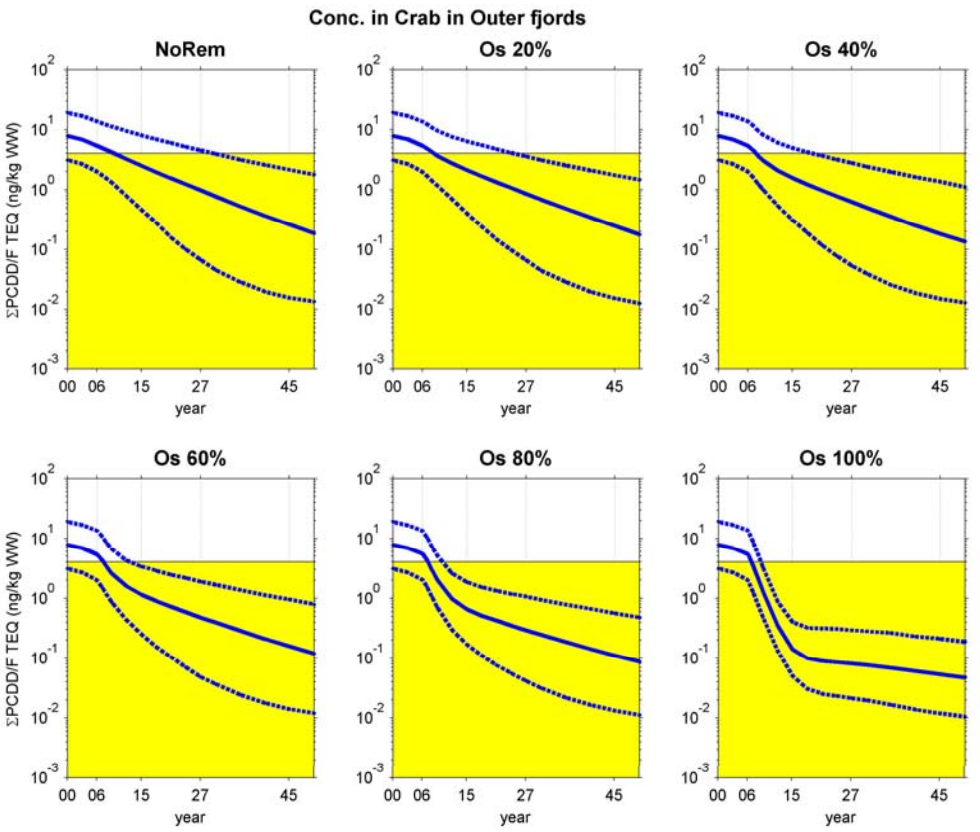
REPORT 5216-2006

SF-tool multimedia model package

Model code description and application examples from the Grenland fjords

Department of Applied Environmental Science (ITM)



Norwegian Institute for Water Research
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Main Office
P.O. Box 173, Kjelsås
N-0411 Oslo, Norway
Phone (47) 22 18 51 00
Telefax (47) 22 18 52 00
Internet: www.niva.no

Regional Office, Sørlandet
Televeien 3
N-4879 Grimstad, Norway
Phone (47) 37 29 50 55
Telefax (47) 37 04 45 13

Regional Office, Østlandet
Sandvikaveien 41
N-2312 Ottestad, Norway
Phone (47) 62 57 64 00
Telefax (47) 62 57 66 53

Regional Office, Vestlandet
Nordnesboder 5
N-5008 Bergen, Norway
Phone (47) 55 30 22 50
Telefax (47) 55 30 22 51

Regional Office Midt-Norge
P.O. Box 1266
N-7462, Norway
Phone (47) 73 54 63 85 / 86
Telefax (47) 73 54 63 87

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Abstract

This report gives a description of an integrated multimedia modelling tool called SF-tool, and application examples from the modelling of the impact of planned contaminated sediment remedial alternatives on the future dioxin and furan levels of cod and crab in the Grenland fjords. The SF-tool (SedFlex-tool) consists of 1) a flexible water-sediment fugacity model code for simulating the sources, sinks and transports of persistent organic pollutants (POPs) in a fjord, estuary or lake system, and 2) a bioaccumulation rate constant model code for simulating the intake and bioaccumulation of POPs in a food web. In addition, the SF-tool contains tools for uncertainty and sensitivity analysis of the model results. The model simulations in the Grenland fjords show that a significant reduction in the concentration levels in cod and crab in the Frierfjorden can first be seen when larger areas of the Frierfjorden are capped, and thus significant portions of the contaminated feeding and habitat sediment areas of cod and crab are cleaned up. The same type of conclusion applies also in the outer fjords remediation scenarios. Furthermore, capping of contaminated sediments in the Frierfjorden will have no significant effect on the future evolution of the sediment concentrations (and hence on the concentrations in cod and crab) in the outer fjords or in the Langesundbukta.

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1. Modellering	1. Modelling
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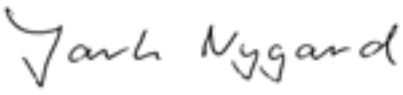
Project manager
Kristoffer Næs

Research manager
Kristoffer Næs



Strategy Director
Jarle Nygard

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SedFlex project

SF-tool multimedia model package

Model code description and application examples from the Grenland fjords

Preface

The development of the SF-tool was part of the SedFlex research project funded by the Research Council of Norway, programme Profo under contract 159214/S30.

The model application to the Grenland fjords presented in this report was done as part of the Rein Fjord project funded by The County Governor of Telemark (Dept. of Environmental Protection) and Interreg Forum Skagerrak II, WP2.

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The project has been managed by Kristoffer Næs (NIVA) and with main scientific contributions from Tuomo Saloranta (NIVA), David Barton (NIVA), Ian Cousin (ITM) and James Armitage (ITM). Contact persons have been Marianne Olsen at the County Governor of Telemark and Lisbeth Lemke Rasmussen (Nordjyllands Amt) for Forum Skagerrak II.

Oslo, August 30, 2006

Tuomo M. Saloranta

Contents

Summary

This report gives 1) a description of an integrated multimedia modelling tool called SF-tool and 2) application examples from the modelling of the impact of planned contaminated sediment remedial alternatives on the future dioxin and furan levels of cod and crab in the Grenland fjords.

The SF-tool (SedFlex-tool) consists of 1) a flexible water-sediment fugacity model code for simulating the sources, sinks and transports of persistent organic pollutants (POPs) in a fjord, estuary or lake system, and 2) a bioaccumulation rate constant model code for simulating the intake and bioaccumulation of POPs in a food web. In addition, the SF-tool contains tools for uncertainty and sensitivity analysis of the model results. The compartment structure in the abiotic and biotic models can be flexibly defined, and both models can be executed both in dynamic and steady state mode.

The model simulations in the Grenland fjords show that a significant reduction in the concentration levels in cod and crab in the Frierfjorden can first be seen when larger areas of the Frierfjorden are capped, and thus significant portions of the contaminated feeding and habitat sediment areas of cod and crab are cleaned up. The same type of conclusion applies also in the outer fjords remediation scenarios. Furthermore, capping of contaminated sediments in the Frierfjorden will have no significant effect on the future evolution of the sediment concentrations (and hence on the concentrations in cod and crab) in the outer fjords or in the Langesundbukta (sediment area at 0-50 m depth, or deeper, considered). This is due to the slowness and ineffectiveness of the transport processes between the sediments of different fjord areas, especially between those separated by shallower sills.

1. Introduction

Numerous fjord and lake sediments are contaminated with persistent organic pollutants (POPs) due to historic emissions from industry and other pollution sources. In many of these sites remedial measures are planned aiming to reduce the impact and exposure of the pollution to the biota. Models can be very valuable tools in helping the planning of remedial measures as they enable the water managers and other stakeholders to holistically investigate the problems and seek for potential solutions and remedial alternatives. Moreover, as models contain a synthesis of the scientific knowledge about the fjord or lake system, use of models in environmental management planning contribute to founding the management on a more scientific basis.

This report presents an integrated multimedia modelling tool called SF-tool, which is suitable for simulating the fate of POPs in aquatic systems. The SF-tool enables also uncertainty and sensitivity analysis of the model results. The SF-tool has so far been applied in connection with environmental management of contaminated sediments in three Norwegian fjords: in the Grenland fjords (as described this report), in Sunndalsfjorden (Armitage and Saloranta, 2005) and in Ranfjorden (Saloranta, 2006). In section 2 a description of the model code and equations are given and in sections 3-4 application examples from the Grenland fjords are presented and discussed. Throughout the following sections the two terms ”model” and ”model code” are addressed a specific meaning and they are defined as in Refsgaard and Henriksen (2004):

model code is a mathematical formulation in the form of a computer program that is so generic that it, without program changes, can be used to establish a model with the same basic type of equations (but allowing different input variables and parameter values) for different study areas.

model is a site-specific model application established for a particular study area, including input data and parameter values.

2. Description of the SF-tool (v.1.1)

The SF-tool (SedFlex-tool) consist of 1) a flexible water-sediment fugacity model code for simulating the sources, sinks and transports of persistent organic pollutants (POPs) in a fjord, estuary or lake system, and 2) a bioaccumulation rate constant model code for simulating the intake and bioaccumulation of POPs in a food web. In addition, the SF-tool contains tools for uncertainty and sensitivity analysis of the model results. The compartment structure in the abiotic and biotic models can be flexibly defined. Figure 1 exemplifies one possible abiotic compartment division with six water and six sediment compartments. The compartments in the biotic model correspond to the design of the food web. Both models can be executed both in dynamic and steady state mode. Steady state solutions are basically solved by calculating the inverse of the rate constant matrix, and the dynamic solutions are solved using Runge-Kutta based methods.

The model codes and the accompanying software for uncertainty- and sensitivity analysis and for illustration of the model results are all coded and executed within MATLAB software (www.mathworks.com). The model applications in the SF-tool can also be compiled, packed and made legally available to persons without MATLAB software license by using MATLAB *Compiler* and *Excel Builder* tools. In this case the model applications can be executed in Excel spreadsheet software environment. The abiotic model code was based on Cousins (2004, internal note) and Mackay (2001), and the biotic model code on Gobas (1993), Hendriks et al. (2001) and Saloranta et al.

(2006). The core of the SF-tool's abiotic model, for example, consists of the following so-called "m-files", i.e., code units:

Abioticinput_v11.m	Subfunction for reading data and parameters for the abiotic model (version 1.1).
Abioticmodel_v11.m	Subfunction which contains the abiotic model code (version 1.1).

Exactly similar model file structure applies also for the biotic model (tag "Abiotic" is only changed with "Biotic" in the name of the m-file). In addition, application specific code modules are coded to control, execute and visualize a single run of the abiotic model as well as of the sensitivity and uncertainty analysis. (The sensitivity and uncertainty analysis modules and the biotic model code are also calling code some additional code located outside the SF-tool's m-files.)

The application specific model parameters and other forcing data are contained in the following four Excel files:

SF_Abio_emissions.xls	Initial/background concentrations for all compartments and emission time series.
SF_Abio_parameters.xls	Parameters for the abiotic model.
SF_Bio_parameters.xls	Parameters for the biotic model.
SF_Chemicals	Data on chemical properties.

The names of all the application specific modules and files are arbitrary and just indicating the template name. They should, of course, be changed to reflect the name of the particular application.

The modelling principle in both the abiotic and biotic model code is based on *rates* of contaminants in and out of the model compartments, expressed in units of, e.g., ng/day. Furthermore, these modelled rates can be divided into three main process types, 1) transports, 2) sinks, and 3) sources. Below we divide the typically modelled rates in water, sediment, air and food web into these three process types. Note that sources and sinks are always located outside the *model domain*, i.e. outside the set of the "core" compartments for which the model "actively" predicts concentrations by using the rate matrix (see equations 3 and 8) in the numerical solutions. Whenever a concentration in a compartment is held constant, or when its concentration is not affected by the other compartments, then this compartment does not belong to the model domain.

Abiotic compartments

Atmosphere: a passive compartment whose fugacity (i.e. concentration) is determined by background fugacity and local emissions.

Water:
Transports: 1) advective exchange (water flow) between neighboring compartments; 2) diffusive exchange with atmosphere (surface water compartments only); 3) organic particle settling from the water compartment above; 4) exchange with sediment by diffusion, sedimentation and resuspension.
Sources: 1) wet and dry deposition from atmosphere (surface water compartments only); 2) local emissions; 3) advection (water flow) from outside the model domain.
Sinks: 1) degradation; 2) advection (water flow) to outside the model domain.

Sediment:
Transports: 1) exchange with water by diffusion, sedimentation (incl. mineralization) and resuspension.
Sources: none.
Sinks: 1) burial to deeper inactive sediment layer; 2) degradation.

Biotic compartments

Transports: 1) predator eats pray in the food web
Sources: 1) uptake from water
Sinks: 1) outflow to water; 2) growth dilution; 3) excretion; 4) metabolic degradation.

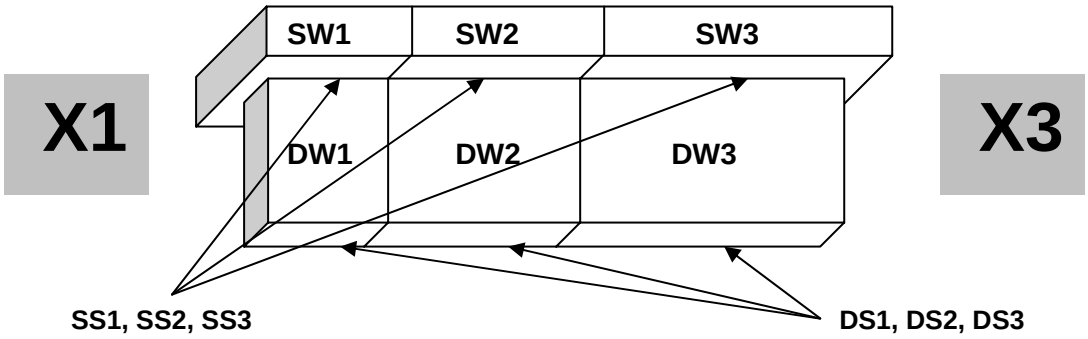


Figure 1. *Example of an arbitrary setup of the surface water (SW), deeper water (DW), littoral (shallow area) sediment (SS) and deeper area sediment (DS) compartments in the SF-tool. The amount of vertical and horizontal divisions is easily changed by the user. X1 and X3 denote the water columns outside the model domain, exchanging water with SW1 and DW1, and SW3 and DW3, respectively.*

2.1 The abiotic model code

The abiotic model code is based on the fugacity concept, described in detail e.g. in Mackay (2001). The fugacity approach uses fugacities *f*, expressed in units of (partial) pressure (Pa), to describe POP concentrations in each compartment, fugacity capacities, or Z-values, (mol m^{-3} Pa^{-1}) to describe the "partition capacity" of a phase, and transport values, or D-values, (mol Pa^{-1} d^{-1}) to describe the transports and transformations of the POPs within and between the model compartments. Equations for calculating Z-values in different phases are listed in Table 1.

Table 1. Definition of fugacity capacities (Z-values, mol m^{-3} Pa^{-1}).

Phase	**Z-value (mol m^{-3} Pa^{-1})**	**Definition of terms**
Water	$Z_w = 1/H$	H is Henry's law constant (Pa m^3 mol^{-1})
POC	$Z_{POC} = Z_w K_{POC} \rho_{OC}$	K_{POC} is POC–water partition coefficient (L_w/kg_{POC}) which is estimated as $K_{POC} = \alpha K_{OW}$, where K_{OW} is the octanol-water partition coefficient, α a scaling coefficient (α~0.35), and ρ_{OC} the density of POC (~1 kg/L).
DOC	$Z_{DOC} = Z_w K_{DOC} \rho_{OC}$	K_{DOC} is DOC–water partition coefficient (L_w/kg_{DOC}) which is estimated as $K_{DOC} = \alpha K_{OW}$ (α ~0.08).
Air	$Z_{air} = 1/RT$	R = 8.314 Pa m^3 mol^{-1} K^{-1}, T = temperature (K).
Aerosols	$Z_Q = K_p Z_{air} = \alpha K_{OA} Z_{air}$	K_{OA} is the octanol-air partition (α~3.8; PAH equation adopted).
Bulk water	$Z_{WT} = Z_w + F_{POC} Z_{POC} + F_{DOC} Z_{DOC}$	F = volume fraction of the subphase (POC or DOC).
Sediment porewater (water + DOC)	$Z_{PW} = Z_w + F_{DOC} Z_{DOC}$	
Sediment solids	$Z_{SS} = F_{POC} Z_{POC}$	
Bulk sediment	$Z_{ST} = \phi Z_{PW} + (1-\phi) Z_{SS}$	ϕ is sediment porosity (-), i.e, volume fraction of pore water.

The mass balance equations of the abiotic model code are devised by adding up 1) all sources that come from outside the model domain, i.e., by direct emissions, by advection from outside waters and by vapour adsorption, rain dissolution, dry and wet deposition from atmosphere, and 2) all the transport D-values (multiplied by the corresponding fugacity) within the model domain that contribute to both inputs of the chemical to a compartment (transports from other model compartments) and output of the chemical from a compartment (degradation, burial to inactive sediment, and transports to other model compartments as well as to outside the model domain). The transport processes within the model compartments include advection (water flow), diffusion, sedimentation, resuspension, as well as volatilisation to the atmosphere. A mass balance for a chemical can then be written in the following form:

$$\frac{dM_i}{dt} = E_i + T_i^{IN} - T_i^{OUT} \quad (1)$$

where subscript i denotes a particular compartment, M denotes mass (mol), and E, T^{IN}, and T^{OUT} (mol d^{-1}) the sum of sources and the sum of incoming and outgoing transports (i.e. D-values multiplied by the corresponding fugacity), respectively. The resulting system of linear, first-order differential equations can also be written more compactly as:

$$\frac{d}{dt}\mathbf{f} = \mathbf{K}\mathbf{f} + \mathbf{S} \quad (2)$$

where **f** is a vector of fugacities (Pa) in the compartments, **S** is a vector of sources (Pa d^{-1}) from outside the model domain into the compartments, and **K** is the specific rate coefficient matrix (d^{-1}), which is constructed using D- and Z-values, and the compartment volumes *V*, in the following way:

$$\mathbf{K}_{ij} = \begin{cases} \dfrac{-\sum D_i^{OUT}}{V_i Z_i} & i = j \\ \dfrac{\sum D_{j \to i}}{V_i Z_i} & i \neq j \end{cases} \tag{3}$$

where *i* and *j* are the *i*th row and *j*th column of the matrix **K** and also denote the particular compartment. D^{OUT} denotes D-values responsible for transport out of the particular compartment, and $D_{j \to i}$ the D-values responsible for transport from compartment *j* to *i*. The equations used to estimate all the relevant D-values are described in Table 2. A source vector originally in units (mol/d) can be transformed to units (Pa/d), required in equation 2, by dividing the values compartment-wise by the corresponding product $V_i Z_i$.

The atmospheric compartment is not part of the main model domain (i.e. it is not among the compartments included in the rate coefficient matrix **K**) and the chemical concentration in atmosphere C_{air} (mol m^{-3}) is simply calculated from the background concentration C_{0_air}, and from the emission E_{air} (mol d^{-1}), turnover time τ (d), and volume V_{air} (m^3) of the atmospheric compartment by:

$$C_{air} = C_{0\_air} + \frac{E_{air}\tau}{V_{air}} \tag{4}$$

In a steady state the left hand side of equation 2 becomes zero (df/dt=0) and the system simplifies to:

$$\bar{\mathbf{f}} = -\mathbf{K}^{-1}\bar{\mathbf{S}} \tag{5}$$

where the overbars denote steady state concentrations. A dynamic solution is, however, often preferred as the model is intended to determine how concentrations in the aquatic systems change in time as a response to changing emissions or remediation measures.

The estimated fugacities can easily be transferred to concentration-units in the different media using equations of the form *C* (mol m^{-3}) = *Z* (mol m^{-3} Pa^{-1}) · *f* (Pa), and to mass transports between the compartments using equations of the form *N* (mol d^{-1}) = *D* (mol d^{-1} Pa^{-1}) · *f* (Pa).

The temperature correction for the three partitioning coefficients (K_{OA}, K_{OW}, K_{AW}) is calculated by

$$\log_{10}(K_{XX}) = \log_{10}(K_{XX\_ref}) - \frac{\Delta U_{XX}}{\ln(10)R}\left(1/T_{amb} - 1/T_{ref}\right) \tag{6}$$

where K_{XX} denotes the particular partitioning coefficient, K_{XX_ref} its value measured in reference temperature T_{ref} [K], T_{amb} [K] denotes the ambient temperature, *R* the gas constant [J mol^{-1} K^{-1}], and ΔU_{XX} the particular change (ΔU_{OA}, ΔU_{OW}, or ΔU_{AW}) in internal energy [J mol^{-1}] (often taken to be equal to the enthalpy of phase change). The Henry's law coefficient *H* is related to K_{AW} by $\log_{10}(H) = \log_{10}(K_{AW}) + \log_{10}(RT)$.

Table 2. Definition of the transport and transformation D-values

Process	D-value (mol d^{-1} Pa^{-1})	Equation and explanation
Bulk water advection (i.e. water, particles and dissolved matter) from water compartment *i* to *j* and to outside of model domain *X*.	$D_{i\rightarrow j}$, $D_{i\rightarrow X}$	$G_{i\rightarrow j}\, Z_{WT\_i}$, $G_{i\rightarrow X}\, Z_{WT\_i}$ where G is the flow rate (m^3/d).
Vertical particle (POC) settling from water compartment *i* to *j* (below *i*).	$D_{settle\_i\rightarrow j}$	$10^6 \cdot C_{POC\_i}\, U_{POC\_i}\, Z_{POC\_i}\, A_{W\_j} / \rho_{OC}$ where C_{POC_i} is the POC concentration (mg/m^3), U_{POC_i} is the POC settling rate (m/d), and A_{W_i} is the surface area (m^2) of the water compartment.
Degradation in compartment *i*.	D_{R_i}	$k_{R\_i}\, Z_W\, V_i$ where k_R is the first-order degradation rate constant (d^{-1}), and V the volume (m^3) of the water phase where the reaction is taking place.
Total transport from air to surface water compartment *i*.	$D_{A\rightarrow i}$	$D_{vv\_i} + D_{rain\_i} + D_{wet\_i} + D_{dry\_i}$ where the individual D-values are defined below.
Volatilisation/vapour adsorption to/from surface water compartment *i*.	D_{vv_i}	$1/(1/k_{VA}\, A_{W\_i}\, Z_A + 1/k_{VW}\, A_{W\_i}\, Z_W)$ where k_{VA} and k_{VW} are the air-side and water-side mass transfer coefficients[1] (m d^{-1}).
Rain dissolution to surface water compartment *i*.	D_{rain_i}	$A_{W\_i}\, U_R\, Z_W$ where U_R is the rain rate (m d^{-1}).
Wet particle deposition to surface water compartment *i*.	D_{wet_i}	$A_{W\_i}\, U_R\, Q\, F_Q\, Z_Q$ where Q is the scavenging ratio[2], and F_Q is the volume fraction of aerosols.
Dry particle deposition to surface water compartment *i*.	D_{dry_i}	$A_{W\_i}\, U_Q\, F_Q\, Z_Q$ where U_Q is the particle dry deposition rate (m d^{-1})
Transport from water compartment *i* to sediment compartment *j*.	$D_{SD\_i\rightarrow j}$	$D_{sed\_i\rightarrow j} + D_{diff\_i\rightarrow j}$ (terms defined below).
Transport from sediment compartment *i* to water compartment *j*.	$D_{SU\_i\rightarrow j}$	$D_{res\_i\rightarrow j} + D_{diff\_i\rightarrow j}$ (terms defined below).
Total sediment deposition from water compartment *i* to sediment compartment *j*.	$D_{sed\_i\rightarrow j}$	$U_{DP\_j}\, A_{S\_j}\, Z_{SS\_j}$ where U_{DP} is the gross sedimentation rate (m d^{-1}) of sediment solids, and A_S is the surface area (m^2) of the sediment compartment.
Sediment resuspension from sediment compartment *i* to water compartment *j*.	$D_{res\_i\rightarrow j}$	$U_{RS\_i}\, A_{S\_i}\, Z_{SS\_i}$ where U_{RS} is the sediment resuspension rate (m d^{-1}).
Sediment-water diffusive exchange from compartment *i* to *j*.	$D_{diff\_i\rightarrow j}$	$k_{SW} A_S\, (Z_W + Z_{DOC\_i})$ where k_{SW} is the sediment-water diffusion mass transfer coefficient (m d^{-1}) for water (including DOC), and A_S is the surface area (m^2) of the corresponding sediment compartment.
Mineralization of sediment solids in sediment compartment *i*.	D_{min_i}	$U_{MIN\_i}\, A_{S\_i}\, Z_{SS\_i}$ Where U_{MIN} is the sediment mineralization rate[3] (m d^{-1}).
Burial of sediment solids in sediment compartment *i*.	D_{bur_i}	$U_{BR\_i}\, A_{S\_i}\, Z_{SS\_i}$ Where U_{BR} is the sediment burial rate[4] (m d^{-1}).

[1] These mass transfer coefficients can be estimated, e.g. by: $k_{VA} = 3.6 + 5U_{10}$, $k_{VW} = 0.0036 + 0.01U_{10}$, where U_{10} is the wind speed at 10 m height (m s^{-1}) (Mackay, 2001).
[2] Scavenging ratio Q (-) denotes the ratio of a raindrop's volume to the volume of the air it sweeps through when falling. In other words, Q denotes how efficiently raindrops "hit" and remove aerosols from the air.
[3] $U_{MIN} = H_{sed}\, ln(2)/t_{MIN}$, where H_{sed} is the depth of the active sediment layer and t_{MIN} is the carbon mineralization half-life.
[4] The sediment burial rate should be equal to the net sediment deposition rate, i.e. $U_{BR\_i} = U_{DP\_i} - U_{RS\_i} - U_{MIN\_i}$.

2.2 The biotic model code

The way the equations are formulated in the biotic model code is very similar to the abiotic model code, except that actual concentrations are used instead of fugacity in the calculations. However, this is just a matter of habit or convenience and, as pointed out above, the conversion between fugacity and concentration units is straightforward. The following brief description of the biotic model code is taken from Saloranta et al. (2006) where more detailed information of the model code can be found, such as equations for parameterisation of the rate constants.

Contaminant flows in a food web are determined by feeding linkages among food web components, and by the organisms' ability to absorb, excrete, and metabolise chemicals from their environment, either the water column or the sediment pore water (Campfens and Mackay, 1997). If a contaminant behaves as a true tracer (i.e., there are no feedback between contaminant concentrations and energy flows between system compartments) then all contaminant flows can be represented as donor-controlled, first-order reactions. The mass balance of contaminants in aquatic organisms is governed by four basic flows between organisms and the environment: intake directly via water/sediment pore water (k_I), intake via food (k_F), outflow directly to water/sediment pore water (k_O), and outflow via egestion and defecation (k_E). Additionally, losses due to growth dilution (k_G) and metabolic degradation (k_M), must be accounted for (Gobas, 1993). As concentrations in organisms and environment are given in different units (per unit wet weight (kg) vs. per unit volume (L)), the intake from water rate constant (k_I) will have dimensions of an affinity constant or a clearance rate (L kg^{-1} d^{-1}). Hence, all rate constants end up with dimension d^{-1} if we assume that organisms have unit density (i.e. kg and L are equal in weight and volume). The resulting system of linear, first-order differential equations can be written, as in equation 2:

$$\frac{d}{dt}\mathbf{c_b} = \mathbf{K}\mathbf{c_b} + \mathbf{S} \tag{7}$$

where $\mathbf{c_b}$ is a vector of contaminant concentrations in the organisms (ng kg^{-1} = ng L^{-1}), **S** is a source vector (ng kg^{-1} d^{-1} = ng L^{-1} d^{-1}) of the intakes directly from water and/or sediment pore water, and **K** is the specific rate coefficient matrix (d^{-1}) constructed using the rate coefficients:

$$\mathbf{K_{ij}} = \begin{cases} -\left[k_O(i) + k_E(i) + k_G(i) + k_M(i)\right] & i = j \\ p_{ij}k_F(i) & i \neq j \end{cases} \tag{8}$$

where p_{ij} is a fraction of organism j in the diet of organism i.

The elements of the source vector **S** are calculated as:

$$S(i) = k_I(i) \cdot c_a(i) \tag{9}$$

where $c_a(i)$ is the contaminant concentration (ng L^{-1} = ng kg^{-1}) in the abiotic environment of the organism i. The total $c_a(i)$ is partitioned into the truly dissolved concentrations C_{diss} in water and sediment pore water by the parameter $\varphi_{sed}(i)$ equal to the fraction of time spent in the sediments for the organism i:

$$c_a(i) = \varphi_{sed}(i)C_{diss\_sed} + \left(1 - \varphi_{sed}(i)\right)C_{diss\_water} \tag{10}$$

In a steady state the time derivative $d\mathbf{c_b}/dt$ becomes zero and equation 7 simplifies, as equation 5, to:

$$\bar{\mathbf{c}}_b = \mathbf{K}^{-1}\bar{\mathbf{S}} \quad (11)$$

where the overbar denotes steady state concentrations.

The rate constants for the different exchange processes are based on relationships to organism properties like size and lipid content, and to contaminant properties like the octanol-water partition coefficient (K_{OW}). All contaminant exchange fluxes are related to vital activities like swimming, gill ventilation, feeding, assimilation, and growth. Thus, one should expect the corresponding rate constants to scale similarly with body size as vital rates do in general, i.e., allometrically with an exponent around -0.25 (Peters 1983). In the SF-tool's biotic model code we have used two different parameterisations of the contaminant exchange rate constants, by Gobas (1993), and by Hendriks et al. (2001). The parameterisation by Gobas (1993) was originally based on a limited data set with a more specific purpose of predicting PCB concentrations in biota of the Laurentian Great Lakes, but has later been generalised to other food webs and substances (e.g. Morrison et al. 1997). The Hendriks et al. (2001) parameterisation, on the other hand, has more general scope in the outset, as resulting from a compilation of almost 2000 different rate constant estimates from a range of different organisms and contaminants. While both model codes use allometric relations as link between vital rates and body sizes, Hendriks et al. (2001) places a more fundamental role on the $1/4^{th}$ power law, while Gobas (1993) uses different exponents for different body size relationships. Assuming a fixed power law exponent reduces the number of these fundamental model parameters to 7 in the in the Hendriks et al. (2001) model code, compared to 11 in the Gobas (1993) model code. We usually refer to the Gobas (1993) model as GOBAS, and to Hendriks et al. (2001) model as the "Power of size" or POS model. The actual equations and standard parameter values of the two model codes are summarised in Saloranta et al. (2006).

2.3 How to set up a model application in the SF-tool

The purpose of the modelling, definition of management objectives and possibly planned remedial operations should be clarified before starting the actual model setup as these may largely influence the selections and decisions made in the model setup. The modelling and management objectives should be written down clearly so that the modeller and manager (and other stakeholders) have mutual understanding of what type of simulations are going to be made, why they are made in that way, what time periods the simulations are run for, what are the most important model compartments and/or species regarding the management interests and objectives, etc.

2.3.1 Compartment division

The first task in the setup of the SF-tool is to decide how to divide the particular fjord, estuary or lake into the different model compartments. The vertical division could represent, for example, surface and deeper water layers with the pycnocline as a natural division depth. The horizontal division could represent, for example, a "hot spot" area close to an industry, the main fjord body, and an outer fjord area after a shallower sill. Properties of these compartments, such as their area, thickness, DOC concentration etc. are given in the model parameter files.

Each water compartment must be associated with one and only one sediment compartment. Thus the number of water and sediment compartments must be equal. When deriving the surface areas of the shallower sediment areas, note that this area is not usually equal to the area of the corresponding surface water compartment, but much less (equal to the area between the coastline and the bathymetric isoline denoting the depth of the surface water compartment).

2.3.2 Chemical properties file

The chemical properties file (SF_Chemicals.xls, Figure 2) lists the values of the following properties for each chemical (required units are indicated in square brackets):

1. Log_{10} of the octanol-water partitioning coefficient in reference temperature (currently set to 25 °C) (K_{OW}) [-]
2. Log_{10} of the (observed) organic carbon-water partitioning coefficient K_{OC_obs} in water column. If given, then these are used in the abiotic model code directly to describe partitioning instead of applying the K_{OW} values. Use "NaN" or "#N/A" for missing values here.
3. Log_{10} of the (observed) organic carbon-water partitioning coefficient K_{OC_obs} in sediment. If given, then these are used in the abiotic model code directly to describe partitioning instead of applying the K_{OW} values. Use "NaN" or "#N/A" for missing values here.
4. Log_{10} of the octanol-air partitioning coefficient in reference temperature (currently set to 25 °C) (K_{OA}) [-]
5. Molecular weight [g mol^{-1}]
6. Minus Log_{10} of the Henry's law constant in reference temperature (currently set to 25 °C) [kPa m^3 mol^{-1}]
7. Toxicity equivalent factor [-]
8. Degradation half-life in water [d]
9. Degradation half-life in sediment [d]
10. Octanol-air change in internal energy (ΔU_{OA}) [kJ mol^{-1}]
11. Octanol-water change in internal energy (ΔU_{OW}) [kJ mol^{-1}]
12. Air-water change in internal energy (ΔU_{AW}) [kJ mol^{-1}]
13. Indicator of which chemicals are included in the current model simulations [1=included, 0=not included]

Note that in cell "A1" there must be a dummy number (e.g. -999) and that the chemical names should start from the cell "B3" for MATLAB to read the file in correctly. The order of the parameter names must not be changed either. (The enthalpy of phase change is sometimes used in place of the change in internal energy.)

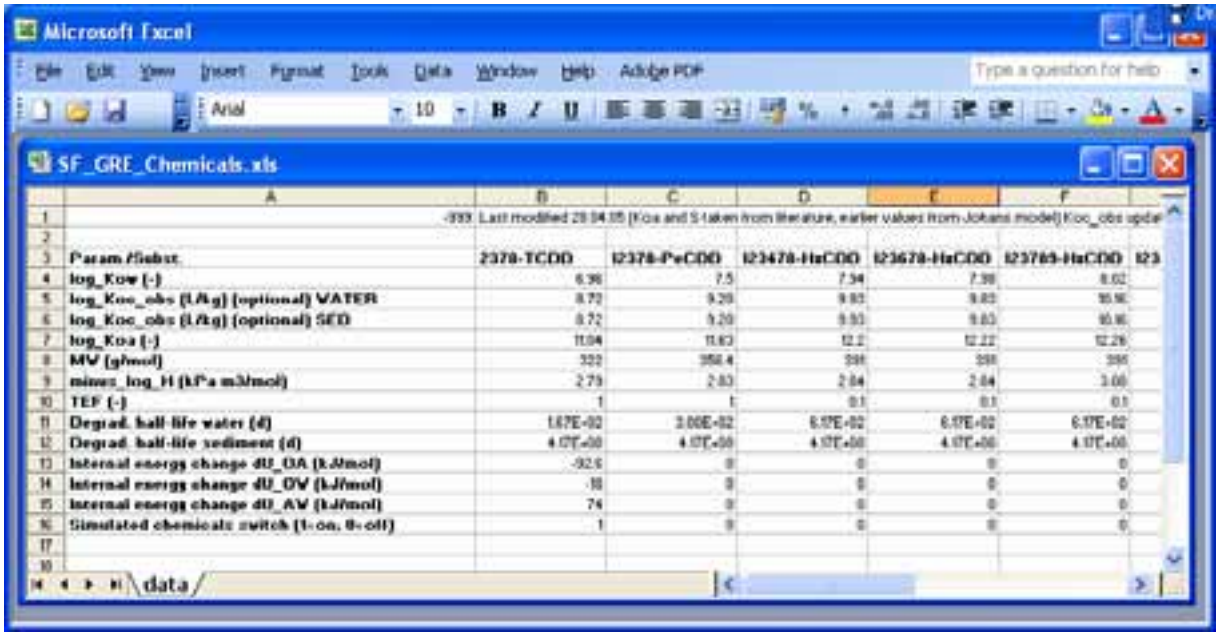


Figure 2. *Example of SF-tool's chemical properties file.*

2.3.3 Abiotic model parameter file

The abiotic model parameter file (SF_Abio_parameters.xls, Figure 3) lists the values of the following compartment-specific model parameters (required units are indicated in square brackets):

Water compartments:

1. Two-digit compartment codes, where the first digit (starting from 1) denotes the horizontal ordering of compartments and the second digit (starting from 1) the vertical ordering. Within each horizontal division, compartments must be ordered by depth starting from the surface compartment.
2. Surface area of the compartment [m^2]
3. Thickness of the compartment [m]
4. Concentration of particulate organic carbon (POC) [mg m^{-3}]
5. Settling rate of particulate organic carbon (POC) [m d^{-1}]
6. Concentration of dissolved organic carbon (DOC) [mg m^{-3}]
7. Indicator of whether degradation is taking place [1=degradation, 0=no degradation]
8. Water temperature [°C]
9. A matrix of water flows between the compartments including water columns outside the model domain (X0 and X3 in Figure 3) [m^3 s^{-1}] (flows are directed from compartments given on rows to those given on columns)

Sediment compartments:

1. Same two-digit compartment codes as with the water compartments, where the first digit (starting from 1) denotes the horizontal ordering of compartments and the second digit (starting from 1) the vertical ordering. The sediment compartments have to be ordered so that their order matches the ordering of water compartments they are coupled to.
2. Surface area of the compartment [m^2]
3. Thickness of the compartment, i.e. of the active, well-mixed sediment layer [m]
4. Volume fraction of particulate organic carbon (POC) in dry sediment solids [-]
5. Mineralization half-life in the sediment [d]
6. Concentration of dissolved organic carbon (DOC) in sediment pore water [mg m^{-3}]
7. Sediment porosity, i.e. volume fraction of water in wet sediment mass [-]
8. Sediment burial rate [m d^{-1}], i.e. net sedimentation rate of sediment solids
9. Sediment resuspension rate [m d^{-1}] of sediment solids
10. Water-sediment mass transfer coefficient [m d^{-1}]
11. Indicator of whether degradation is taking place [1=degradation, 0=no degradation]
12. Sediment temperature [°C]

Air compartment:

1. Precipitation rate [m d^{-1}]
2. Air side mass transfer coefficient over water surface [m d^{-1}]
3. Water side mass transfer coefficient under water surface [m d^{-1}]
4. Scavenging ratio [-]
5. Volume fraction of aerosols in air [-]
6. Dry deposition rate [m d^{-1}]
7. Flushing time of the air compartment [d]
8. Volume of the air compartment [m^3]
9. Temperature of the air compartment [°C]

Note that in cell "A1" there must be a dummy number (e.g. -999) and that the order of the parameter names, as well as the amount and order of empty lines and columns shown in Figure 3 must not be changed. The values not required can be marked with "#N/A". As a help to understand and derive the less obvious parameter values, such as the mass transfer coefficients and parameters of the air compartment, see e.g. Mackay (2001).

There should, of course, be a water mass balance in the flow matrix, so that the inflows to the individual compartments, as well as to the model domain as a whole (e.g., inflows from X0 and X3 in Figure 3), are equal to the corresponding outflows.

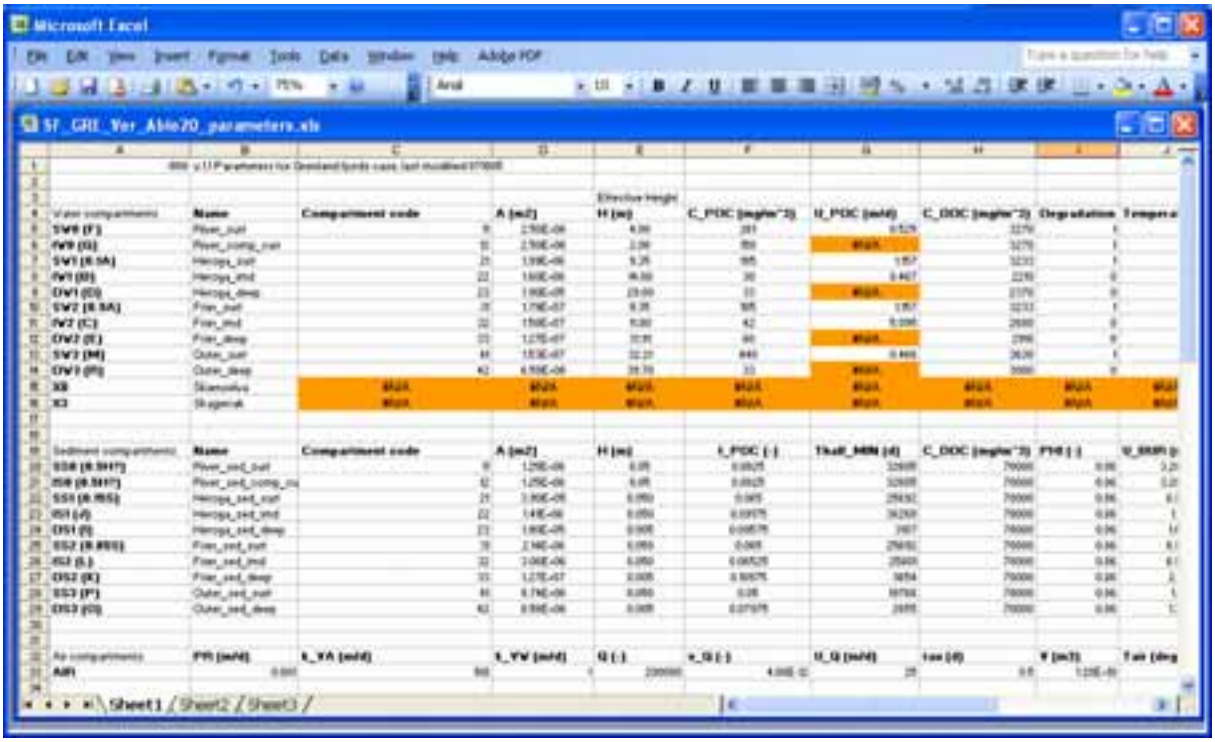


Figure 3. (continued on next page)

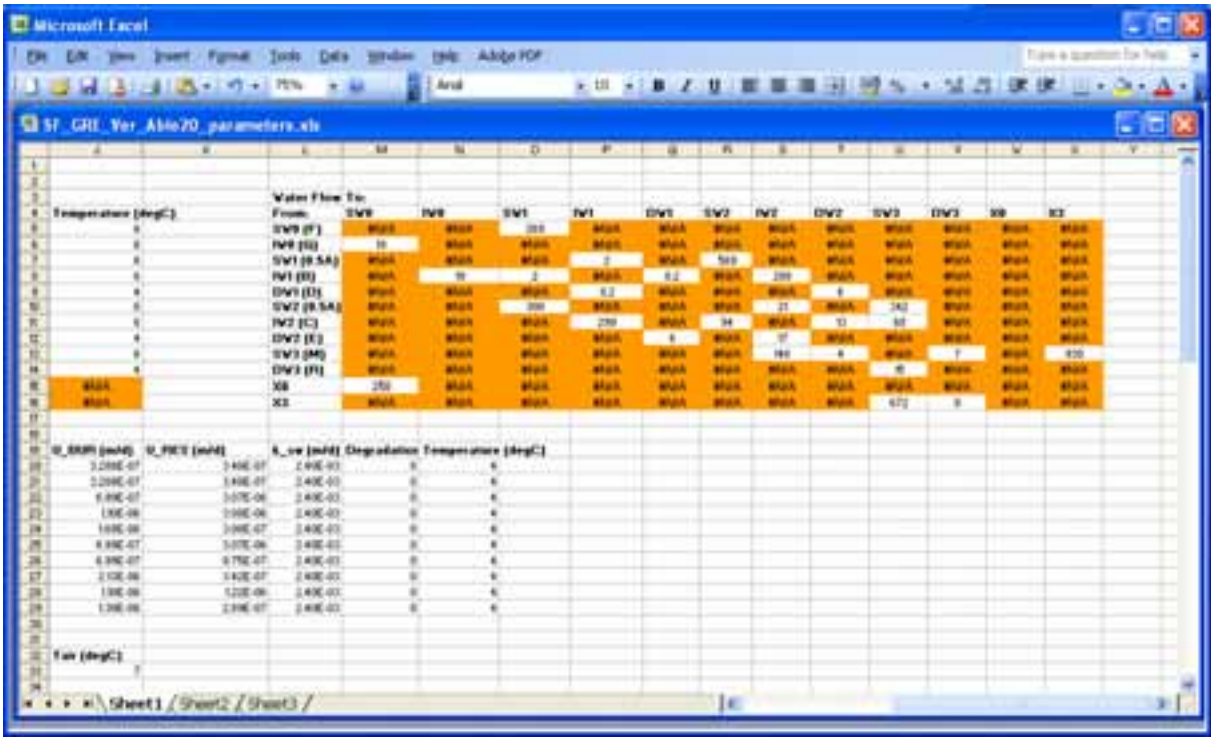


Figure 3. *Example of the SF-tool's abiotic model parameter file.*

2.3.4 File for abiotic emissions and initial/background concentrations

The background and initial concentrations [g m^{-3}] as well as emission time series [g d^{-1}] are listed in the corresponding file (SF_Abio_parameters.xls) as shown in Figure 4. Initial values are given for all model compartments (excluding air and the water columns outside the model domain [X0 and X3 in Figure 4]), emission time series for those model compartments that receive emissions, and background concentrations for the air compartment and for the water columns outside the model domain (X0 and X3 in Figure 4).

Note that in cell "A1" there must be a dummy number (e.g. -999) and that the chemical names should start from the cell "D5" for MATLAB to read the file in correctly. The order of the chemicals must be the same as in the chemical properties file, and the order of the compartment names in the initial/background concentration section of the emission file must follow the example shown in Figure 4; first air compartment, then water compartments, then sediment compartments, and finally the water columns outside model domain. The same internal ordering as in the parameter file within these groups must be followed. A free amount of empty rows are allowed between the emission time series for each compartment receiving emissions but the dates (year, month, day) must be inserted on the columns A-C. The assignment of the different emission time series to the correct compartments is done in the model code so their order in the Excel sheet is not fixed. In the model code it is assumed that emissions before the first given value are equal to this value. Similarly, emissions after the last given value are equal to this value.

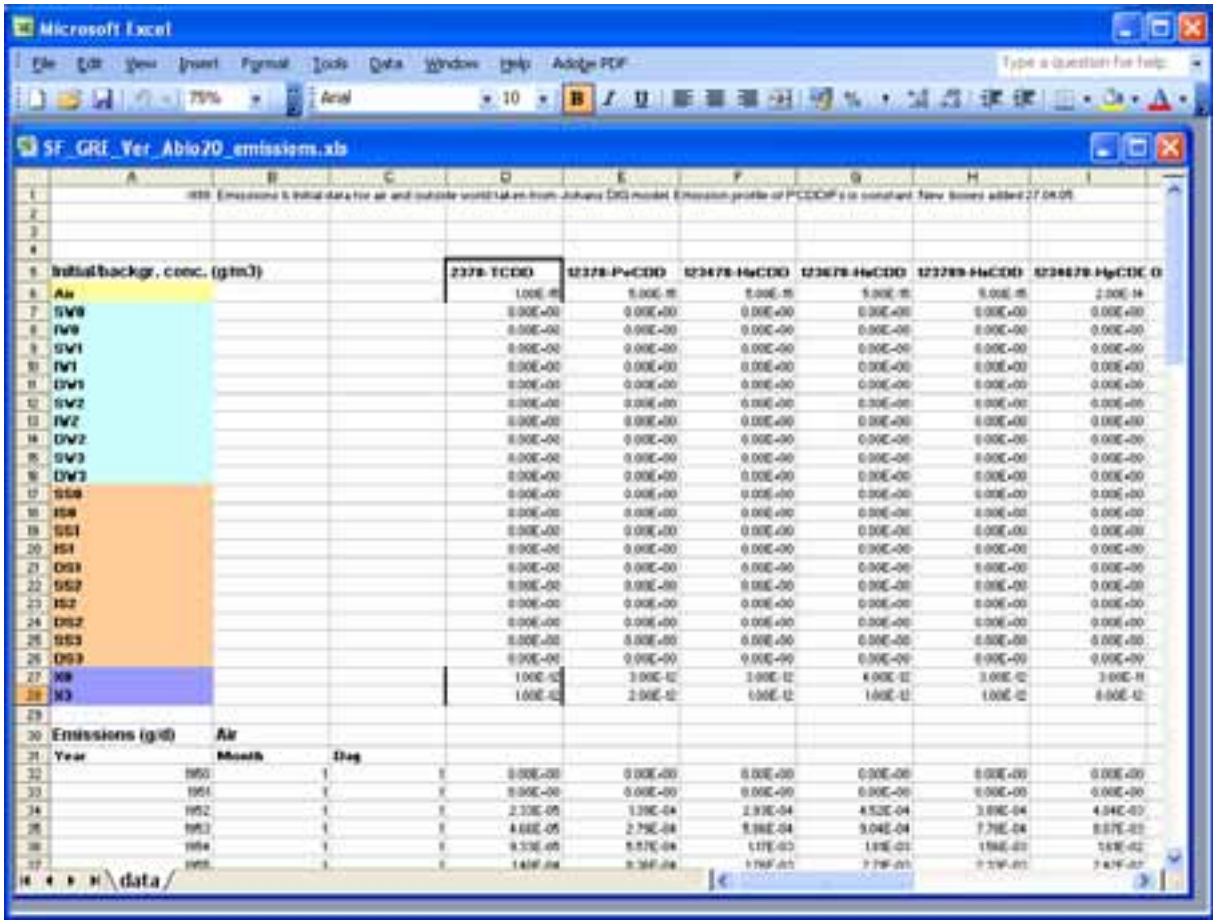


Figure 4. *Example of the SF-tool's file for initial/background concentrations and emission time series.*

2.3.5 Biotic model parameters

The biotic model parameter file (SF_Bio_parameters.xls, Figure 5) lists the values of the following compartment-specific (i.e. species or species groups) model parameters (required units are indicated in square brackets):

1. Matrix of diet preferences (fraction of each pray in the particular organism's diet) [-] (species given on rows eat those given on columns)
2. Body volume [L = kg]
3. Lipid fraction [-]
4. Metabolic degradation rate [d^{-1}]
5. Fraction of the organism's time spent in sediment (porewater) [-]

Note that in cell "A1" there must be a dummy number (e.g. -999) for MATLAB to read the file in correctly. The order of the species must be the same in the rows (data starting from 3rd row) and columns (data starting from 2nd column) of the diet matrix. The order of the parameter names following the diet matrix must not be changed either.

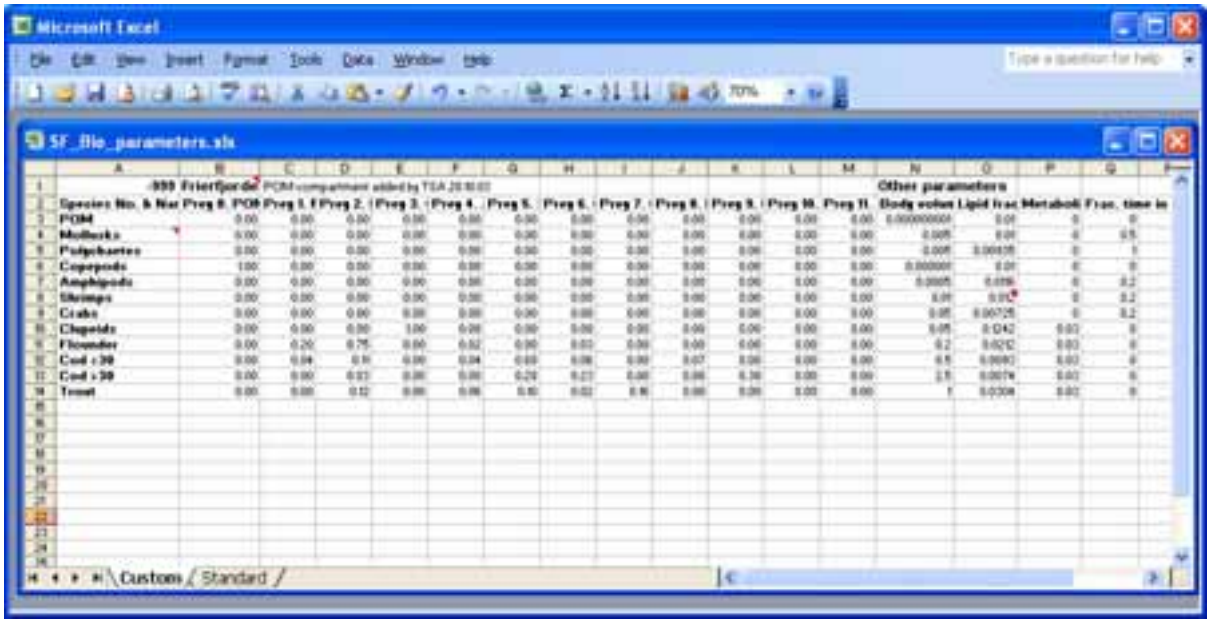


Figure 5. *Example of the SF-tool's biotic model parameter file.*

3. Simulating the fate of dioxins in the Grenland fjords

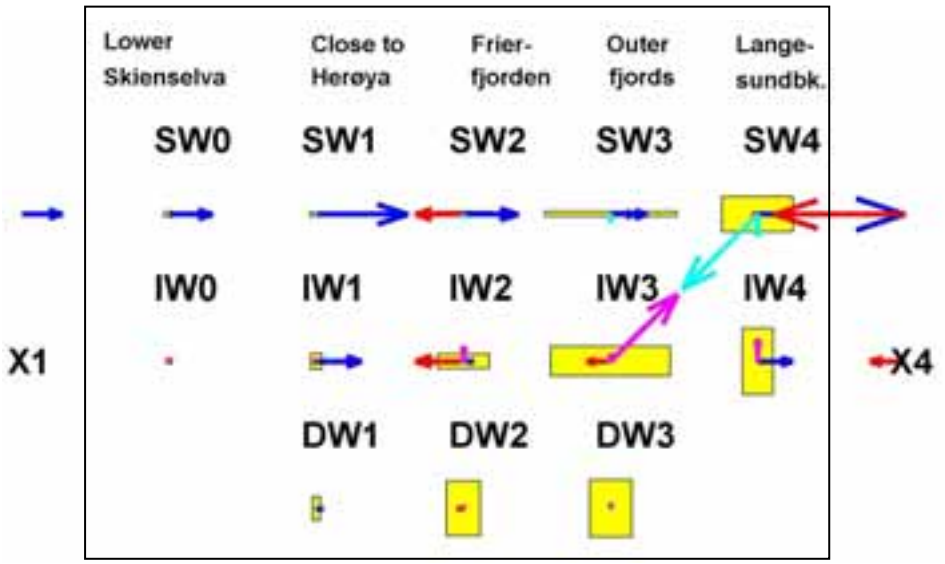
The Frierfjorden is the innermost branch of the Grenland fjord system in the southern Norway (58^o 5' N, 9^o 38' E). It has a surface area of ~20 km^2 and mean and maximum depths of 40 m and ~100 m, respectively. The sill depth at the mouth of the fjord is ~25 m. A magnesium production plant began operating in 1951 by the island Herøya in the innermost part of the Frierfjorden, and large amounts of polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) and other chlorinated organic pollutants were formed as by-products during the chlorination of magnesium oxide to yield water-free magnesium chloride. The PCDD/Fs discharges from the plant to sea water have been in the orders of kilograms per year calculated as 2378-TCDD (tetrachlorinated dibenzo-*p*-dioxin) toxicity equivalents. However, installation of cleaning devices at the plant in the end of the 1980s, reduced the direct emissions to less than 10 grams annually. The magnesium plant was closed down in 2002 and as a result direct PCDD/F emissions ceased. This pollution has been so severe that Norwegian authorities have issued advices against consumption of fish and shellfish caught in the area. A major environmental issue at present is the need and effect of remedial actions against the contaminated fjord and harbour sediments. To that end, the consequences on concentrations in biota and effect on the dietary advices both immediately and over time is critical (Saloranta et al. 2006). This called for modelling the fate of PCDD/Fs in the abiotic and biotic system in the fjord, and in the projects SedFlex and Rein Fjord the SF-tool was applied to simulate the impacts of different contaminated sediment remedial alternatives on the PCDD/F levels in cod and crab.

The following results were originally described in four separate research notes written by T. Saloranta for the Fylkesmannen i Telemark as part of the Rein Fjord project. Note that a version 1.0 of the SF-tool is used in the simulations described in this section. The largest difference compared to the version 1.1. (described in section 2) is the missing temperature dependency of the partitioning coefficients (equation 6). Testing between the two model code versions indicated, however, that the code difference did not affect the results significantly in the Grenland fjords case. Moreover, as the abiotic model could more or less replicate the results from another similar model for the Grenland fjords ("DIG model", Persson et al., 2006), this made us confident that the abiotic model code in the SF-tool is well verified and free from major bugs. In the Grenland fjords case we use results from already existing biotic simulations by Saloranta et al. (2006) (see section 3.3).

3.1 Model application setup for the Grenland fjords

The selected compartment structures in the abiotic and biotic model applications of the Grenland fjords case study are shown in Figure 6. The abiotic compartment volumes and surface areas are shown in Figure 7. These were calculated using GIS-tools and digital bathymetric maps. The surface compartments are restricted to 0-5 m depth interval, except in the Langesundbukta surface compartments (SW4, SS4) where 0-50 m interval is used (the surface and intermediate compartments are lumped into one). The intermediate compartments are restricted to 5-24 m depth interval, except in the outer fjords where 5-50 m interval is used. In the Langesundbukta the intermediate compartment is not applied but compartments IW4 and IS4, which cover the 50 m to bottom interval, correspond to deeper waters. The deep water compartments cover the rest of the water masses (from 24 to the bottom in the Frierfjorden and area close to Herøya, and from 50 m to the bottom in the outer fjords). Typical water residence times in the surface compartments are couple of days, in the intermediate compartments 10-20 days, and in the deep compartments ~1 year.

a)



b)

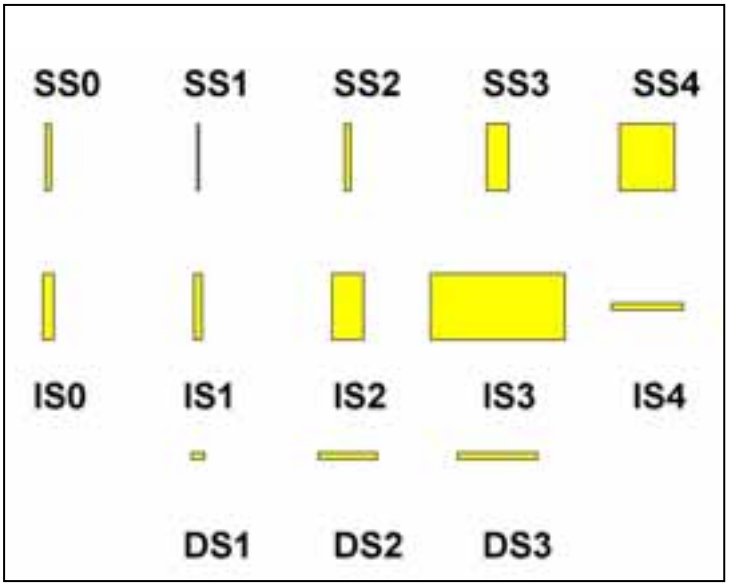
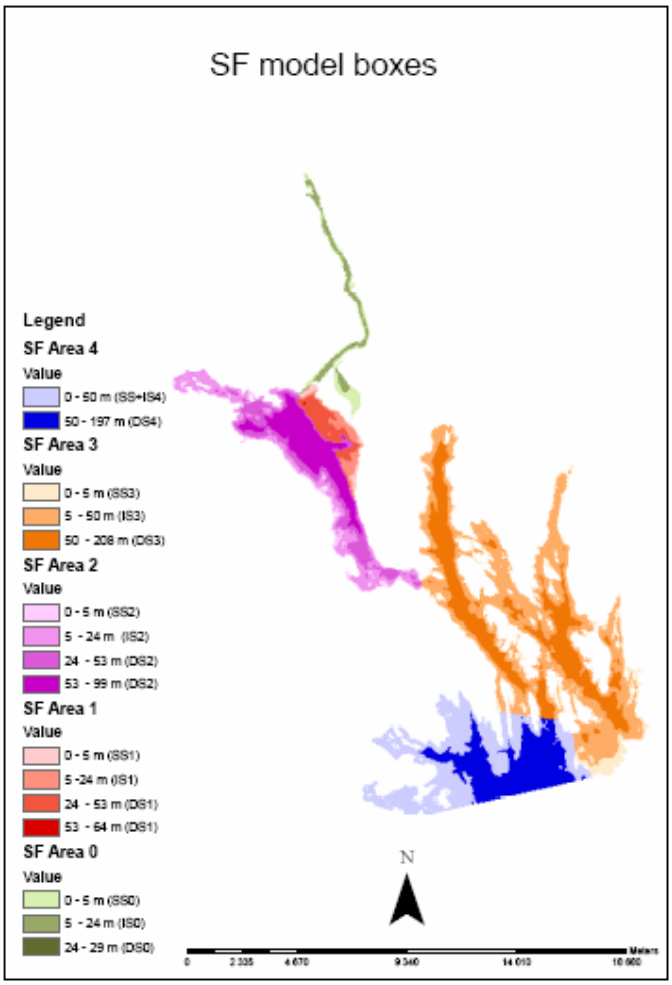


Figure 6. (continued on next page)

c)



d)

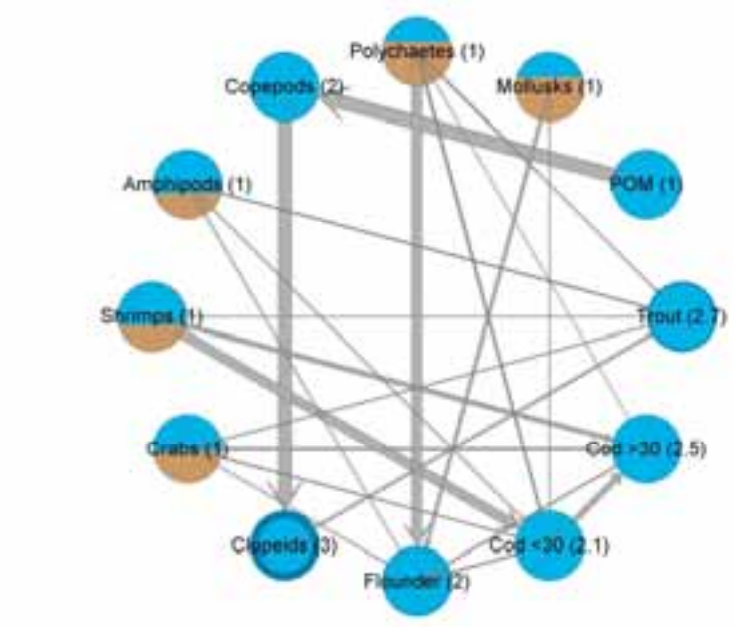


Figure 6. (continued on next page)

Figure 6. *a) Schematic illustration of the surface water (SW), intermediate water (IW), and deep water (DW) compartments in the SF-tool application on the Grenland fjords. The corresponding locations in the Grenland fjords are denoted above. The heights and widths of the "boxes" denote the relative depths and areas of the compartments (see Appendix A for more details on compartment characteristics). The arrows denote the magnitude of water flow between the compartments. Note that each water compartment is associated with a corresponding sediment compartment shown in (b). c) A bathymetric map showing the basis for compartment division in the model application. d) The food web of the Frierfjorden. Light brown color denotes the fraction of time spent in sediments and the darker blue ring the organisms' lipid fractions. Numbers in parentheses denote the effective trophic levels of the organisms.*

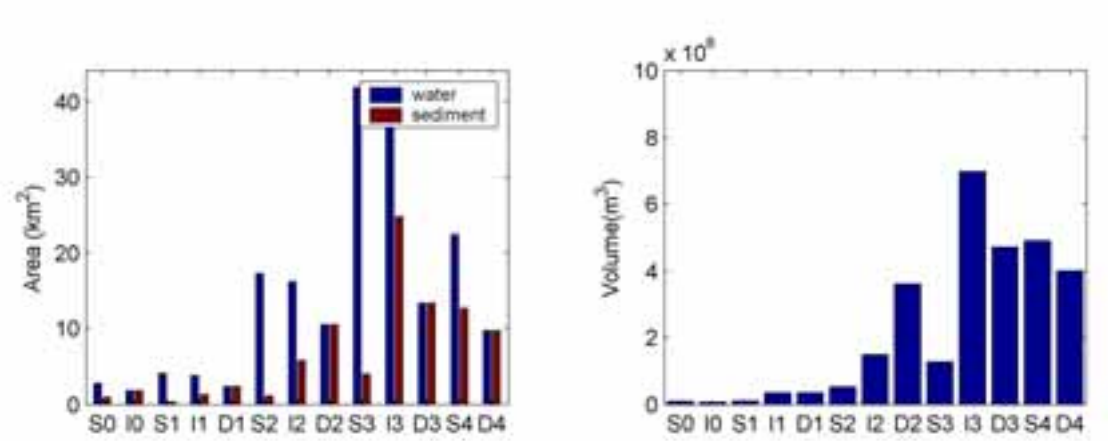


Figure 7. *Surface areas and volumes of the 13 water (and 13 sediment) compartments in the SF-tool abiotic model application for the Grenland fjords. "S" denotes surface, "I" intermediate, and "D" deep compartment. The number indexes denote: 0) lower River Skienselva, 1) close to Herøya, 2) Frierfjorden, 3) outer fjords 4) Langesundbukta (Skagerrak).*

The SF-tool's abiotic model was set up with parameters and other forcing data from the following sources (nominal values for the abiotic model parameters are shown in Appendix A):

- Data on chemical properties were obtained from Govers and Krop (1998) (K_{ow}), van der Berg et al. (1998) (TEF), Harner et al. (2000) (K_{oa}) and Persson et al. (2006).
- Data and values for abiotic model parameters, background concentrations, emission time series, and water flow were obtained from Persson et al. (2006). However, as the compartment structure and the compartment areas and volumes are somewhat different in the present application, some of the water flow values from Persson et al. (2006) are rescaled and some new flow values for the outermost fjord area are newly estimated. Generally the parameter values of the outer fjords compartments were applied also for the Langesundbukta compartments.

A major task in this study was to simulate how the cumulative cleaning up of the model sediment compartments in the Frierfjorden in 2006 would affect the PCDD/F levels in 1) Frierfjorden, 2) outer fjords and 3) Langesundbukta compartments (volume- and area-weighted average concentrations of the selected water and sediment compartments; see section 3.3), and how these changes would affect the PCDD/F concentrations in cod and crab. As the sediments seem to be the main source of PCDD/Fs for cod and crab (Saloranta et al., 2006), we focus mostly on the sediment concentrations in the following presentation of the model results.

The case study was started by running the abiotic model with nominal (non-calibrated) parameter values and comparing the results against observed particle-bound PCDD/F concentrations in the sediment of the Grenland fjords. The particle-bound concentrations were carbon-normalised and they are expressed in sums of the 17 simulated PCDD/F congeners in 2378-TCDD toxicity equivalent units (van der Berg et al., 1998). This initial model evaluation showed that the abiotic model predicts particle-bound concentrations around year 2000 reasonably well for most of the compartments. However, the model simulations overestimated observed concentrations in 1989 and around year 2000, especially in the Frierfjorden intermediate sediment compartment (IS2).

In order to obtain better fit between the model simulations and observations, and on the basis of the results from sensitivity analysis (see section 3.2), we selected to re-evaluate the burial and resuspension rates used by Persson et al. (2006). Their burial rates were estimated from excess ^{210}Pb-activity of vertically sliced sediment cores at eight stations in the Grenland fjords, and the rates varied from 638 to 1942 g m^{-2} year^{-1}. Their burial rate for the river Skienselva was estimated to 300 g m^{-2} per year assuming similarities with two other river systems, upper Hudson River and the Canadian Fraser River. The organic matter mineralisation rates used by Persson et al. (2006) (32 and 38 g m^{-2} year^{-1} for the shallow and deep sediments, respectively) were based on published values from literature for the Fanafjord of western Norway. The resuspension rates used by Persson et al. (2006) were expressed as a fraction of the gross sedimentation, and this fraction was fitted so that the gross sedimentation flux agreed with the flux measured in sediment traps (one trap in the Frierfjorden, and one in the Breviksfjorden).

Our new estimates of the burial rates in the fjord area were kept in the same range as in Persson et al. (2006), but the strong vertical differences (e.g. between intermediate and deep sediment of the Frierfjorden, boxes “L” and “K” in Persson et al. (2006)) were smoothed out. Thus burial rate for all surface sediment compartments was set to 650 (g m^{-2} yr^{-1}), for the intermediate sediment compartment in the Frierfjorden (IS2) to 1500 (g m^{-2} yr^{-1}). Furthermore, the deep sediment compartments were assumed to have 20% larger burial rates than in the intermediate compartments, and the outer fjords and Langesundbukta areas were assumed to have 1.5 times smaller burial rates. The resuspension fraction for the river compartments (SS0, IS0) was set to 0.6 and for the intermediate sediment compartment in the Frierfjorden (IS2) to 0.45, instead of 0.2 and 0.3 used in Persson et al. (2006). We also adjusted the depth of the active sediment layer H_{sed} from 0.5 cm to 2 cm for the deep sediment boxes outside Frierfjorden (i.e. DS3 and DS4). This modification is made to reflect the probably better oxygen conditions and thus larger H_{sed} in the deeper parts of the outer fjords than estimated in the DIG model parameterization (Persson et al., 2006). Figure 8 summarizes the applied sediment-related rates, and Table 3 shows the revised parameter values and those used by Persson et al. (2006).

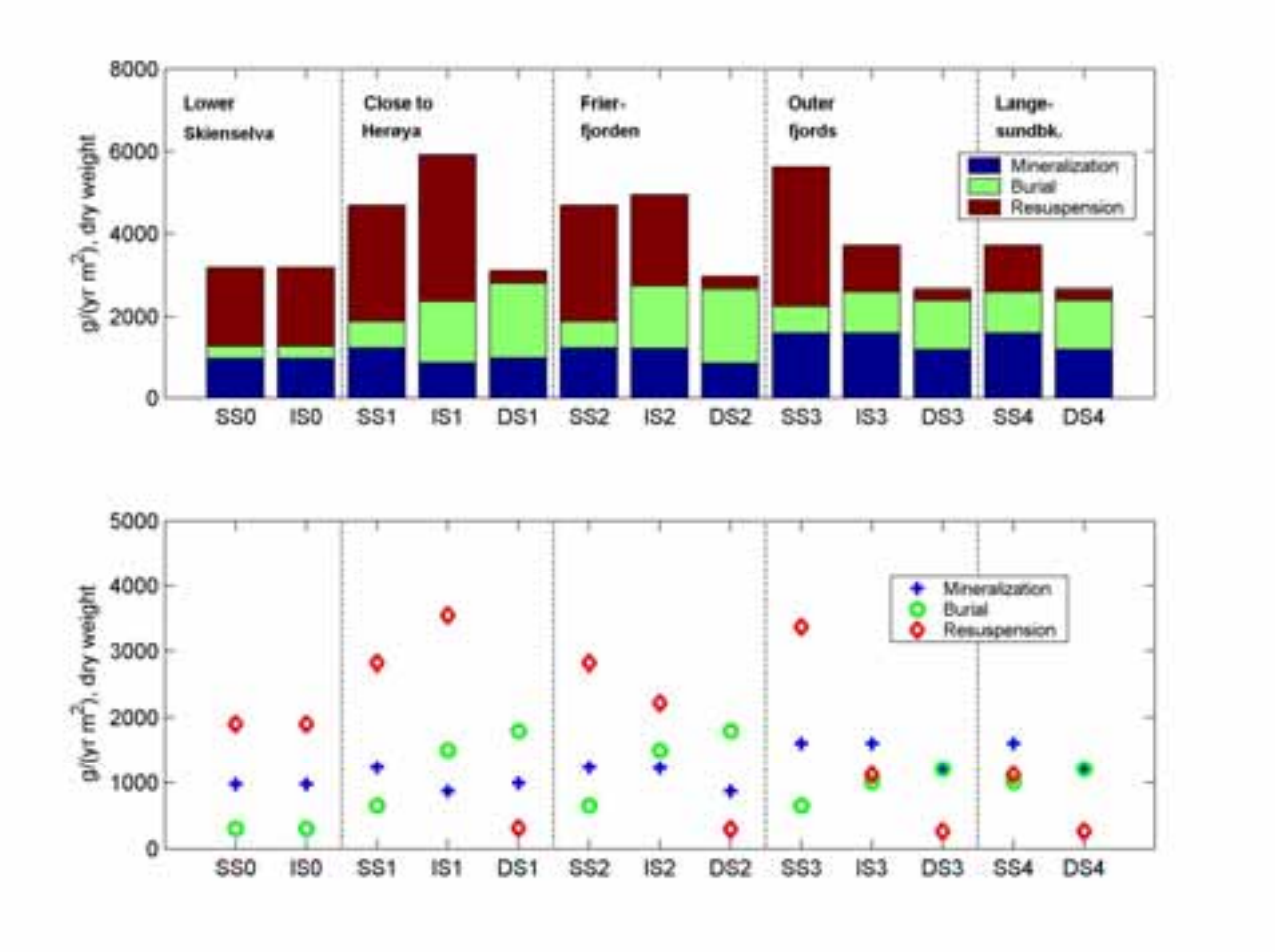


Figure 8. *Applied burial, resuspension and mineralization rates (grams of dry sediment per year per m^2) in the Grenland fjords model application. The three rates shown in the lower figure are stacked in the upper "bar-plot" figure to show the gross sedimentation rates (equal to the sum of the three rates).*

Table 3. Comparison of the revised burial rate (Bur) and fraction resuspended (Res) parameter values in the SF-tool (SF) and those used by Persson et al. (2006) (DIG).

Comp.	H (SS0, SS1)	I (DS1)	J (IS1)	K (DS2)	L (IS2)	O (DS3, DS4)	P (IS3, IS4)	S (SS1,2,3,4)
Bur_SF ($g\ m^{-2}\ yr^{-1}$)	300	1800	1500	1800	1500	1200	1000	650
Bur_DIG ($g\ m^{-2}\ yr^{-1}$)	300	1534	1000	1942	638	1186	1000	638
Res_SF (-)	0.6	0.1	0.6	0.1	0.45	0.1	0.3	0.6
Res_DIG (-)	0.2	0.1	0.6	0.1	0.3	0.1	0.3	0.6

As Figure 9 shows, the abiotic model predicts now particle-bound concentrations in 1989 and around year 2000 reasonably well, also in the Frierfjorden intermediate sediment compartment (IS2).

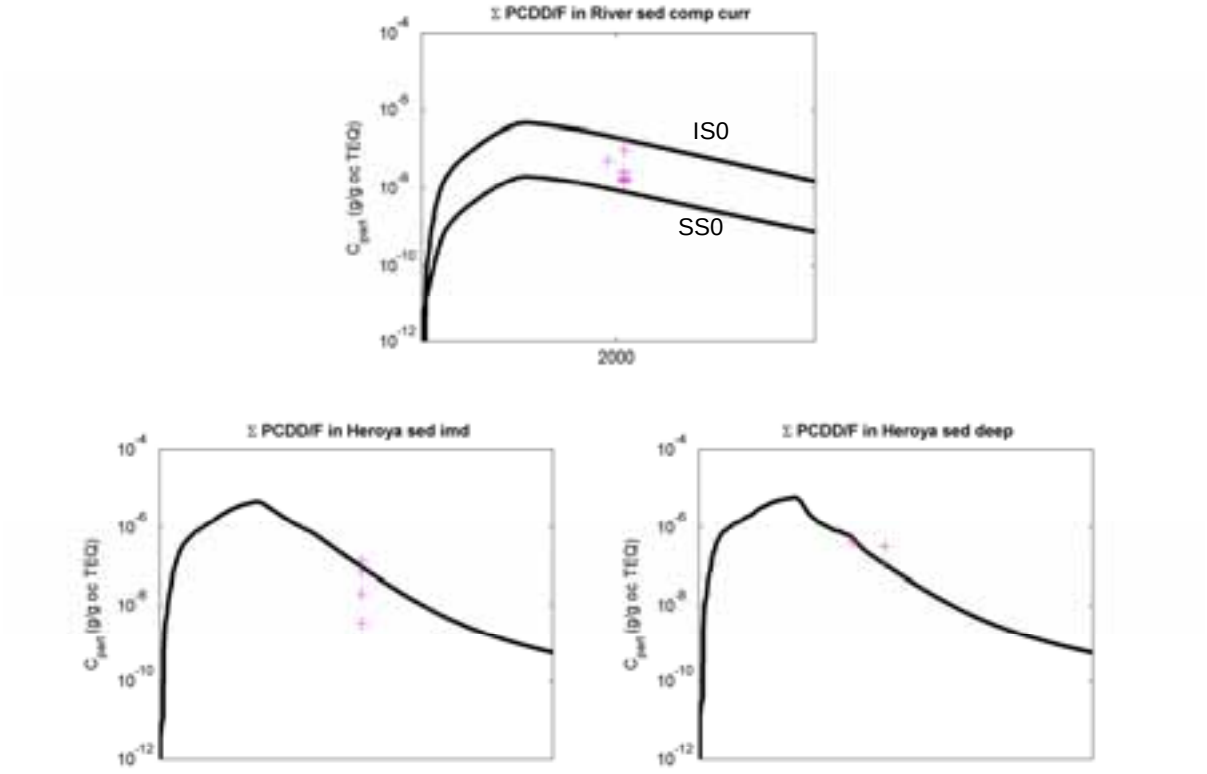


Figure 9. (continued on next page)

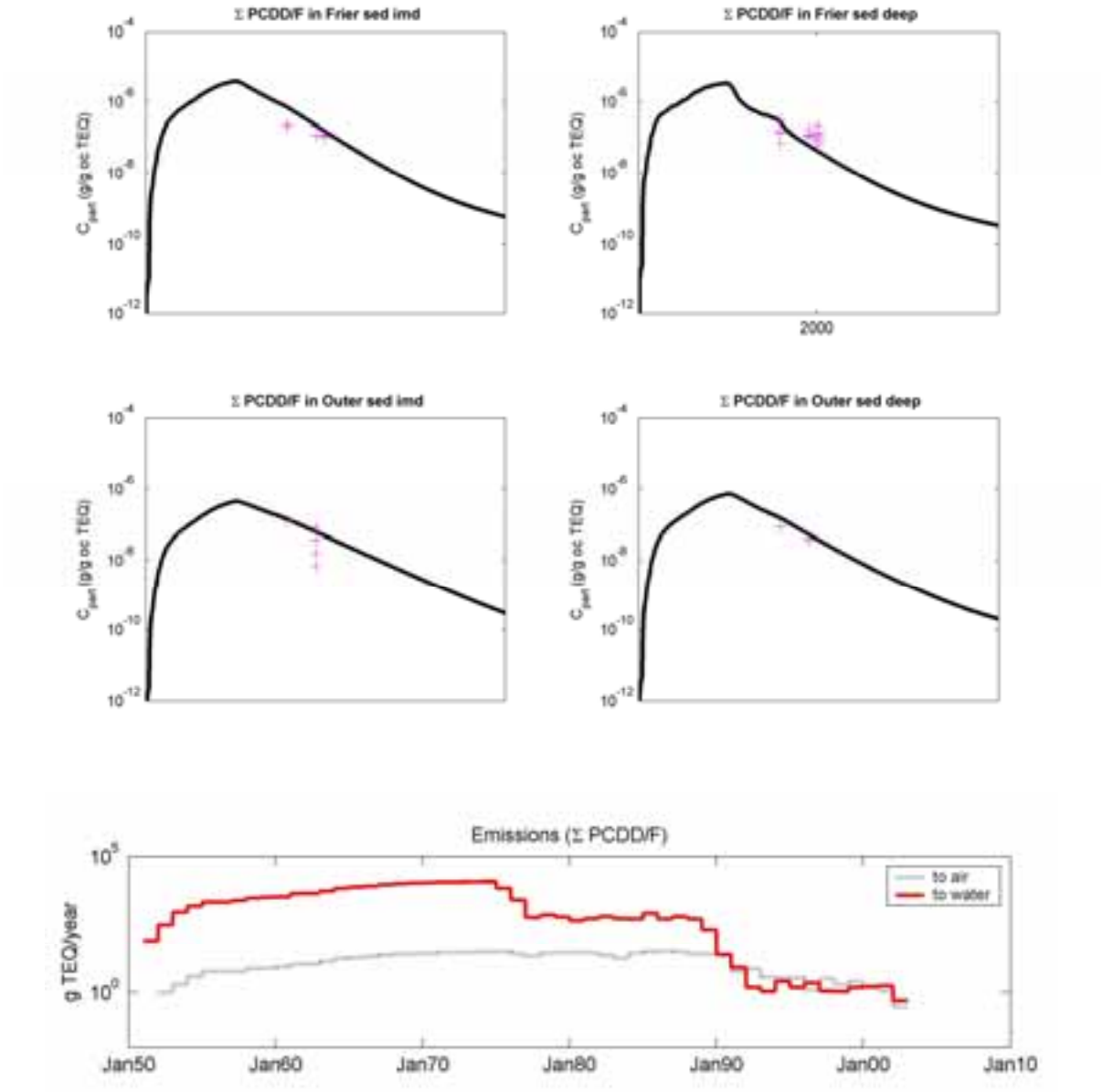


Figure 9. *Abiotic model simulated sediment particulate PCDD/F concentrations for period 1950-2050 with nominal parameter values. Crosses show observed concentrations based on samples from a 1-3 cm thick slice of the surface sediment. The lowermost subfigure shows the smission time series used for model forcing. The emission to water is directed to compartment SW1 (surface water close to Herøya).*

3.2 Sensitivity analysis of the abiotic model

The sensitivity analysis of the abiotic model was performed using Extended FAST technique (Saltelli et al., 2000). The results shown here are from a very similar previous model application for the Grenland fjords. Table 4 lists the min-max ranges that were defined for the 17 model parameters that were included in the sensitivity analysis (most of these are actually scaling factors for the actual parameters; parameter values apply throughout all the relevant compartments).

The model output, for which parameters' sensitivity was monitored, were sums of 2378-TCDD, 123678-HxCDF and OCDF concentrations in Friefjorden (volume- and area-weighted average concentrations of the six Frierfjorden water and sediment compartments including area close to Herøya). These sums were expressed in toxicity equivalent units (van der Berg et al., 1998) in years 2000, 2005, 2015, and 2050. The model was run for 1997-2050 with initial concentrations for 1997 taken from a previous model run. Sampling rate in FAST was two times the Nyquist frequency taking into account four harmonics of the basic frequency, and the selected total number of model runs was ~57000.

Table 4. Minimum-maximum ranges for the 17 abiotic parameters included in the sensitivity analysis. "(scal.)" denotes cases where the nominal parameter value is scaled within the given range.

Parameter	Min	Max	Unit	Remark
phi	0.75	0.95	-	sediment water content (porosity)
burial	0.2	5	(scal.)	scaling of sediment burial rate
resus	0.2	5	(scal.)	scaling of sediment resuspension rate
seddiff	0.1	10	(scal.)	scaling of sediment-water diffusion mass transfer coeff.
miner	0.2	5	(scal.)	scaling of sediment mineralization rate
C_init	1/3	3	(scal.)	initial concentration level at simulation start
H_shl	0.5	2	(scal.)	scaling of shallower area sed. active depth
H_deep	0.5	5	(scal.)	scaling of deeper area sed. active depth
Kow	1/3	3	(scal.)	scaling of K_{ow}
Koc_obs	1/3	3	(scal.)	scaling of K_{oc_obs}
flow	0.5	2	(scal.)	scaling of water flow
emiss	0.5	2	(scal.)	scaling of emissions
Cback	1/3	3	(scal.)	scaling of background conc. in river and sea water outside the model domain
A_DOC	0.05	20	(scal.)	scaling of DOC partitioning coeff.
U_poc	1/3	3	(scal.)	scaling of POC settling velocity
POC_wat	0.5	2	(scal.)	scaling of water POC conc.
Foc_sed	0.5	2	(scal.)	scaling of OC volume fraction in sediment

When considering the difference in dissolved sediment pore water concentration levels between 2000-2015 and 2000-2050 (Figure 10) the model results were most sensitive for burial and resuspension rates, as well as for the thickness of the shallower sediment active layer and sediment water content.

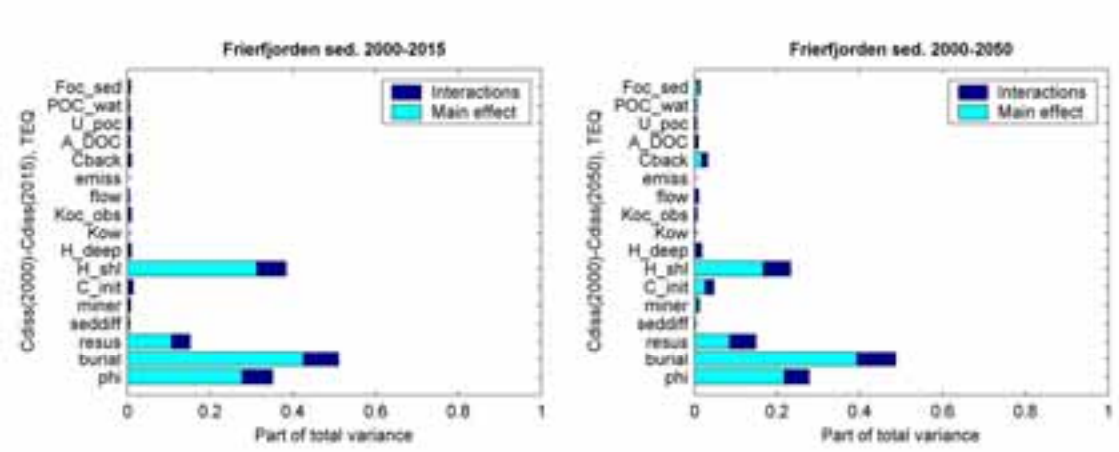


Figure 10. *Sensitivity analysis of the abiotic model output in the Frierfjorden. The difference in dissolved concentration levels between 2000-2015 (left panel) and 2000-2050 (right panel) for sum of 2378-TCDD, 123678-HxCDF and OCDF (toxicity equivalent units) are considered. "Main effect" denotes the parameter's contribution alone (first order effect), and "interactions" its contribution due to higher order interactions with other parameters.*

3.3 Simulating remedial measures in the Frierfjorden

To produce simulation results for the remediation scenarios in terms of probability distributions, rather than single values, an uncertainty analysis of the abiotic model in the SF-tool was done. 11 parameters were selected for this analysis, on the basis of the results from the sensitivity analysis. In the uncertainty analysis, the model was run 2500 times with randomly chosen values for the selected parameters sampled on the basis of the distributions and rank correlation matrix given in Tables 5-6. Results were saved on each simulation round and finally the simulation results data set, covering 6 different scenarios, in 5 different fjord areas, for 17 PCDD/F congeners, in 18 different points in time, and for 2500 uncertainty analysis runs, consisted of 23 million distinct concentration values. This kind of repeated model simulation with random parameter value sampling is also called Monte Carlo simulation. The values of the rest of the model parameters, not included in uncertainty analysis, were fixed to their nominal values.

Note that the variation of both burial and resuspension rates was made independent of other compartments in compartments IS1 and IS2. Note also that the range of burial rates in the uncertainty analysis attempts to take into account the spread between estimated mean burial rates for the Frierfjorden: 638-1942 g m^{-2} yr^{-1} in Persson et al. (2006), and ~400 g m^{-2} yr^{-1} in Pederstad et al. (1993). The higher estimates shown in Table 3 give better fit with the observed sediment concentrations around year 2000, while lower burial rate estimates are seemingly needed in order to reproduce the estimated ~8% mean yearly decrease in cod liver concentrations in 1991-2001 (Bjerkeng and Ruus, 2002). This again underlines the important role these rates play in the model, and that a more thorough parameter estimation study is needed to try to fully resolve this discrepancy. For the purpose of this study we have selected the uniform distribution favouring lower burial rates than in Table 3 in the uncertainty analysis for cod and crab.

The abiotic model was then run for 17 PCDD/F congeners for the period 1997-2051 with six remediation scenario alternatives. The simulated remediation measure was taking place in August 1, 2006, and consisted of capping the contaminated sediment areas with clean sediment mass (having otherwise the same properties as the capped contaminated mass). The (minimum) thickness of the

capped layer was the same as the active sediment layer depth (see Appendix A). The simulated scenarios were the following:

1. **scenario "NoRem"** where no remediation measures are made.
2. **scenario "R"** where the model sediment compartments SS0 and IS0 (i.e. lower River Skienselva) were capped. (~3 km^2, i.e. 12 % of the total area of the Frierfjorden including lower River Skienselva and area close to Herøya).
3. **scenario "R+Hs"** where the model sediment compartments SS0, IS0, SS1, and IS1 (i.e. lower River Skienselva and areas close to Herøya down to 24 m depth) were capped. (~5 km^2, i.e. 19 % of the total area).
4. **scenario "R+Hs+Fs"** where the model sediment compartments SS0, IS0, SS1, IS1 SS2, and IS2 (i.e. lower River Skienselva , as well as areas close to Herøya and in the rest of Frierfjorden down to 24 m depth) were capped. (~11 km^2, i.e. 47 % of the total area).
5. **scenario "R+Hs+Fs+Hd"** where the model sediment compartments SS0, IS0, SS1, IS1, DS1, SS2, and IS2 (i.e. lower River Skienselva , areas close to Herøya down to the deepest point, and areas in the rest of the Frierfjorden down to 24 m depth) were capped. (~14 km^2, i.e. 57 % of the total area).
6. **scenario "R+Hs+Fs+Hd+Fd"** where the model sediment compartments SS0, IS0, SS1, IS1, DS1, SS2, IS2, and DS2 (i.e. lower River Skienselva, as well as all sediment areas close to Herøya and in the rest of the Frierfjorden down to the deepest point) were capped. (~24 km^2, i.e. 100 % of the total area).

Table 5. Probability distribution functions (PDF) for the 11 parameters included in the uncertainty analysis. "CF" denotes confidence factor, i.e. it gives the lower and upper 95% confidence limits when the median values is divided and multiplied by CF, respectively. "(scal.)" denotes cases where the nominal parameter value is scaled with the given PDF. For explanation on parameter abbreviations, see Table 4.

Parameter	**PDF**	**Mean/median/mode**	**Spread**
phi [-]	Triangular	0.85	0.75-0.95 (min-max)
burial (scal.)	Uniform	0.65	0.3-1 (min-max)
resus (scal.)	Lognormal	1	5 (CF)
H_shl [m]	Triangular	0.05	0.02-0.1 (min-max)
Koc_obs (scal.)	Lognormal	1	10 (CF)
flow (scal.)	Lognormal	1	1.3 (CF)
C_init (scal.)	Lognormal	1	3 (CF)
POC_wat (scal.)	Lognormal	1	1.3 (CF)
Foc_sed (scal.)	Lognormal	1	1.3 (CF)
C_back_X1 (scal.)	Lognormal	1	2 (CF)
C_back_X4 (scal.)	Lognormal	1	2 (CF)

Table 6. Non-zero rank correlations between the parameters included in the uncertainty analysis. For explanation on parameter abbreviations, see Table 4.

Parameter 1	**Parameter 2**	**Rank correlation**
burial	*POC_wat*	0.75
H_shl	*resus*	0.5
POC_wat	*Foc_sed*	0.25
phi	*H_shl*	-0.5

In order to transfer the simulated abiotic concentration time series to concentration levels in cod and crab we used the methodology described in Saloranta et al. (2006) who simulated the intake and bioaccumulation of PCDD/Fs in the Frierfjorden food web (Figure 1) with a similar model code as contained in the SF-tool. They also performed a sensitivity analysis of the biotic model which pointed out the dissolved concentrations in water and sediment (i.e. the output from the abiotic model) as well as the fish metabolic degradation rate as the most influential model factors.

Saloranta et al. (2006) also applied results from the general theory for linear systems and showed that, among others, it is possible to calculate the fraction of an organism's PCDD/F concentration which originates from sediment pore water S_{sed} (the remaining fraction originating from water, i.e. $S_{wat} = S_{sed} - 1$). As the biotic model code is formulated as a linear system, then for any arbitrary time-invariant model parameter values this means that, e.g. a 20 % reduction in the water and sediment pore water levels of the dissolved phase will lead to a similar reduction in the simulated concentrations of all the organisms (taking into account the response time of the biotic system, of course). These assumptions give us a rather robust modelling strategy for the biotic system, in which we use the biotic model only to calculate the S_{sed} and S_{wat} values for the target organism(s), and to estimate the organisms' response times. After this we can use the simulated reductions of the dissolved PCDD/F levels in water and sediment pore water together with S_{sed} and S_{wat} and the estimated response times to derive corresponding reductions in the PCDD/F levels in the target organism(s). In this way we can use the observed concentrations in the target organism(s) as the starting point, and thus eliminate the propagation of the possible bias of the concentration levels from the abiotic model output into the biotic predictions. Namely, while abiotic models, such as ours, generally often can well predict the levels of the total PCDD/F concentrations, they can more easily fail in predicting well the truly dissolved concentration levels due to lack of understanding of the complicated partitioning phenomena (see e.g. Persson et al., 2002). However, if we can assume that the solid-water partitioning will remain unchanged in time, then a simulated reduction in the total concentrations levels would imply an equal reduction also in the dissolved levels (which would in turn induce a similar reduction in the PCDD/F levels in the organisms, taking into account S_{wat} and S_{sed}, and the response times, of course).

Saloranta et al. (2006) showed that S_{sed} was 100 % for both cod and crab, i.e. that they gain practically their entire PCDD/F load from the sediment (either directly or via food web). Consequently, we used the simulated time series of sediment pore water as the forcing for cod and crab. Furthermore, we focused on three different fjord areas assuming that both cod and crab will stay and feed entirely within them. These areas were 1) Frierfjorden (0-50 m depth interval for both cod and crab due to often prevailing low oxygen concentrations in deeper waters); 2) outer fjords (0-50 m depth interval for crab and the whole water column for cod); 3) Langesundbukta (0-50 m depth interval for crab and the whole water column for cod). The response time of the biotic system to changes in their abiotic forcing was set to 2 years for both cod and crab, based on Saloranta et al. (2006). After one (two) response time(s) the system has covered 63% (86%) of its way towards the new (quasi) steady state.

Figure 11 shows the results from the uncertainty analysis where the relative reductions in the dissolved sediment pore water concentrations since 2000 are transferred to sum of PCDD/F concentration (in 2378-TCDD toxicity equivalent units, taking into account the difference between the abiotic and biotic PCDD/F congener compositions) time series in cod and crab by assuming initial median whole body PCDD/F concentration in the Frierfjorden in 2000 of 20 ng/kg wet weight in cod, and 27 ng/kg wet weight in crab, according to observations made in the DIG-project (Næs et al., 2004). The initial concentrations in the outer fjords and Langesundbukta were selected to be lower by factors 3 and 9 of those in the Frierfjorden, respectively, based on Bjerkeng and Ruus (2002). We also added an additional uncertainty (i.e. standard error of the median) by a confidence factor of 3 on the biotic initial conditions in 2000 and assumed that the co-variation in the abiotic and biotic initial concentrations in 2000 have a rank correlation of 0.95.

Figure 11, the main end product of our Frierfjorden study, shows among others that the median of the 2500 simulated PCDD/F concentration time series in cod will in the “NoRem” scenario fall below the EU limit of the dietary health advisory around 2015, while in the ”R+Hs+Fs” scenario it had reached this limit around 2009. If one, however, wants to be more cautious and consider the 95th percentile of all the 2500 simulations, then Figure 6 shows that the simulated PCDD/F concentration in cod will in the ”R+Hs+Fs” scenario fall below the EU limit of the dietary health advisory around 2012, while in the “NoRem” scenario not before ca. 2040.

Figure 12 shows simulation results for cod and crab in the Frierfjorden from an alternative scenario where remediation measures are made in 2010 instead of 2006. In the same year 2010, the oxygen conditions deeper in the Frierfjorden are assumed to have greatly improved and consequently the cod is assumed to stay in the whole water column down to the deepest point (100 m, i.e. 50 m deeper than in the scenarios presented in Figure 11) and thus be exposed to the entire sediment area of the Frierfjorden. Also the depth of the active sediment layer is assumed to have increase from 0.5 cm to 5 cm, and already buried sediment 10 years back (corresponding to a bulk sediment burial rate of 5 mm/yr) is assumed to become included in the active sediment layer again. The results show that the deepening of the active sediment layer does not influence dramatically the mean sediment concentration cod is exposed to (a slight increase occurs, though). This is due to the combination of following factors: i) increased portion of the deeper sediment area in the mean value calculation, ii) concentration increase due to activation of already buried sediment in 2010, and iii) the generally somewhat lower concentration levels in the deep sediment compared to the intermediate sediment. However, since the feeding area of cod is increased in 2010 by 33 %, the effect of the remediation measures (except in the full capping option “R+Hs+Fs+Hd+Fd”) becomes less pronounced, as relatively smaller areas of the total feeding area are capped. Due to the changes in the deep sediment properties after 2010 it also now takes about 10 years longer time until the median concentration level in cod in scenario “NoRem” reaches the 4 ng/kg ww limit. Note, however, that these timeline estimates are particularly sensitive to parameterization of the sediment properties (burial, resuspension, active layer thickness).

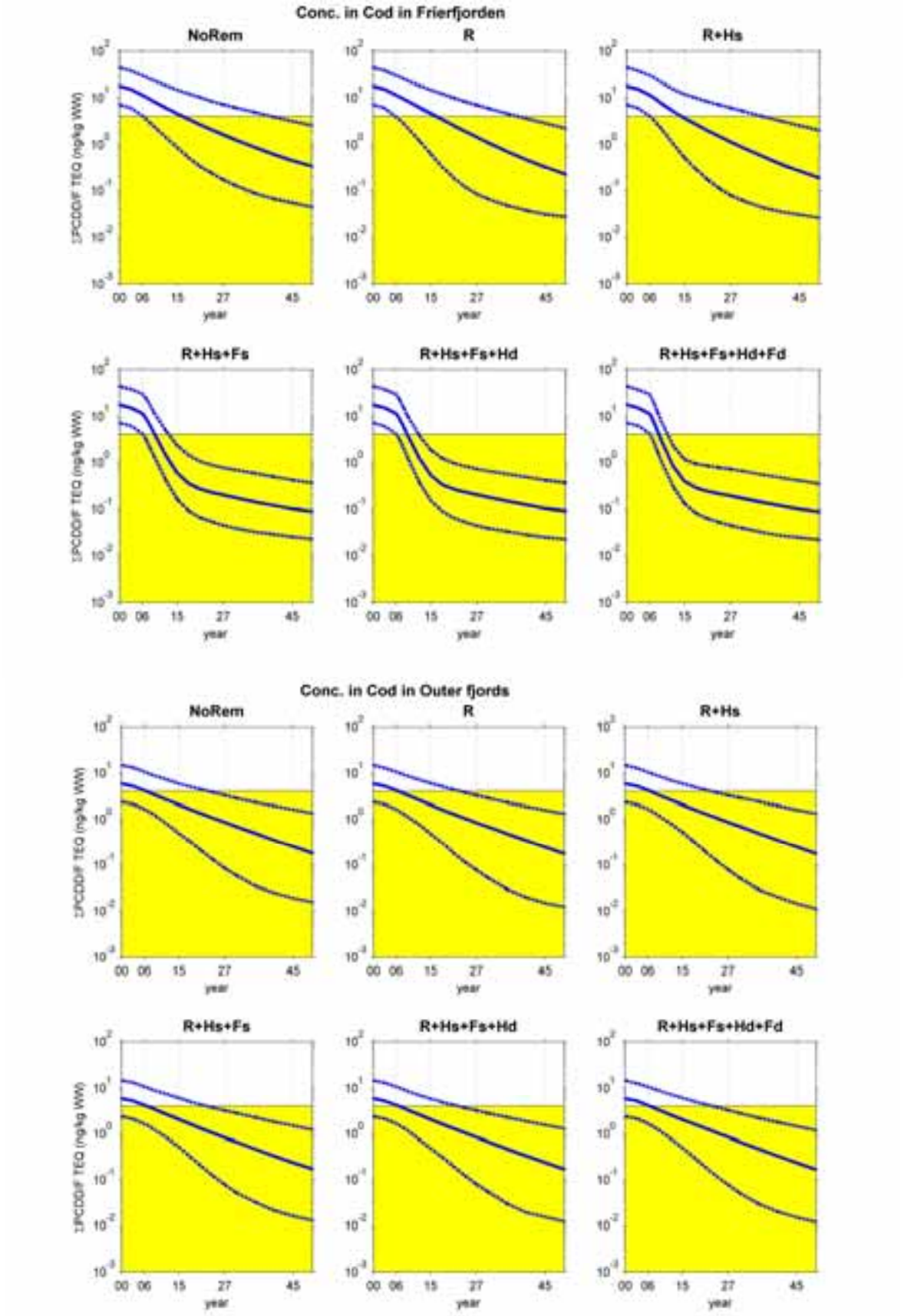
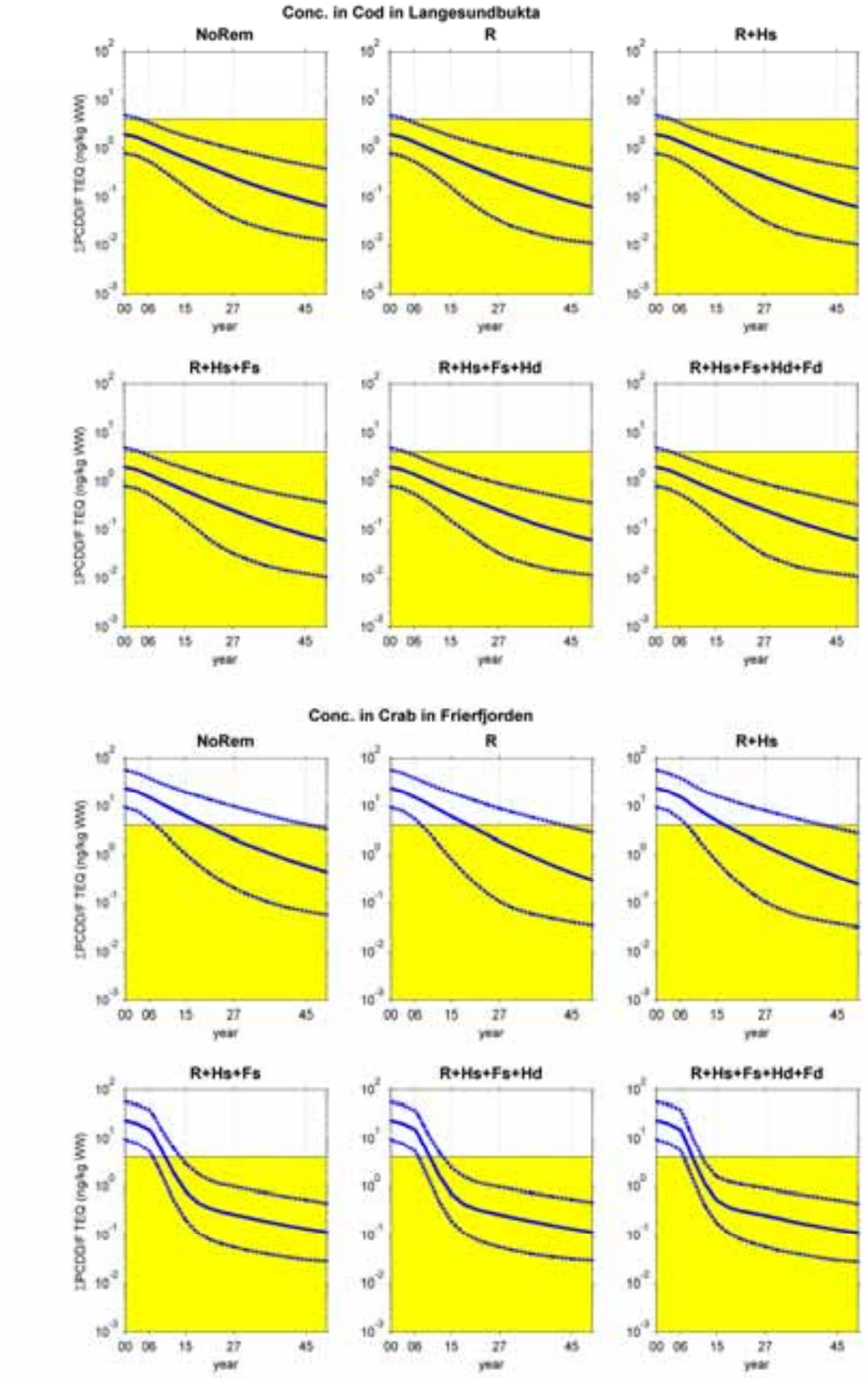


Figure 11. (continued on next page)



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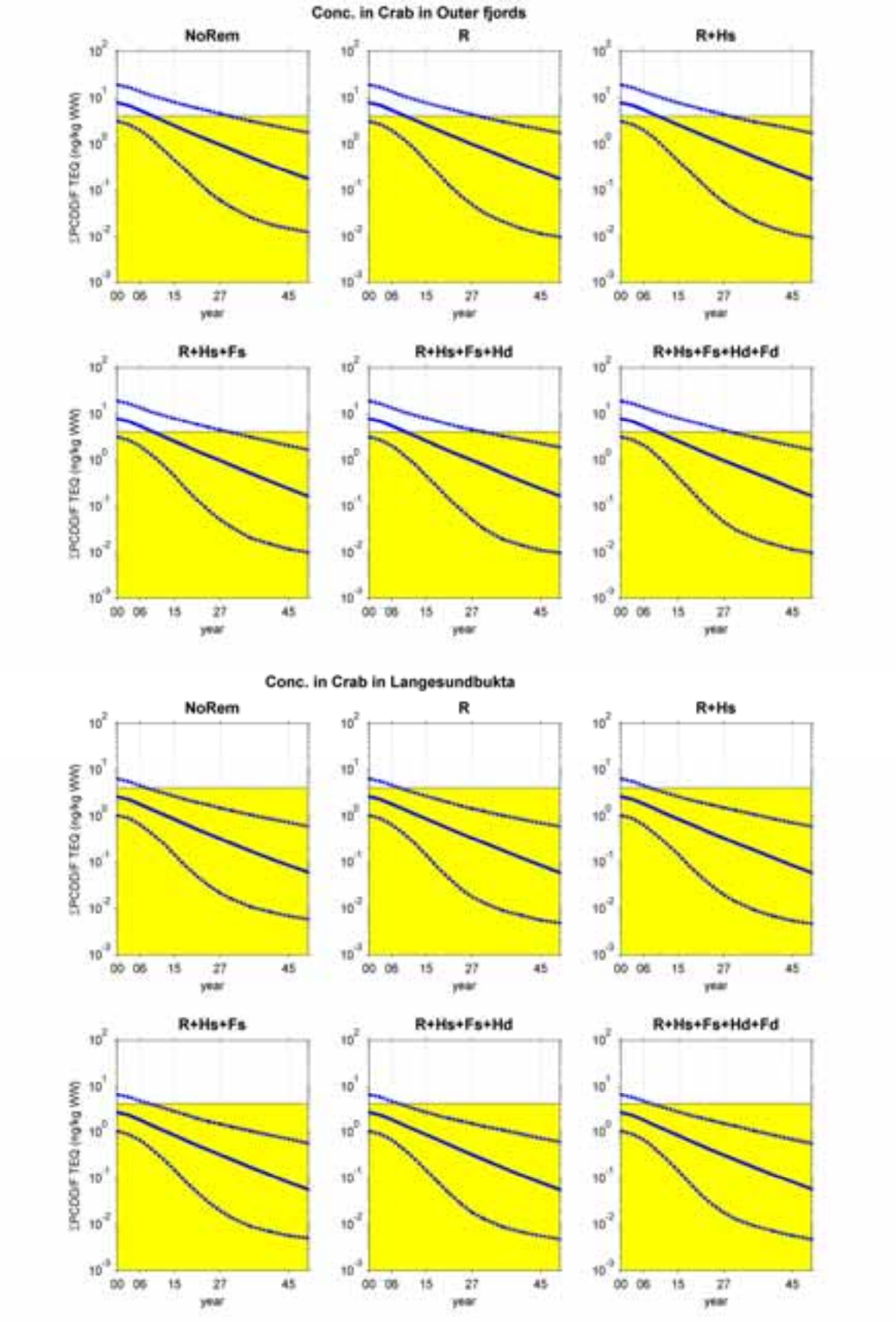

Figure 11. (continued on next page)

Figure 11. *Time evolution of the sum of 17 PCDD/F congeners (concentrations expressed in toxicity equivalent units) in cod and crab in the Frierfjorden, outer fjords, and Langesundbukta under six different remediation scenarios. Thick solid lines denote the median, and dashed lines the 5th and 95th percentiles, based on the 2500 model runs executed in the uncertainty analysis. The yellow shaded area denotes concentrations below the EU limit value of 4 ng/kg wet weight for dietary health advisory (VKM, 2004, cited in SedFlex project note by D. Barton).*

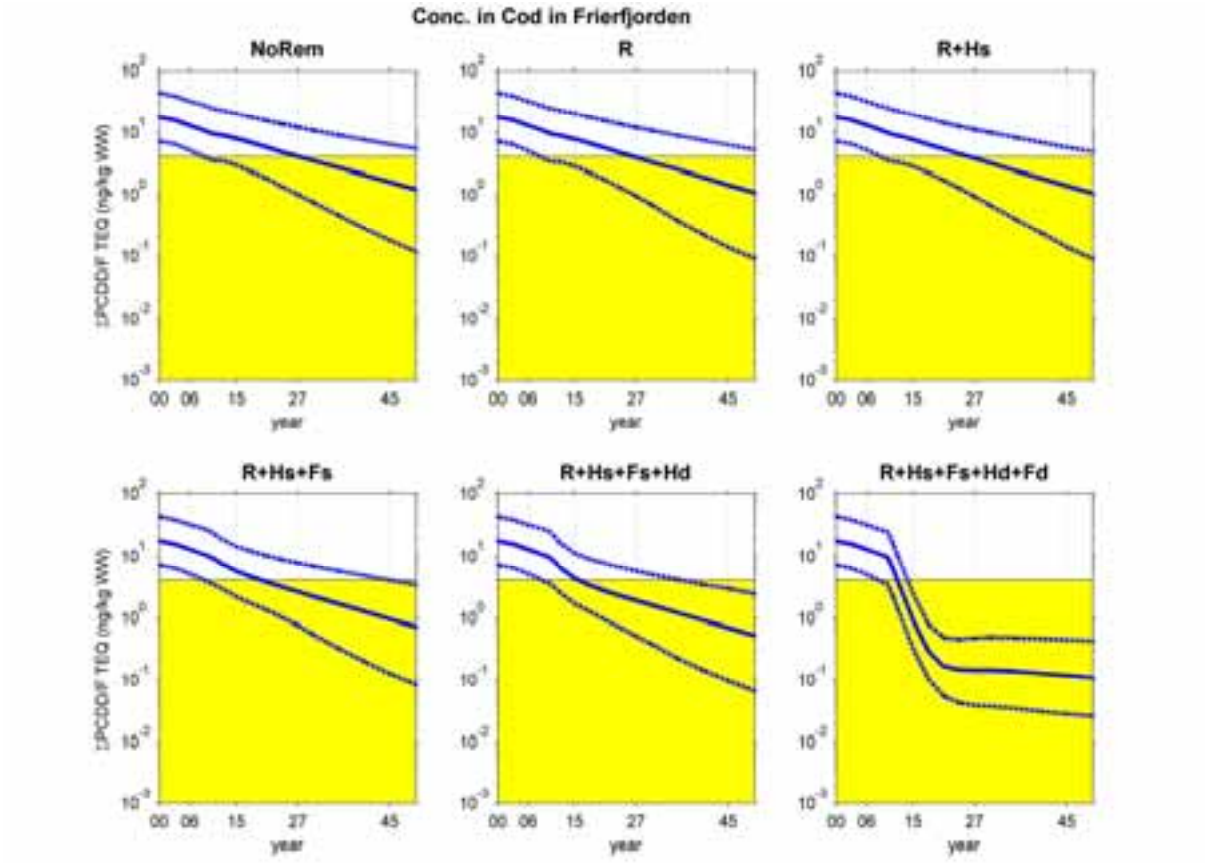

Figure 12. *As in Figure 11 for cod in the Frierfjorden, but where the six different remediation scenarios and greatly improved oxygen conditions in the deeper water column and sediments occur in 2010.*

3.4 Simulating remedial measures in the outer fjords

In the following we describe the simulated remediation scenario analysis for the "outer fjords" (model area 3, i.e., the fjord system seawards of the Brevik sill, excluding the outermost Langesundbukta area; see Figure 1). This study is a direct continuation of the simulated remediation scenario analysis for the Frierfjorden (section 3.3).

This study was started by running the abiotic model with nominal (non-calibrated) parameter values and comparing the results against observed particle-bound PCDD/F concentrations in the sediment.

The particle-bound concentrations were carbon-normalised and they are expressed in sums of the 17 simulated PCDD/F congeners in 2378-TCDD toxicity equivalent units (van der Berg et al., 1998). The new measurements from November 2005 are also shown in Figure 13.

As Figure 13 shows, the abiotic model predicts particle-bound concentrations in 1989 and around year 2000 reasonably well, but the decreasing concentration trend is somewhat larger than estimated by Bjerkeng and Ruus (2002) for concentrations in cod liver (~8% decrease per year). As in the Frierfjorden case (section 3.3) we have selected to scale the nominal burial rates with the uniform distribution 0.3-1 favouring lower burial rates, and thus giving better fit with the observation-based concentration decline rate in the uncertainty analysis for cod and crab.

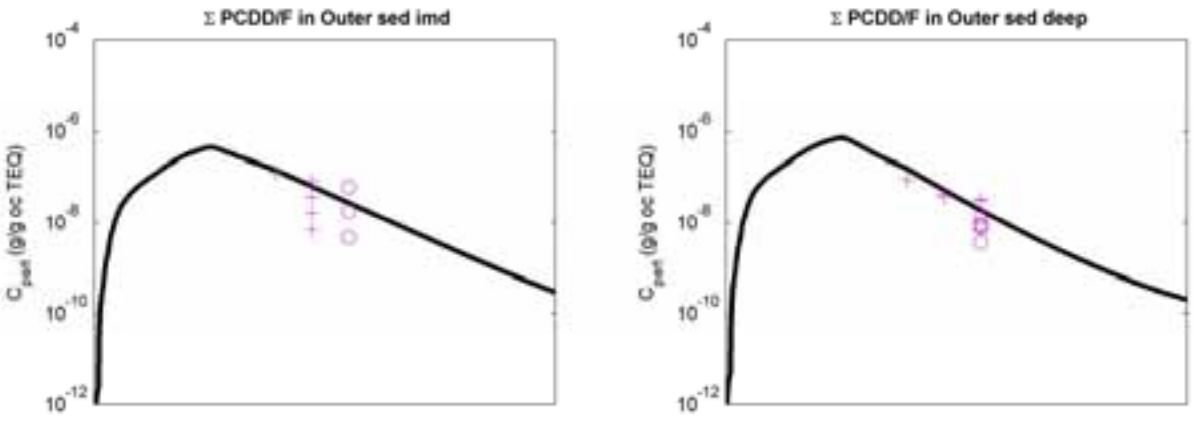

Figure 13. *Abiotic model simulated sediment particulate PCDD/F concentrations in two outer fjord sediment compartments for period 1950-2050 (nominal model parameter values). Crosses show observed concentrations based on samples from a 1-3 cm thick slice of the surface sediment. The circles denote those new observations from November 2005 that are situated outside the main fjord channel (i.e., outside Eidanger-Breviksfjorden).*

To produce simulation results for the remediation scenarios in terms of probability distributions, rather than single values, an uncertainty analysis of the abiotic model in the SF-tool was done. In the uncertainty analysis, the model was run 2500 times with randomly chosen values for the selected parameters sampled on the basis of the distributions and rank correlation matrix described in Tables 5-6. The only modification made was that the probability distribution for the thickness of the active sediment layer (used in the uncertainty analysis), which in the Frierfjorden case (section 3.3) applied only for the shallow and intermediate sediment compartments, is now extended to apply also for the deep sediment compartments

The abiotic model was then run for 17 PCDD/F congeners for the period 1997-2051 with six remediation scenario alternatives. The simulated remediation measure was taking place in August 1, 2006, and consisted of capping the contaminated sediment areas with clean sediment mass (having otherwise the same properties as the capped contaminated mass). The (minimum) thickness of the capped layer was the same as the active sediment layer depth. The simulated scenarios were the following:

1. **scenario "NoRem"** where no remediation measures are made.
2. **scenario "Os 20%, "** where 20 % of the model sediment compartments SS3 and IS3 (i.e. outer fjords down to 50 m depth) were capped. (~5.7 km^2, i.e. 14 % of the total area of the outer fjords).
3. **scenario "Os 40%, "** where 40 % of the model sediment compartments SS3 and IS3 were capped. (~11.4 km^2, i.e. 27 % of the total area of the outer fjords).
4. **scenario "Os 60%, "** where 60 % of the model sediment compartments SS3 and IS3 were capped. (~17.2 km^2, i.e. 41 % of the total area of the outer fjords).
5. **scenario "Os 80%, "** where 80 % of the model sediment compartments SS3 and IS3 were capped. (~22.9 km^2, i.e. 55 % of the total area of the outer fjords).
6. **scenario "Os 100%, "** where 100 % of the model sediment compartments SS3 and IS3 were capped. (~28.6 km^2, i.e. 68 % of the total area of the outer fjords).

The response times of cod and crab (set to 2 years, based on Saloranta et al. (2006)) to changes in their abiotic forcing was taken into account in the results. The simulation results in Figure 14 show that in order to gain a significant reduction in the concentration levels in cod and crab living in the outer fjords (cod assumed to stay and feed down to the deepest point of ~200 m, and crab down to 50 m depth) large areas of the outer fjords should be capped, cleaning up significant portions of the contaminated feeding and habitat sediment areas of cod and crab. The remediation scenarios for cod have less effect than for crab since the deeper areas (<50 m) remain uncapped in all scenarios.

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We produced also simulation results for cod and crab from an alternative scenario where the areas outside the main fjord channel (Eidanger-Breviksfjorden) are assumed to be decoupled from the main channel (although ideally they could be defined as a new model compartment). These more "periferic" outer fjord areas show generally lower (up to ~one order of magnitude) concentration levels in 2005 than the main channel (see Figure 13). The sediment areas and volumes of this main channel are taken from Persson et al. (2006) and the vertical water fluxes in the outer fjords are set to 50% of their previous values in order to scale them to reduced surface area. The same remediation scenarios as above are used, but now the absolute and relative capping areas are different, as shown below:

1. **Eidanger-Brevik scenario "NoRem"**, 0%, 0 km^2
2. **Eidanger-Brevik scenario "Os 20%"**, 11%, 1.7 km^2
3. **Eidanger-Brevik scenario "Os 40%"**, 23%, 3.5 km^2
4. **Eidanger-Brevik scenario "Os 60%"**, 34%, 5.2 km^2
5. **Eidanger-Brevik scenario "Os 80%"**, 46%, 7.0 km^2
6. **Eidanger-Brevik scenario "Os 100%"**, 57%, 8.7 km^2

Comparison (not shown) reveals very similar results between the whole fjord and the main-channel-only alternatives, which is not surprising since the sediment properties (which remain unchanged) dominate the future development of sediment concentration levels. Thus, it seems that results from the whole fjord simulations can be "downscaled" to apply also for the main channel, as long as similarly local cod (and crab) populations can be assumed (this might not be a valid assumption, though, especially for cod).

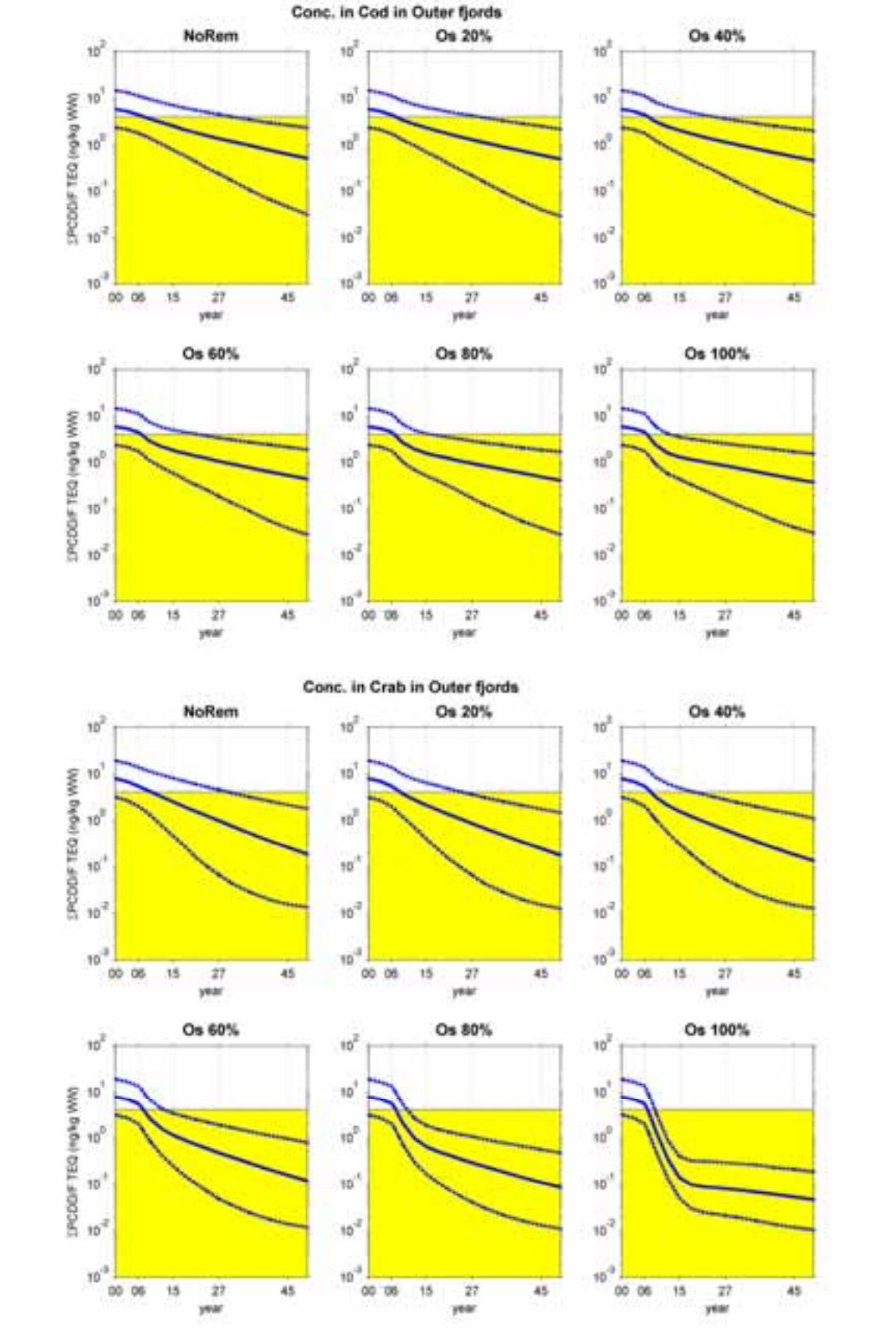

Figure 14. (continued on next page)

Figure 14. *Time evolution of the sum of 17 PCDD/F congeners (concentrations expressed in toxicity equivalent units) in cod and crab in the outer fjords under six different remediation scenarios. Thick solid lines denote the median, and dashed lines the 5th and 95th percentiles, based on the 2500 model runs executed in the uncertainty analysis. The yellow shaded area denotes concentrations below the EU limit value of 4 ng/kg wet weight for dietary health advisory (VKM, 2004, cited in SedFlex project note by D. Barton).*

Figure 15 shows the net flux of the sum PCDD/Fs (in 2378-TCDD toxicity equivalents) over the Brevik sill (i.e. from Area 1 to 2) and from the sediments of the whole Frierfjorden and from the lower River Skienselva (Areas 0, 1, and 2).

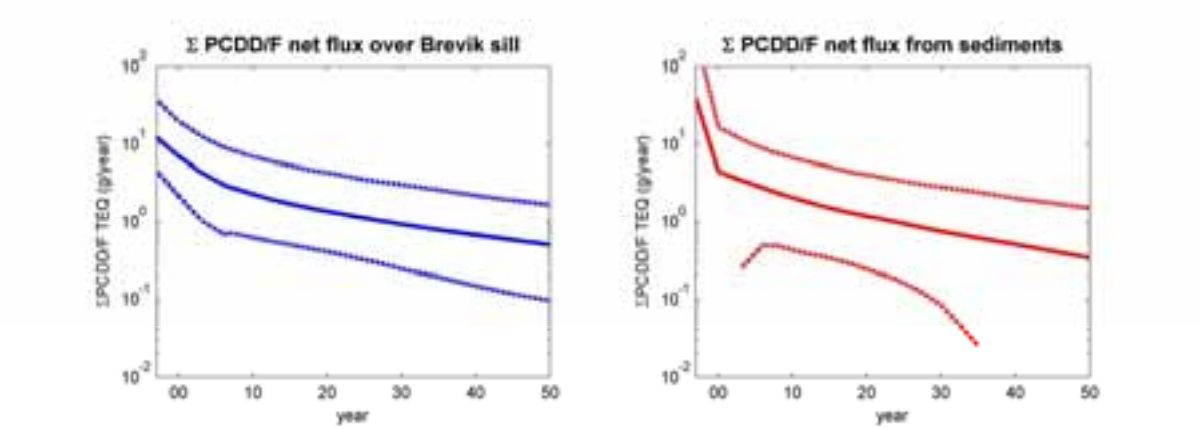

Figure 15. *The net flux of the PCDD/Fs (sum of 17 congeneres, in 2378-TCDD toxicity equivalents) over the Brevik sill (i.e. from Area 1 to 2) and from the sediments of the whole Frierfjorden and from the lower River Skienselva (i.e., Areas 0, 1, and 2). Thick solid lines denote the median, and dashed lines the 5th and 95th percentiles, based on the 2500 model runs executed in the uncertainty analysis.*

4. Conclusions and final remarks

The main conclusion based on the simulations with the SF-tool in the Grenland fjords (see Figures 10 and 13) are the following:

- A significant reduction in the concentration levels in cod and crab in the Frierfjorden can first be seen when larger areas of the Frierfjorden (see Figure 11, scenario R+Hs+Fs) are capped, and thus significant portions of the contaminated feeding and habitat sediment areas of cod and crab are cleaned up. The same type of conclusion applies also in the outer fjords remediation scenarios (Figure 14).
- Capping of contaminated sediments in the Frierfjorden will have no significant effect on the future evolution of the sediment concentrations (and hence on the concentrations in cod and crab) in the outer fjords or in the Langesundbukta (sediment area at 0-50 m depth, or deeper, considered). This is due to the slowness and ineffectiveness of the transport processes between the sediments of different fjord areas, especially between those separated by shallower sills. However, capping of contaminated sediments in the Frierfjorden will have an effect (figure not shown), although small (reduction by a factor of ~2), in the concentration level in the water column of the outer fjords and Langesundbukta (0-50 m, or deeper, water column considered).
- Capping of contaminated sediments in lower River Skienselva and in the shallower parts of the area close to Herøya will have no significant effect on the future evolution of the concentration levels in cod and crab in the Frierfjorden, in the outer fjords or in the Langesundbukta. This is due to the reason pointed out above, as well as due to the relatively small areas and somewhat lower concentration levels in the lower River Skienselva and Herøya compartments (see Figure 9). In addition, cod and crab are not assumed to feed or stay in the river domain (the shallower parts of the area close to Herøya cover ~10 % of their assumed Frierfjorden habitat).
- Generally the model simulations seem to indicate that if one aims to make effective remediation measures affecting the PCDD/F levels in the organisms, one should start covering at areas where the organisms live and feed, where the sediment burial and resuspension rates are smallest, and where the active sediment layer depth and present concentration level are highest.

In addition to the model assumptions already described in this note, the following remarks should be borne in mind when drawing conclusions from the simulations presented in this note:

- The spatial resolution in the model is quite coarse, and thus e.g. the compartment depth intervals (e.g. 5-24 m representing the intermediate compartments in the Frierfjorden) and areas should be taken tentatively, when e.g. planning the remediation measures. Moreover, homogeneous conditions are assumed within each compartment and the spatial variation within the compartments is not taken into account. E.g. in the Frierfjorden it is assumed that all deep sediment compartments (in the model defined as areas below 24 m) have anoxic conditions, while in reality the depth where anoxic condition begin to occur may vary from year to year and will most probably not be in the mean exactly at 24 m, as defined in the coarse vertical resolution of the model (three vertical layers). To investigate the effect of enhanced oxygen conditions in the Grenland fjords we also run a simulation where all the sediment compartments were assumed to have the active layer depth of 5 cm (not shown). However, this caused no significant changes in the above conclusions. Also the simulated concentration levels represent the average cod and crab in the particular fjord domain, and variation in individual crab or cod concentrations, e.g. due to different exposure from different local habitats within the fjord domains, is not included in the results.

- The starting point values for cod and crab in 2000 are based on samples from only that single year (an uncertainty by 95 % confidence factor of 3 is, however, assumed for these starting point values). Thus interannual variability is not taken into account here. The longer time series of concentrations in cod liver from Bjerkeng and Ruus (2002) could be used in the future to construct starting point values which would be based on mean estimates from a longer period.
- The solid-water partitioning parameter which accounts for the bioavailability of the PCDD/Fs is assumed constant in the model. This is still a poorly know parameter, and especially its future evolution is uncertain and difficult to predict. However, if it would change drastically in the future, e.g. due to non-linear sorption dynamics, this would likely cause changes in the future PCDD/F levels in the organisms which are not taken into account in the present simulations.
- If one would like to narrow down the uncertainty estimates in the model simulations, one should focus on more accurately estimating the four most influential parameters pointed out in the sensitivity analysis. Of these the active sediment layer depth and sediment porosity are easier to measure than the burial and resuspension rates.
- In Figures 10, 11 and 13 important parameter uncertainties in the abiotic model are taken into account together with the uncertainty of the selected starting points of median concentration level in cod and crab. This type of model parameter uncertainties are also called *technical uncertainties*. Its worth remembering, however, that the relative intercompartmental differences in the parameter values are not affected by our uncertainty analysis. For example, uncertainties in the details of the described flow regime or intercompartmental differences in the burial rate are not taken into account as we only consider scaling (up or down) of the whole flow regime and all the nominal burial rates in the different compartments. There may also be significant uncertainties of another type which are not accounted for in a usual uncertainty analysis, e.g uncertainties in how well the scientific knowledge behind the algorithms in the model code describes reality (*methodological uncertainties*) or uncertainties due to presently unknown processes of PCDD/F behavior in a fjord (*epistemological uncertainties*).

5. References

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Appendix A.

Below is shown the Excel worksheet containing the model nominal parameter values used in the simulations.