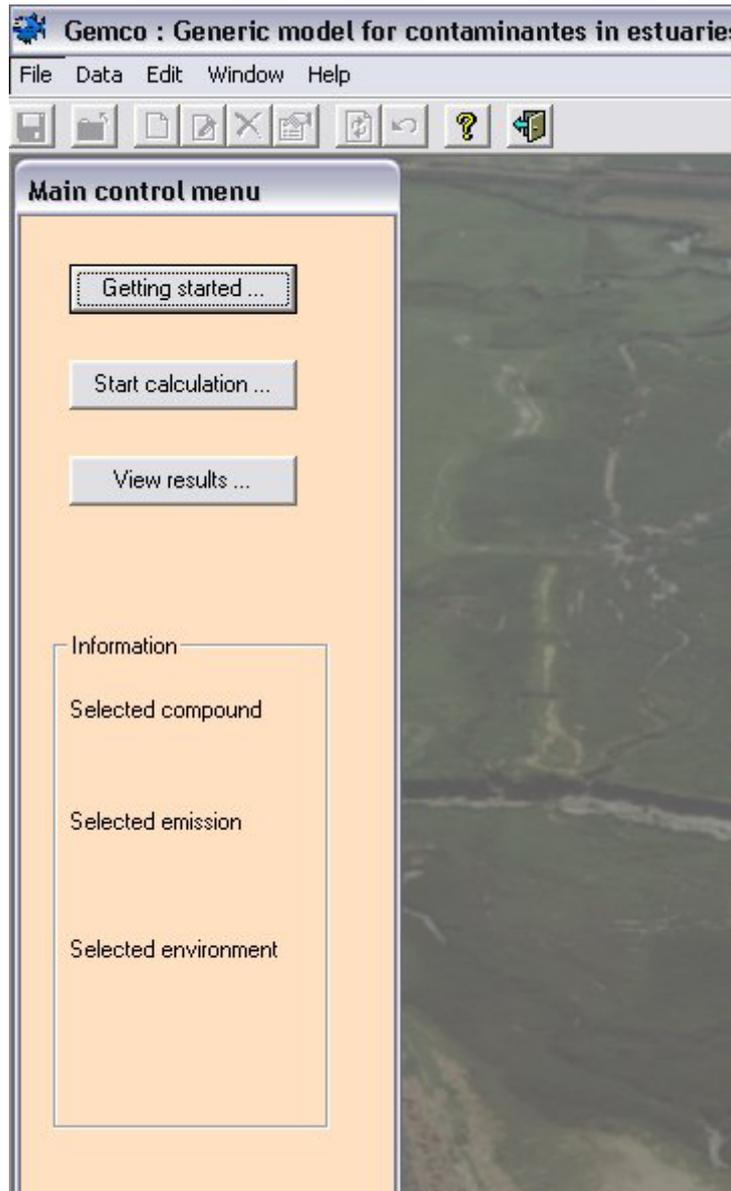
4   Starting a calculation

There are three levels of detail in the estuary definition that you can select. The first level provides four different generic 'annual averaged' estuaries. In the second level you can select the seasonal (summer/winter) scenarios for the generic estuaries. The third level provides access to user defined specific estuaries.
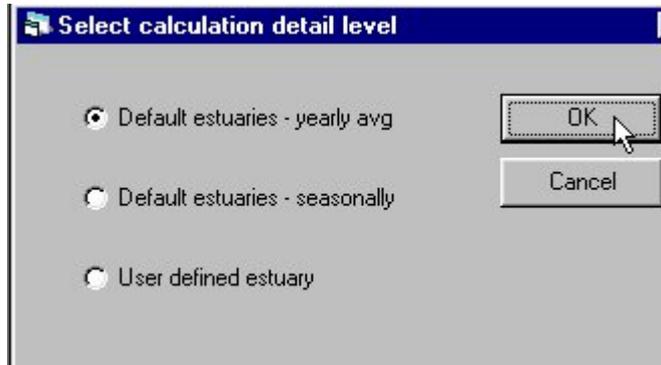
Doing a calculation implies the following actions:

- select tier level

- selecting a chemical compound

- selecting an estuary

- selecting an emission of a compound in the estuary

- calculate concentrations

- view results

After selecting the tier level, you can select from a list of pre-defined compounds, emissions and estuaries. The selected items are shown on the main menu info box on the left.
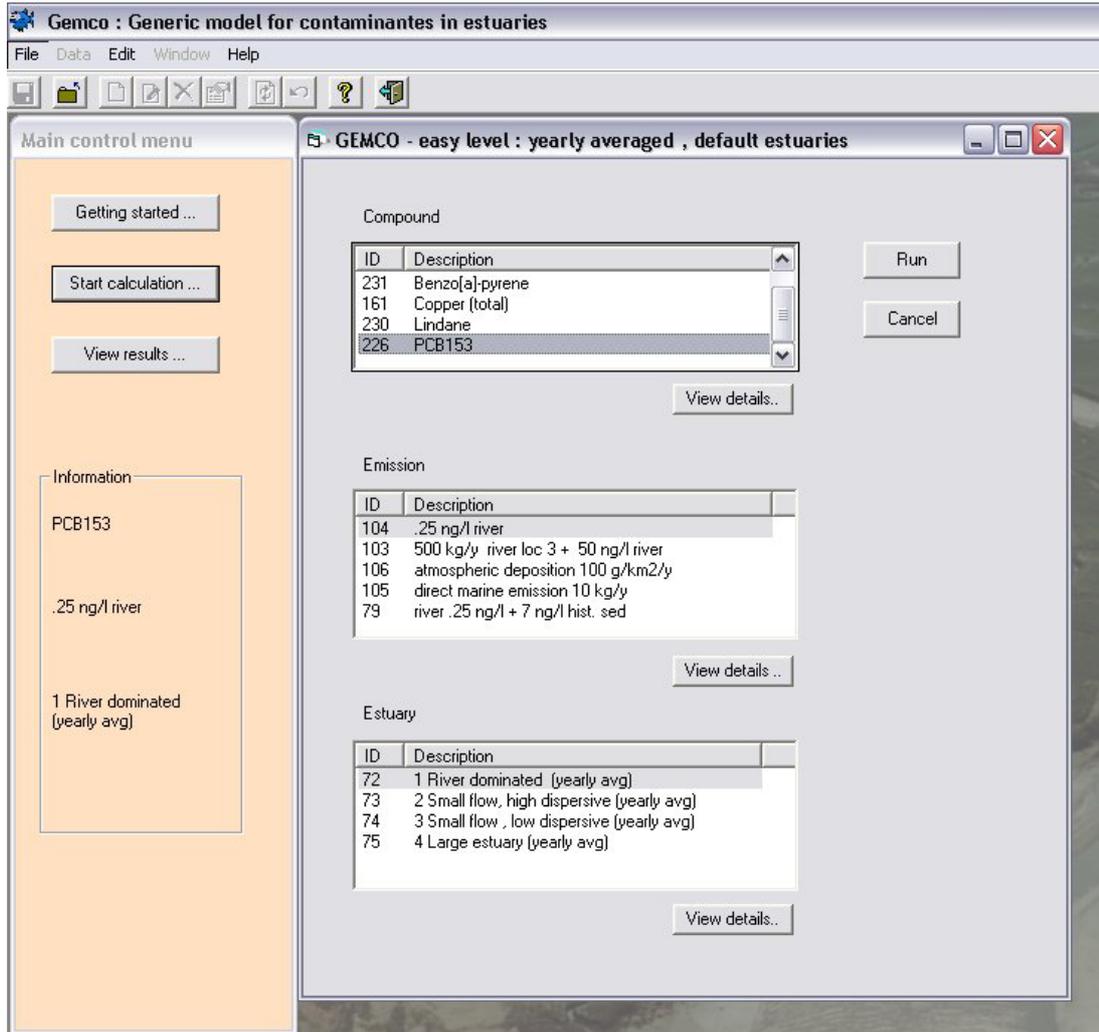
To run press "OK" button. The program will start the calculation and show the results.

The view details buttons show the properties of the selected items. You can not change the properties in this view mode. To add, edit or delete predefined items you must use the EDIT function in the menu bar.

5   Edit, copy, add or remove compounds

In GEMCO you can edit, copy and remove pre-existing compound data. Items that have been used in calculations can not be edited or removed as long as the result from the calculation is stored in the database.

Tip: You can copy the data and change the values in the copy

You can remove previous calculations through the menu bar: EDIT - Run list...
To access the compound data use "EDIT - Compound list" in the menubar.
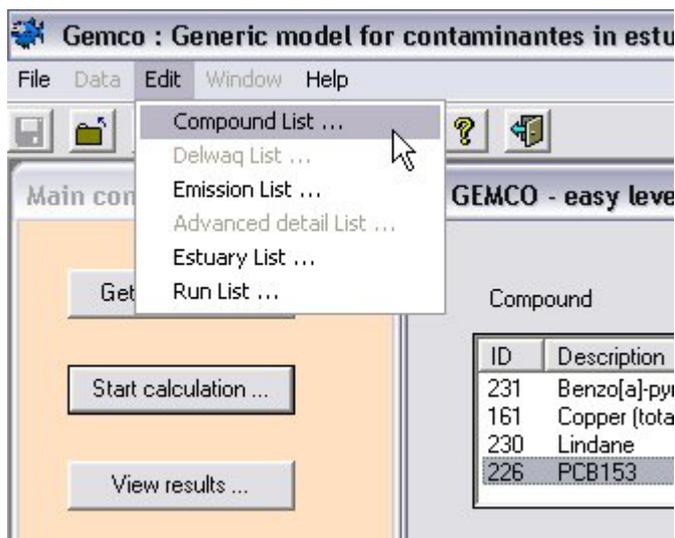
This will show a list of all available compounds in the database. You can add, copy, edit or delete a compound by using the buttons below the list. Clicking on the column header will sort the column alphabetically.
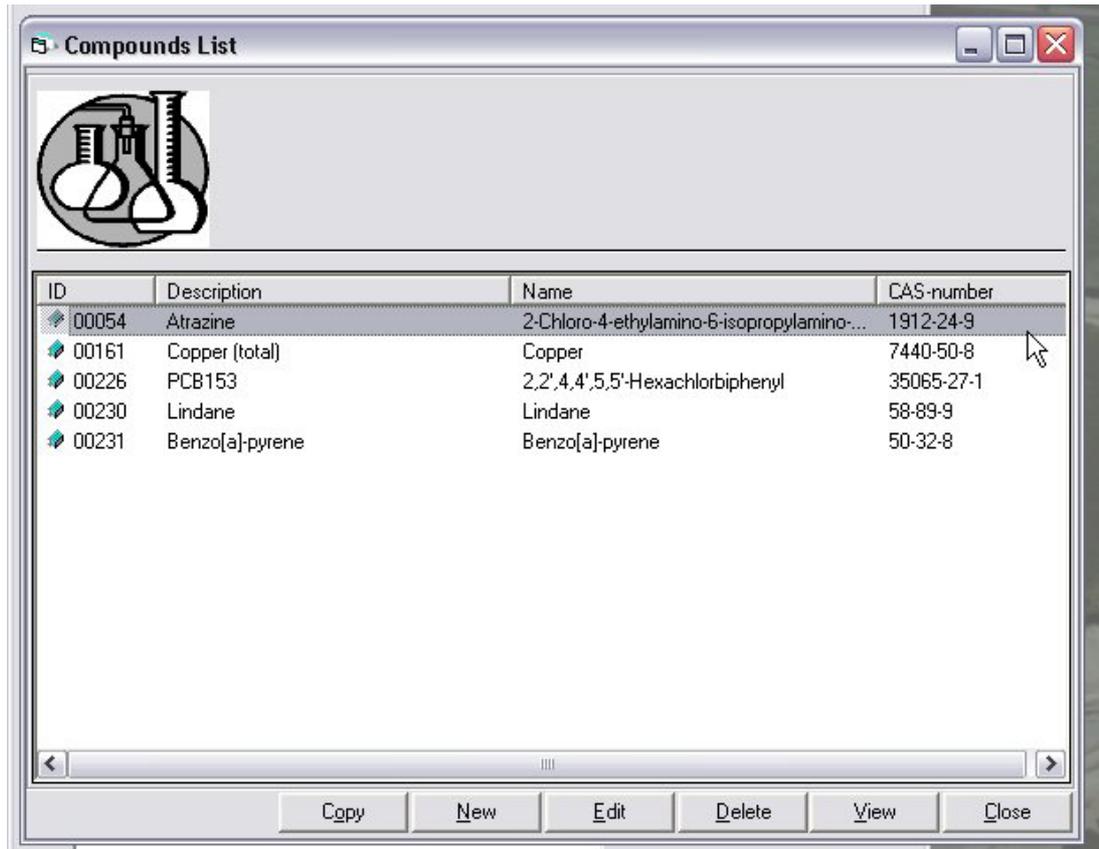
Clicking the Copy, New or Edit button will bring you to the detail input screen. The View button shows the same information but you can not change anything in the View mode.

6   Detailed compound information

Clicking the Copy, New or Edit on the compound list screen will bring you to the detailed compound input screen:

List of compound details:
- Description :   User defined description of the compound
- Name :   Chemical name of the compound
- CAS number :   CAS number of the compound
- Type: Select between "Heavy metal" or "Organic compound"
- Molecular mass :
  Molecular mass of compound, unit: gram / mol
- log(Kow)
  Octanol - water coefficient. Expressed as 10-log value. Disabled for metals.
- Kd :
  Sediment - water partition coefficient, unit: liter / gram. Disabled for organic compounds.
- Henry's coefficient :
  Henry's coefficient, equilibrium between gas and water phase concentrations. Pressing the question mark will enable the QSAR to estimate this parameter : He = Molecular mass * Vapour pressure / Solubility

- Partition coefficient between water and organic carbon log(Koc)

Organic carbon - water partition coefficient, disabled for metals. Expressed as 10-log. Pressing the question mark will enable the QSAR module to estimate this parameter. Two methods are available:

Sablic
$\log(Koc) = 0.1 + 0.81 * \text{Log}(Kow)$

Else
$\log(Koc) = \text{Log10}((1 / (10 \char94 (8 - pKa.)) + 1)) * 10 \char94 (\log(Kow))$

- Degradation rates

You can specify individual degradation rates for biodegradation, hydrolysis and photolysis in water and for compounds bound to sediment. Please note that the photolysis rate is the 24h depth averaged rate. Degradation rates are disabled for metals.

- Biotransformation correction factors

  These factors allow for correction of calculated concentrations in various levels in the foodchain.
  Corrected concentration = (1 - biotransformation factor) * original concentration

- Bioaccumulation: alpha water

- Uptake efficiency from water

7   Edit, copy, add or remove emissions

To change an emission scenario go to the menu "Edit - Emissions list"
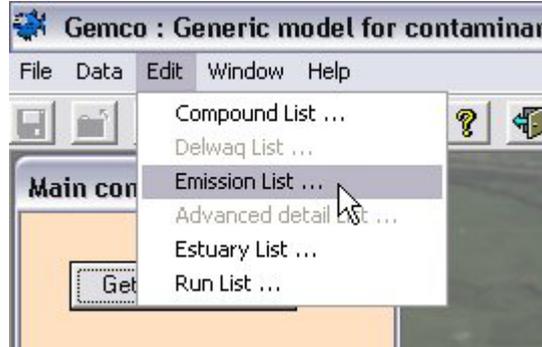
This will show a list of all available emission scenarios in the database. You can add, copy, edit or delete an emission scenario by using the buttons below the list. Scenarios which have been used in a calculation can not be changed unless the results from the previous calculation are removed first (data integrity). Clicking on the column header will sort the column alphabetically.
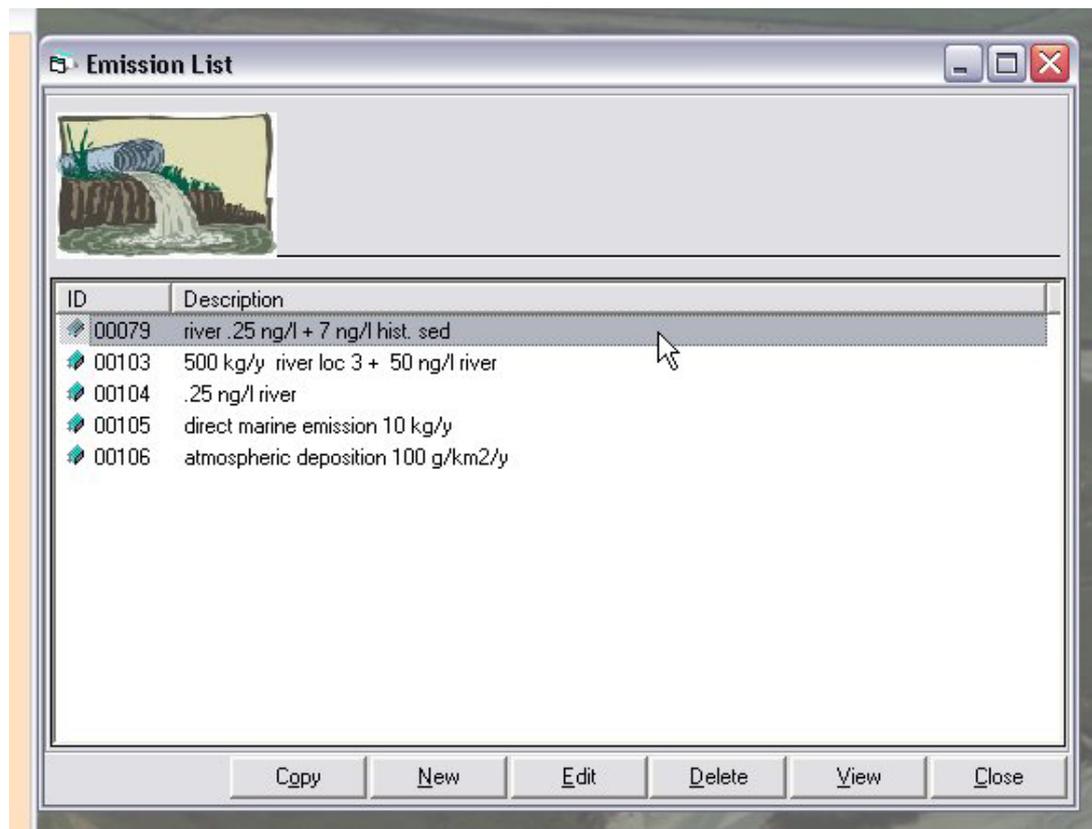
Clicking the Copy, New or Edit button will bring you to the detail input screen.

8   Emission details

Clicking the Copy, New or Edit button on the emission list window will bring you to the detail input screen.
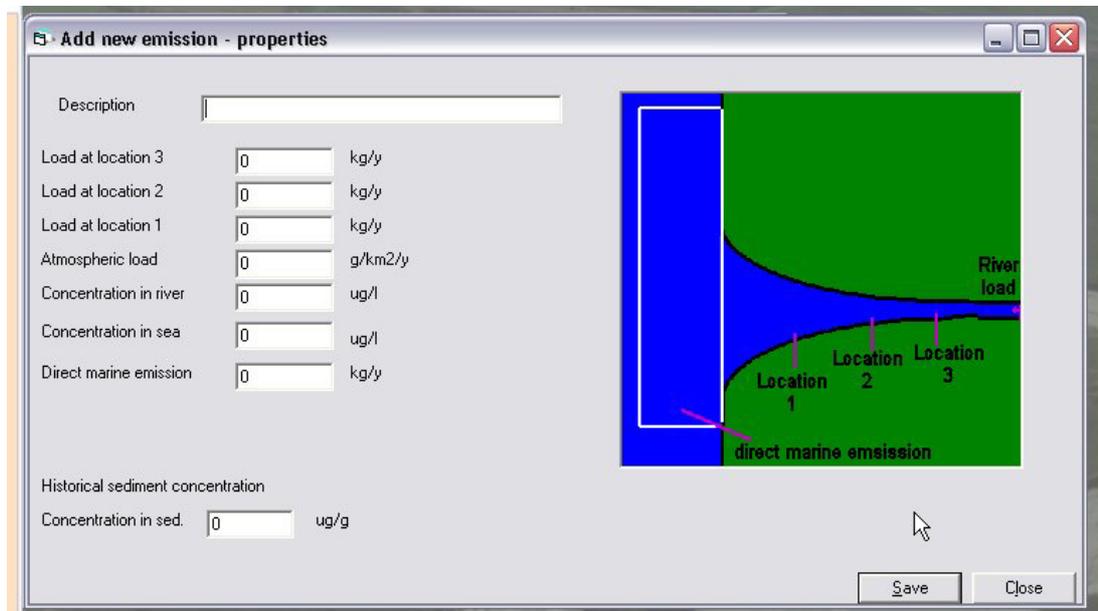
The user can select a number of emission input types:
- Direct river load (concentration in the river)
- Direct emission into the estuary

  There are three predefined schematised emission locations defined on the "south" border of the estuary. The locations are defined relative to the length of the estuary. Location 3 is at 50 % of the estuary length, location 2 at 25% and location 1 at 12.5 % (0 % is defined as the sea-estuary interface). Due to the generic nature of the estuary schematisation the locations are to be considered as indicative of the position along the estuary. Further detailing would require detailed description of the conditions close to the emission. This is beyond the scope of this generic risk assessment.

- Atmospheric deposition

  Is defined as an average uniform load (g/km2/y). It is considered to be uniformly distributed over the estuary and consisting of both wet and dry deposition. A good estimate of the atmospheric deposition anywhere in Europe can be obtained from the ADEPT model (TNO / Delft Hydraulics, 2003)

- Background concentration in sea
- Historical sediment concentration

 Normally this value should be set to zero. In cases where emissions have been reduced

in the last period, but these changes are not yet reflected in the sediment trapped in the estuary, this parameter can be used as a correction for the calculated sediment concentration values. If the calculated concentration that reflects the current emissions is higher than the historical background concentration, the calculated sediment concentration is used. If the historical (known) background concentration is higher than the current calculated concentration, the known concentration is used.

9   Copy, edit, add or remove estuaries

In GEMCO you can edit, copy and remove pre-existing estuary data. The user can not change the default estuaries.
Tip: You can copy the data and change the values in the copied item

Also items that have been used in calculations can not be edited or removed as long as the results from the calculation is stored in the database. You can remove previous calculations through the menu bar : EDIT - Run list... Select EDIT - Estuary list in the menu bar to access the list of defined estuaries.
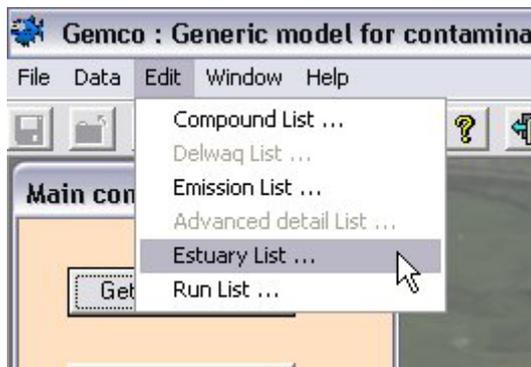
This will show a list of all available estuaries in the database. You can add, copy, edit or delete an estuary by using the buttons below the list. Default estuaries and estuaries that have been used in a calculation can not be changed unless the results from the previous calculation are removed first (data integrity). Clicking on the column header will sort the column alphabetically.
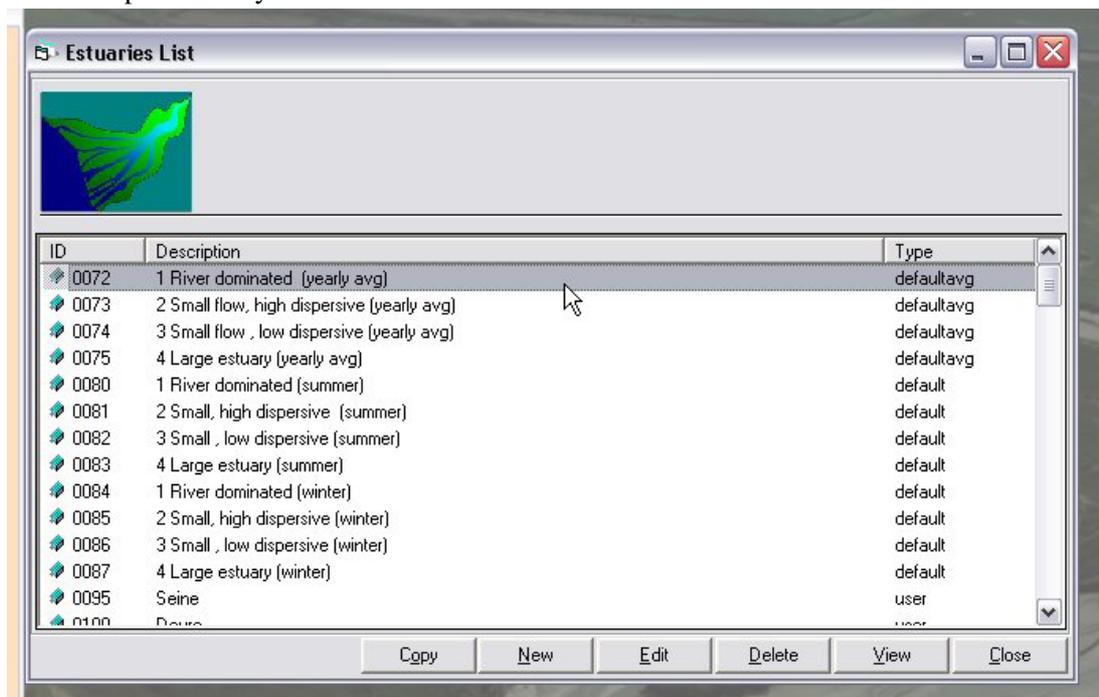
10   Estuary details

Clicking the Copy, New or Edit button in the estuary list window will bring you to the detail input screen.
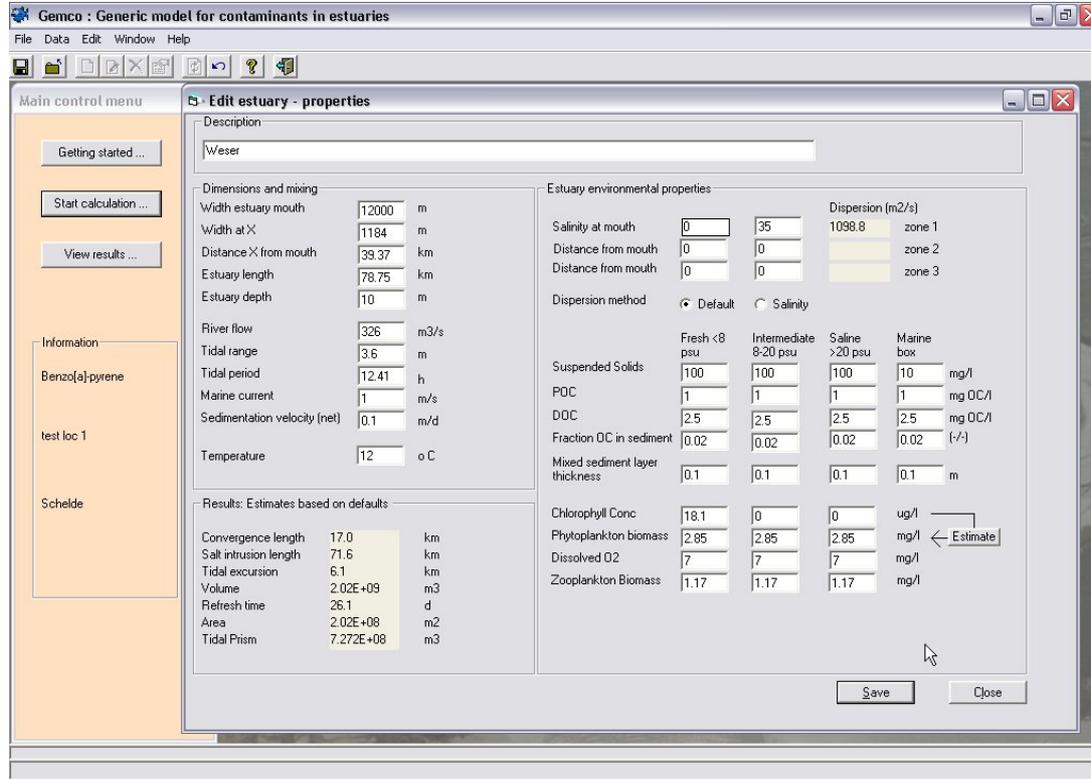
The following parameters are used to define an estuary:

- **Estuary shape**

Estuary geometry can be defined by a number of indicators, such as width (B), length and depth (h). The width convergence length is a term for the shape of the estuary.
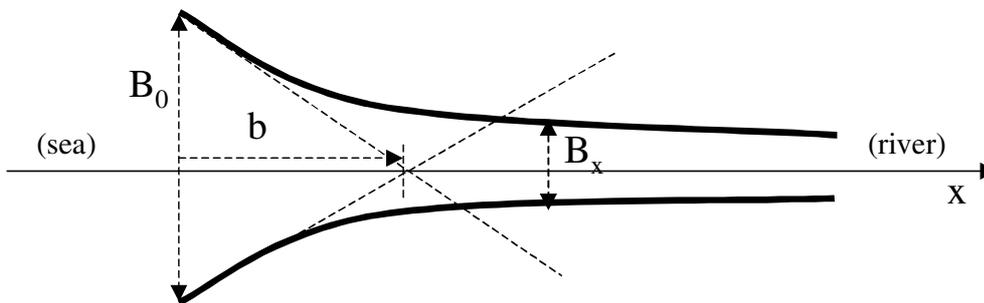
For the determination of the width convergence length it is necessary to use estuary width several kilometres from the mouth. Strongly converging estuaries, like the Seine, have a small converging length 'b', whereas estuaries with quite parallel banks will have a large convergence length. Examples for this type are the Gironde, Severn and Scheldt. The width convergence length (Savenije, 1992) can be written as:

$$B = B_0 \exp\left(-\frac{x}{b}\right)$$

- o **Width estuary mouth B0** (m), this figure is bound to be a bit arbitrary, please consider the default estuary shape and select the most appropriate value.

- o **Width estuary at distance X** from estuary mouth Bo

- o **Distance from estuary mouth** where width Bx is defined

- o **Estuary length**: must be (slightly) larger than the salt intrusion length. Please note that the estuary length is defined on basis of salinity, not tidal influence.

- o **Estuary depth** : uniform average depth

- o **Marine long-shore current**: averaged long-shore current is applied for the estimation of concentrations in the adjacent marine box with a fixed size of 40 km length, 10 km width and 10 m deep

- **Exchange definition**

  - o **River flow** : annual / seasonal averaged flow

  - o **Tidal range** : average value

  - o **Tidal period** : use default value 12.41 h appropriate for most estuaries in Europe, or specify a location specific value

  - o **Dispersion methods**

    Default
    Calculates the tide-averaged longitudinal dispersion coefficient based on the estuary shape and exchange parameters as derived by Savenije and WL (WL, 2003a). Please note that the GEMCO estuary is a very simplified schematisation of an estuary. Due to this simplification, mixing processes that occur in estuaries that are caused by shape, varying bathymetry and such are not explicitly modeled. These processes are represented in the dispersion coefficient.

$$\alpha_0 = 220 \frac{h_0}{a} \sqrt{\frac{E_0 \cdot T \cdot g \cdot h_0}{Q_f \cdot A_0}}$$

$$D_0 = \alpha_0 \cdot Q_f$$

$$K = 4.38 \frac{h_0^{0.36}}{B_0^{0.21} b^{0.14}}$$

$$D(x) = D_0 [1 - \frac{K \cdot a \cdot Q_f}{D_0 \cdot A_0} (\exp(\frac{x}{a}) - 1)]$$

$$L = b \ln \left(\frac{220}{K} \frac{h_0^2}{b^2} \sqrt{\frac{E_0 T g B_0}{Q}} + 1 \right)$$

L	[m]	salt intrusion length
E_0	[m]	tidal excursion
K	[-]	Van der Burgh's coefficient ($0 < K < 1$)
B	[-]	estuary convergence length
A	[-]	estuary cross-section area convergence length
H_0	[m]	depth at estuary mouth
B_0	[m]	width at the mouth of estuary
T	[s]	tidal period
Q_f	[m³/s]	river discharge

As can be seen in the formula above, the calculated longitudinal dispersion depends on the cross sectional area Ao which decreases upstream. Therefore the dispersion will decrease upstream. The dispersion shown in the user interface is the value at the mouth of the estuary.

Salinity measurements

One preferred method to derive the tide-averaged longitudinal dispersion is by the use of estuarine salinity as a tracer of the tidal mixing (Stommel, 1953; Thomann et al., 1987, WL, 2003).

$$D = \frac{-\dfrac{Q_f a}{A_0} \cdot \exp(\dfrac{x_2 - x_1}{a}) + \dfrac{Q_f a}{A_0}}{\ln(\dfrac{S_2}{S_1})}$$

Qf:	net estuarine flow at given tributary	(m³/s)
S:	salinity	(ppt)
D:	tide-averaged dispersion	(m²/s)
A0:	cross sectional area	(m²)
x:	distance from mouth	(m)

Salinity is taken as 0.1 psu at the end of the estuary (river part) and is taken as the user specified salinity at the estuary mouth. The user must specify salinity at 2 other locations in the estuary. The distance is defined as distance from the sea-estuary border (Bo).

- **Temperature**

   Temperature is the average water temperature in degrees Celsius

- **Salinity at the mouth**

Salinity at the estuary mouth / marine box in PSU

The following parameters are defined separately for different salinity zones and the marine compartment.

- Suspended solids : average silt concentration in water column (mg/l)
- POC : particulate organic carbon concentration : g OC.m-3
- DOC : dissolved organic carbon concentration : g OC.m-3
- Fraction organic carbon in sediment : (g/g)

- Chlorophyll concentration (ug/l)
- Phytoplankton biomass (mg/l)
- Zooplankton biomass (mg/l)
- Dissolved oxygen : average dissolved oxygen concentration(mg O2/l)

11   Viewing results

When you finished a calculation the result screen will pop up automatically. You can always access the result screen by pressing the VIEW RESULTS button on the main menu.
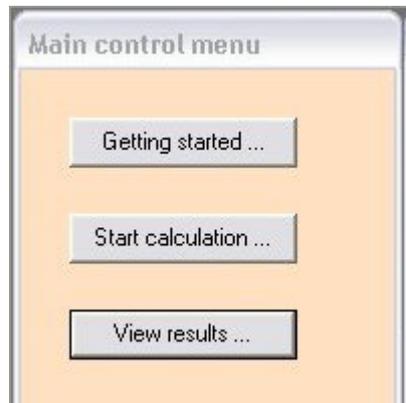
The result window has several features:

1. Select results from a previous calculation

2. View statistical output for abiotic an biotic concentrations

3. View xy graph of calculated concentrations

4. View spatial distribution of calculated concentrations

5. Print a results report
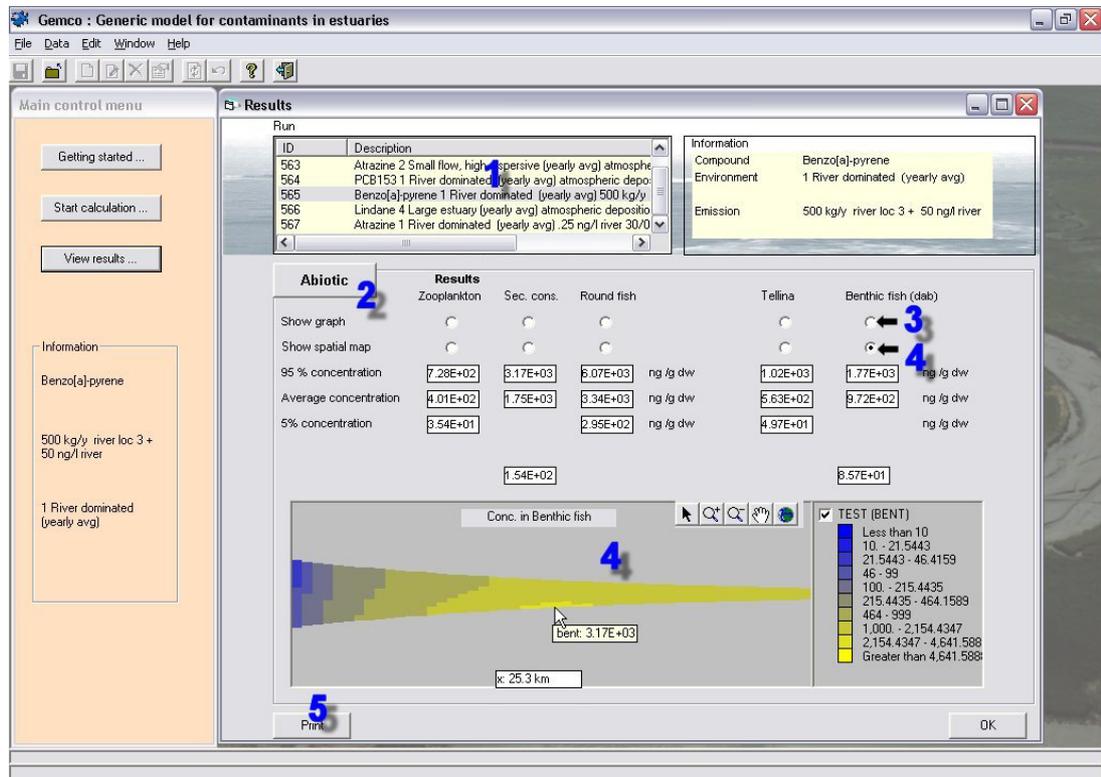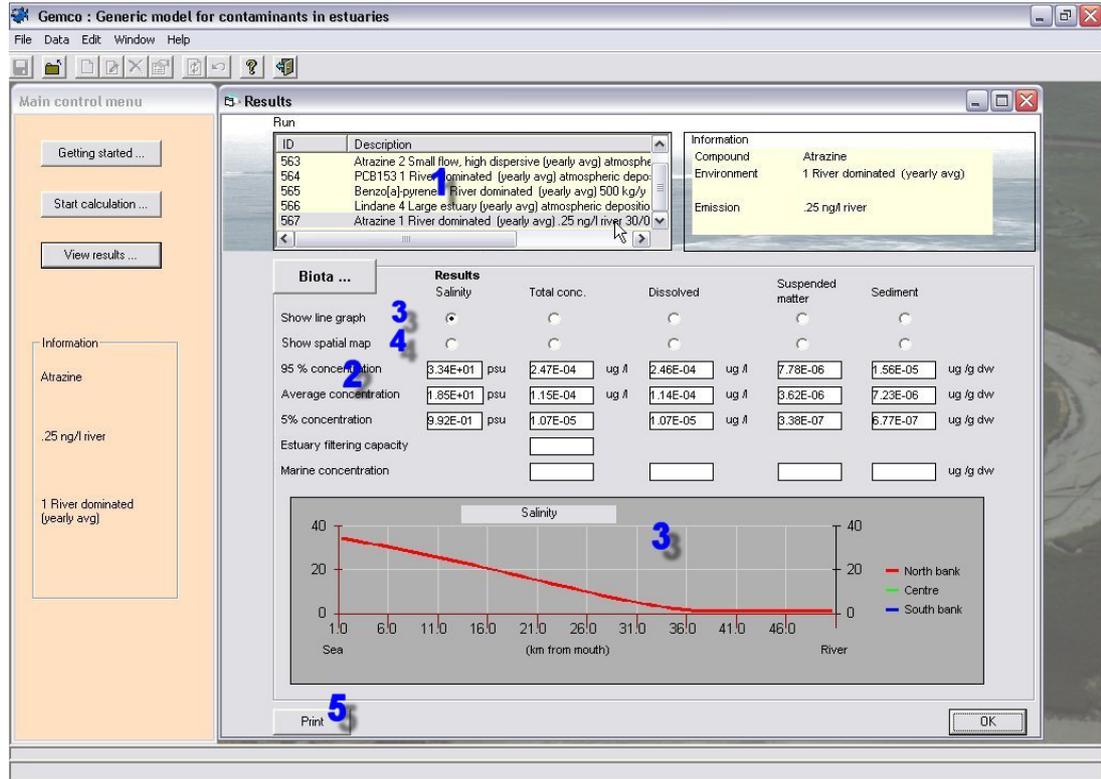
As the model is a steady state model, the calculated concentrations do not vary in time (in a given scenario). The calculated statistics refer to the area. The 95 percentile value is the value that is exceeded in 5% of the estuary. The 5-percentile value is exceeded in 95% of the

estuary.

The results for the abiotic compartments are:

- **Salinity** (p.s.u.), ideal to be used for assessing the performance of the model for dissolved compounds.
- **Total conc.**: Total concentration (ug/l) - includes dissolved and compounds adsorbed to suspended material. The model uses a averaged suspended solids concentration. In reality suspended solids concentrations show large fluctuations in time. As the total concentration of adsorbing compounds is directly related to the suspended solids concentration, it will show similar behaviour. Dissolved concentration and concentration level on the sediment show less fluctuations and are more suited to compare to long term average measurements.
- **Dissolved**: dissolved compound concentration(ug/l)
- **Suspended matter**: concentration of compound on suspended solids(ug/g dry weight)
- **Sediment**: concentration of compound on sediment (ug/g dry weight)
- **Estuarine filtering capacity**: ratio of the sum of all chemical removal rates (sedimentation, biodegradation, volatilisation etc) and the total input of the chemical by the river.

Results: concentrations in biota.

The results for the foodweb model are only available for compounds for which the foodweb model is valid : organic compounds with Kow values between 4.5 and 9. Otherwise the Biota button will be disabled.
- **Zooplankton**: concentration of contaminants in zooplankton (ng/g dry weight)
- **Sec. cons.**: concentration in secondary consumers (ng/g dry weight)
- **Round fish**: concentration in round fish (ng/g dry weight)
- **Tellina**: concentration Tellina (ng/g dry weight)
- **Benthic fish**: concentration in pelagic fish (ng/g dry weight), e.g. dab (*Limanda limanda*)

Print: Pressing the print button will print all the input parameters and results for the selected run to the installed printer.

Deleting previous calculations
To delete previous calculations select EDIT in the menubar and then RUN LIST. A window will show all existing calculations. Select the one to remove and then press the DELETE button. The compound, emission and estuary associated with a calculation will remain in tact.