

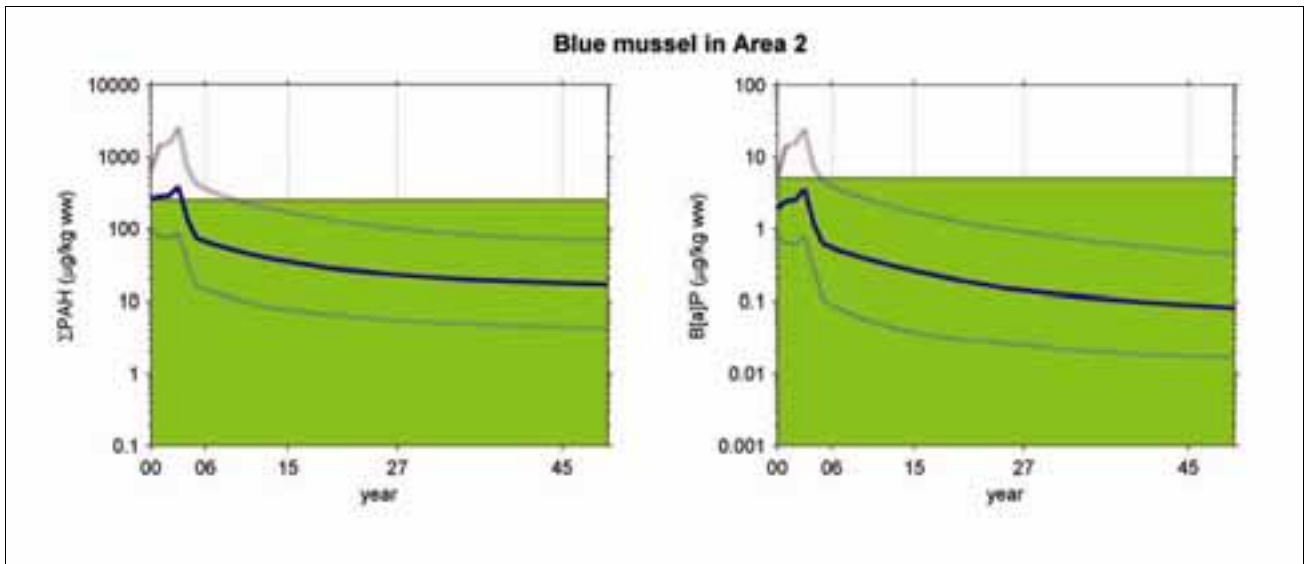


REPORT SNO 5113-2005

# Simulating the Fate of Polycyclic Aromatic Hydrocarbons (PAHs) in the Sunndalsfjord



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<p><b>Abstract</b></p> <p>As part of the ongoing discussion on remedial actions against PAH contaminated sediments in the Sunndalsfjord, the SedFlex-Tool was applied to the Sunndalsfjord system in order to investigate the magnitude PAH transport from the inner Sunndalsfjord (i.e. near Sunndalsøra) to outer fjord areas (e.g. the Tingvollfjord), concentrations of PAHs in blue mussels in the Tingvollfjord if future emissions from the Sunndal plant are assumed to be zero, and how the concentrations of PAHs in the sediments in the Sunndalsfjord and Tingvollfjord will change with time. Main conclusions are:</p> <ul style="list-style-type: none"> <li>- The transport of PAHs from the inner Sunndalsfjord to outer fjord areas in 2000 was initially estimated to be approximately 1000 kg year<sup>-1</sup>, dominated by the flux from the contaminated sediments.</li> <li>- The total PAH and Benzo[a]Pyrene concentrations in blue mussels inhabiting the surface layer (0 – 5 m) in the Tingvollfjord will fall rapidly once direct emissions to the system cease. The model also demonstrated that inputs from background atmospheric and riverine sources control the long-term levels of PAHs in blue mussels, rather than remobilization of contaminants from the sediments</li> <li>- The initial total PAH levels in sediments (surface, intermediate and deep) in the Sunndalsfjord and Tingvollfjord were estimated to be approximately 11 720 µg kg<sup>-1</sup> and 1035 µg kg<sup>-1</sup> respectively. The model indicated that these levels decline relatively quickly and reach levels approximately 2-3 orders of magnitude lower over the simulation period (2000 – 2050).</li> </ul>
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# **Simulating the Fate of Polycyclic Aromatic Hydrocarbons (PAHs) in the Sunndalsfjord**

## **Preface**

This project has been performed according to project description form NIVA of October 3, 2005. Reference is made to purchase order 2331023 of October 24, 2005 from Hydro Aluminium Sunndal.

Grimstad, December 20, 2005

*Kristoffer Næs*

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## Abbreviations

PAHs	-	polycyclic aromatic hydrocarbons
DOC	-	dissolved organic carbon
POC	-	particulate organic carbon
$K_{OW}$	-	octanol-water partition coefficient
$K_{OA}$	-	octanol-air partition coefficient
$K_{AW}$	-	air-water partition coefficient
$K_{DOC}$	-	dissolved organic carbon-water partition coefficient
$K_{OC}^{OBS}$	-	observed organic carbon-water partition coefficient
BaP	-	benzo[a]pyrene
ww	-	wet weight / fresh weight

## Norsk oppsummering

I forbindelse med tiltaksplaner mot PAH-forurensede sedimenter (PAH= polysykliske aromatiske hydrokarboner) i Sunndalsfjorden ønsket Hydro Aluminium Sunndal å utføre modellsimuleringer for å belyse viktigheten og tidsutviklingen knyttet til PAH i sedimentene i Sunndalsfjorden og i Tingvollfjorden. Modellpakken SF-Tool (SedFlex-tool) ble derfor benyttet for å simulere kilder, sluk og flyt av PAH i Sunndalsfjorden. Modellpakken SF-Tool ble nylig utviklet på Norsk institutt for vannforskning (NIVA) og består av (1) en abiotisk modellkode for å simulere fysisk-kjemiske prosesser av persistente organiske miljøgifter i vann og sediment i fjorder og innsjøer, (2) en biotisk modellkode for å simulere opptak, utskillelse og bioakkumulering av disse miljøgiftene i akvatiske næringskjeder, og (3) programverktøy for å gjennomføre usikkerhets- og følsomhetsanalyser på de to modellene. I modellen blir vannkolonnen og sedimentet i fjorden/innsjøen delt både horisontalt og vertikalt i såkalte "bokser", som utgjør modellens romlig oppløsning (innen hver boks antas homogene egenskaper). I Sunndalsfjorden ble vannmassene vertikalt delt i et overflatelag (0-5 m), et intermediært lag (5-120 m), og et dyplag (120 m-max. dybde). Horisontalt ble fjorden delt i en "hot-spot" del (Area 1) fra Sunndalsøra til Flåøya, en indre fjord fra Flåøya til Tingvoll (Area 2), og en ytre fjord fra Tingvoll og utover (Area 3).

I simuleringene skulle det belyses følgende spørsmål:

- Hva er transporten av PAH fra innerst i Sunndalsfjorden (Area 1) til Tingvollfjorden (Area 2)?
- Hvilken konsentrasjon vil modellen predikere for PAH i blåskjell i Tingvollfjorden basert på en null-utslippssituasjon fra Hydro Aluminium Sunndal etter 2003?
- Hvorledes vil konsentrasjonen av PAH i sedimentene i Sunndalsfjorden og Tingvollfjorden utvikle seg over tid og hva blir effekten av dette på innholdet av PAH i blåskjell.

I modellstudiet kom vi til følgende konklusjoner:

- 1) Transporten av sum PAH ( $\Sigma\text{PAH}_{16}$ ) fra innerst i Sunndalsfjorden (Area 1) til Tingvollfjorden (Area 2) i 2000 var estimert til ca. 1000 kg/år (medianestimat, Figur 11). Transporten var dominert av fluksen fra forurensede sedimenter, spesielt fra de store sedimentarealene i den intermediære (5 – 120 m) og den dype (120 – max. dybde) modellboksen. Denne horisontale transporten representerer ca. 2.5% av den totale massen som er beregnet til å ligge i det øverste (0-5 cm) sedimentlaget innerst i Sunndalsfjorden (Area 1). Simuleringer viser at denne transporten avtar over tid og ble for eksempel i 2015 estimert til ca. 100 kg/år (median). Konfidensintervaller basert på usikkerhetanalyse av modellsimuleringene viser (Figur 11) at disse transportestimatene har en tidsavhengig usikkerhet på opptil en størrelsesorden i begge retninger.
- 2) Ut fra reelle observasjoner ble konsentrasjonen av sum PAH og benzo[a]pyrene (B[a]P) i blåskjell i 2000 estimert til henholdsvis  $255 \mu\text{g kg}^{-1}$  and  $2 \mu\text{g kg}^{-1}$  våtvekt. Ved å bruke disse konsentrasjonene som startverdier for blåskjell i 2000, og anta at skjellene lever i det 0-5 m dype området i Tingvollfjorden (Area 2), har modellen predikert tidsutviklingen frem til år 2050 (Figur 12). Resultatene viser at konsentrasjonsnivåene faller raskt etter at emisjonene til luft og vann fra Hydro Aluminium Sunndal er antatt å ha stoppet i 2004. Nivåene vil også raskt falle under grensene for kostholdsrad ( $\Sigma\text{PAH}_{16} > 250 \mu\text{g kg}^{-1}$  ww; B[a]P  $> 5 \mu\text{g kg}^{-1}$  ww; grønn område i Figur 12). Modellsimuleringene viste også at det er bakgrunnskonsentrasjoner i luft og innstrømmende vann som dominerer fremtidsutviklingen i PAH-nivåene i blåskjell i Tingvollfjorden (på 0-5 m dybde). Fluksen fra sedimentet blir mindre viktig her, mest pga. stor vanntilførsel fra elva, dessuten pga. det relativt lite sedimentarealet som er i kontakt med 0-5 m vannkolonne.

- 3) Modellsimuleringene indikerte at konsentrasjonsnivåene i sedimentet på 0-5 m vanndybde avtar 2-3 størrelsesordener i løpet av simuleringsperioden 2000-2050 (Figur 9). Konfidensintervaller basert på usikkerhetsanalyse av modellsimuleringer (Figur 9) viser igjen at konsentrasjonsnivåestimatene har en tidsavhengig usikkerhet på opptil to størrelsesordener i begge retninger.

Det er viktig å legge merke til at vår fokus har vært på 0-5 m vannkolonne med tilhørende sedimentområde (og blåskjell), og at resultatene dermed som regel bare gjelder for denne delen av fjordområdet (Figur 11 som unntak). Det er også viktig å legge merke til modellresultatenes usikkerheter og deres følsomhet for forskjellige parameterverdier, som vist i Figurene 7-13. Siden vi mangler gode observasjoner for mange nøkkelparametere, ville et målrettet undersøkelsesprogram kunne hjelpe til å redusere usikkerhetene ved modellprediksjonene. Spesielt viktige måleparametere å kartlegge i det henseende for den 0-5 m dype vannkolonnen (se Figurene 7, 8, og 13) ville vært bl.a.: (1) nåværende PAH-konsentrasjoner i ellevann, i luft over fjorden, og i blåskjell; (2) simulerte konsentrasjoner i luft over fjorden tilbake i tiden når emisjoner var ennå signifikante (for eksempel 2000-2003); (3) PAH-konsentrasjoner, sedimentasjon-, begravning- og resuspensjonsrater i sedimentet samt tykkelser på det aktive sedimentlaget.



## Summary

The SF-Tool was applied to the Sunndalsfjord system in order to investigate the following questions:

- What is the transport of PAHs from the inner Sunndalsfjord (i.e. near Sunndalsøra) to outer fjord areas (e.g. the Tingvollfjord)?
- What concentrations of PAHs will the SF-Tool predict for blue mussels in the Tingvollfjord if future emissions from the Sunndal plant are assumed to be zero?
- How will the concentrations of PAHs in the sediments in the Sunndalsfjord and Tingvollfjord change with time and what will be the consequences for the PAH content in blue mussels?

Based on the modelling exercise, the following conclusions have been made.

1. The transport of PAHs from the inner Sunndalsfjord to outer fjord areas in 2000 was initially estimated to be approximately  $1000 \text{ kg year}^{-1}$ , dominated by the flux from the contaminated sediments. This flux represents approximately 2.5% of the mass of PAHs calculated to be present in the sediments. It is important to realize that this flux is largely due to remobilization of contaminants from the intermediate (5 – 120 m) and deep (120 – max. depth) sediments of the system, which was seen to have a limited influence on the water column in the surface layer (0 – 5 m).
2. The total PAH ( $\Sigma\text{PAH}_{16}$ ) and B[a]P concentrations in blue mussels inhabiting the surface layer (0 – 5 m) in the Tingvollfjord, initially estimated to be approximately  $255 \mu\text{g kg}^{-1}$  ww and  $2 \mu\text{g kg}^{-1}$  ww respectively, fall rapidly once direct emissions to the system cease. The model indicated that PAH levels in blue mussels from this area will fall below the dietary advisory thresholds established by the Norwegian Scientific Committee for Food Safety ( $\Sigma\text{PAH}_{16} > 250 \mu\text{g kg}^{-1}$  ww ; B[a]P  $> 5 \mu\text{g kg}^{-1}$  ww) in a relatively short period due to the steep decline in surface water column concentrations following the cessation of direct emissions. The model also demonstrated that inputs from background atmospheric and riverine sources control the long-term levels of PAHs in blue mussels, rather than remobilization of contaminants from the sediments.
3. The initial total PAH levels in sediments (surface, intermediate and deep) in the Sunndalsfjord and Tingvollfjord were estimated to be approximately  $11\,720 \mu\text{g kg}^{-1}$  and  $1035 \mu\text{g kg}^{-1}$  respectively. The model indicated that these levels decline relatively quickly and reach levels approximately 2-3 orders of magnitude lower over the simulation period (2000 – 2050). The decline in sediment concentrations had less influence on the long-term time development of PAH levels in blue mussels in the surface layer, which stabilize in response to background atmospheric and riverine inputs (as discussed above).

It is important to once again stress that the conclusions from this exercise are applicable only to the surface compartment rather than the system in its entirety. The behaviour of PAHs in the intermediate layer, which could also support blue mussels, might be more heavily influenced by PAHs in the sediment bed as exchange between this layer and the atmosphere (via the surface layer) is limited.

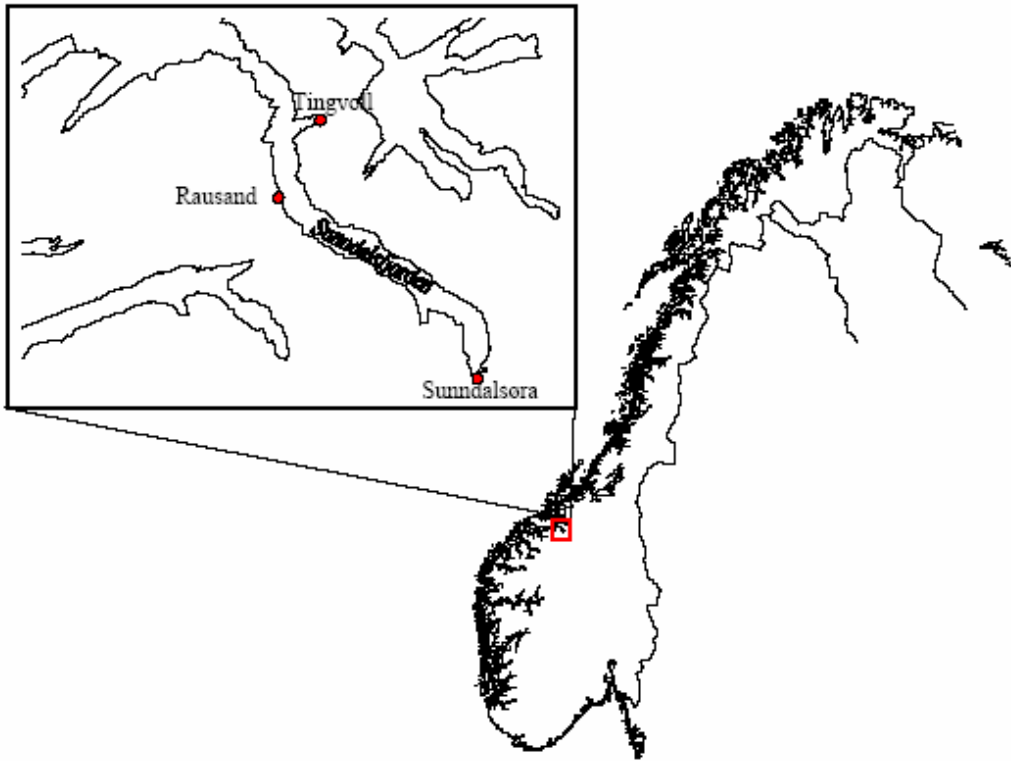
It is also important to appreciate the significant uncertainties and sensitivity of the model output related to the lack of specific data for key parameters, such as initial and background concentrations. In light of these data gaps, a first course of action could be to conduct a limited monitoring campaign focusing on at least:

- 1) Background concentrations in air and water in the Sunndalsfjord (both current levels and historical levels, e.g. simulated by a model)
- 2) Current levels in blue mussels in all surface layers (0 – 5 cm)

Information on sediment concentrations in surface areas throughout the fjord would also be useful as well as quantitative information on sediment dynamics (e.g. settling, burial and resuspension rates) in the system. With this information, the robustness of the model predictions could be greatly improved.

## Background on the Sunndalsfjord

The Sunndalsfjord, shown in Figure 1 is approximately 60 km in length and between 2 – 3 km wide and is located in the western part of Norway. Due to historical effluent discharge from an aluminium reduction plant situated at the head of the fjord, sediments and indicator organisms have been found to be significantly contaminated with PAHs (Næs et al., 1995, Næs and Oug, 1998, Næs et al., 1999, NIVA 2003).



*Figure 1.* Location of the Sunndalsfjord

Recent technological improvements have greatly reduced primary emissions of PAHs to the system and the long-term fate of 'legacy' contaminants sequestered in sediment is now of interest. One approach for investigating this issue is the use of multimedia environmental models, which attempt to quantitatively describe the behaviour of a contaminant based on its physical-chemical properties and the properties of the system of interest (Mackay, 2001).

Persson et al. (2003) recently developed a model to describe the fate of dioxins and furans in the Grenland fjords. This model served as the template for the SF-Tool, a multimedia environmental model implemented in MATLAB ([www.mathworks.com](http://www.mathworks.com)) that can be readily adaptable to other aquatic systems.

Details of the SF-Tool model development, structure and application to the Grenland fjords are documented in Saloranta (2005). In brief, the model consists of an abiotic component, which simulates the transport and distribution of contaminants in the system of interest and a biotic component, which simulates the uptake and elimination of those compounds in a representative food web.

## **Purpose of Modelling Exercise**

The SF-Tool was applied to the Sunndalsfjord system in order to investigate the following questions :

- What is the transport of PAHs from the inner Sunndalsfjord (i.e. near Sunndalsøra) to outer fjord areas (e.g. the Tingvollfjord)?
- What concentrations of PAHs will the SF-Tool predict for blue mussels in the Tingvollfjord if future emissions from the Sunndal plant are assumed to be zero?
- How will the concentrations of PAHs in the sediments in the Sunndalsfjord and Tingvollfjord change with time and what will be the consequences for the PAH content in blue mussels?

The modelling strategy for this application is therefore to forecast concentrations in abiotic and biotic components of the system starting from the levels of PAHs currently observed. Direct emissions from the aluminium plant after 2003 were assumed to be zero. Details of the model parameterization procedure are now discussed.

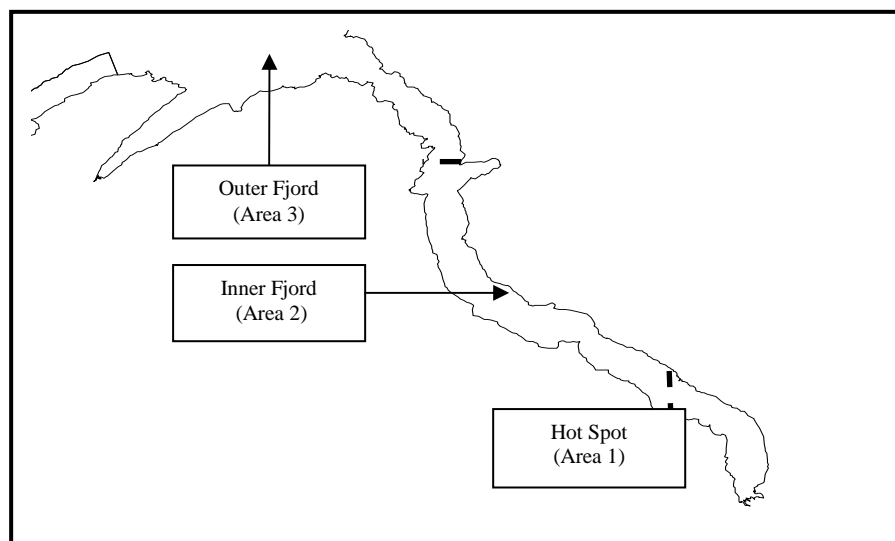
# Parameterization of the Abiotic Model Component

The abiotic component of the SF-Tool requires the user to enter data describing 1) the basic physical characterization of the system 2) environmental properties of the system 3) physical-chemical properties of the contaminants of interest and for this application, 4) initial concentrations in environmental media. Emission data for 2000 – 2003 were also used. Note that all parameter values used are summarized in the Appendix.

## Basic Physical Characterization

### *Sediment and Water Compartments*

The Sunndalsfjord system was first divided into three main areas, as shown in Figure 2. The boundary between the ‘hot spot’ area (Area 1) and the inner fjord (Area 2) was based on a PAH sediment quality assessment using the classification guidelines suggested by the Norwegian Institute for Water Research (NIVA, 2003). As is typical for a fjord system (Aure and Skjodal, 2003), the water mass structure was divided into three layers, representing 1) overlying brackish water 2) intermediary water (to sill depth) and 3) deep water (sill depth to max. depth). Each water mass (i.e. surface, intermediate and deep) has an associated sediment compartment, yielding 6 compartments in each area for a total of 18 compartments. Once the boundaries were established, the area and average depth of each compartment (m<sup>2</sup>) were estimated using GIS software.



**Figure 2.** Main Areas in the Sunndalsfjord Model

### *Atmosphere Compartment*

The atmospheric compartment was initially parameterised assuming a mixing height of 1000m and an area equivalent to the total area of the surface water of the fjord. Based on expert judgement, the calculated volume was then increased by a factor of 10 in order to account for possible dilution effects related to rapid transport of emitted PAHs out of the model domain due to prevailing wind conditions. This effect and thus the volume of the atmospheric compartment were considered uncertain and were therefore included in the sensitivity and uncertainty analysis. The 5<sup>th</sup>, 50<sup>th</sup>, and 95<sup>th</sup> percentiles of this volume in the uncertainty analysis correspond to atmospheric concentrations of 2.5, 16, and 151 ng/m<sup>3</sup> for the sum of 16 PAH congeners in 2002 (emissions are estimated to be 10 tons in this year; see

NIVA, 2003). For comparison, a mean air concentration of 366 ng/m<sup>3</sup> for the sum of 30 PAH congeners in the vicinity of the aluminium plant was observed in 2002 (Hagen, 2003). Furthermore, total PAH air concentration of ~100 ng/m<sup>3</sup> was simulated 3-5 km offshore the plant by Gjerstad (2003) (summer period, prevailing winds blowing from northwest, emissions of 13.5 tons per year). This type of atmospheric dispersion model could be further employed to simulate the mean PAH concentrations in the air above the whole fjord; this is, however, out of the scope of the current project.

### Environmental Properties

Important environmental properties required for the SF-Tool input parameter files and the data sources and gaps are listed below. Efforts to address data gaps are then discussed.

<i>Parameter</i>	<i>Sources</i>
Temperature (water)	Internal NIVA database (dataoversikt.xls)
Concentration of DOC in	
Water Column	No specific data
Sediment Porewater	No specific data
Concentration of POC in	
Water Column	No specific data
Flow Regime	
River discharge	L'Abée-Lund et al. (2004), NPCA (1999)
Fjord circulation	No specific data
Sediment characteristics	
Organic carbon content	Internal NIVA database (dataoversikt.xls), Næs et al. (1999), Næs and Oug (1998).
Porosity	Persson et al. (2003)
Active layer depth	Persson et al. (2003)
Sediment dynamics	
Deposition	Internal NIVA database (dataoversikt.xls)
Resuspension	No specific data
Burial	No specific data

The following steps were taken to address the data gaps outlined above :

#### 1) DOC and POC in the system

Average concentrations of dissolved organic carbon (DOC) and particulate organic carbon (POC) in the water column from two other Scandinavian fjords (Næs et al., 1998 and Persson et al., 2003) were used as initial values for the Sunndalsfjord system. Alperin et al. (1999) reported that DOC in marine sediment porewater is typically 1 order of magnitude greater than DOC in the water column. This ratio was therefore applied to the Sunndalsfjord.

#### 2) Fjord circulation

Aure and Skjoldal (2003) reported that water exchange in the Sunndalsfjord system is good despite its length and containment due to the deep sill (120 – 140 m) and two 1 km wide entrances joining the outer fjord to the coastal system. This qualitative assessment was used to compare the Sunndalsfjord to the Grenland fjord system, which has a sill depth of only 23 m. Intermediate and deep water

exchange rates reported for the Grenland fjords by Persson et al. (2003) were then used as a reference to establish initial estimates of the flow regime.

### 3) Sediment dynamics

Descriptions of sediment dynamics in other systems (Mackay, 1989, Persson et al., 2003, Palm et al., 2004) were consulted in an attempt to derive values for the Sunndalsfjord that result in a plausible relationship among the values for deposition, resuspension and burial. However, it should be noted however that the lack of specific data regarding these parameters is a major uncertainty.

## Physical-chemical Properties

<i>Parameter</i>	<i>Sources</i>
Partitioning	
$K_{OW}$	Beyer et al. (2002), Mackay et al. (2000)
$K_{AW}$	Beyer et al. (2002), Bamford et al. (1999)
$K_{OA}$	Beyer et al. (2002), Harner and Bidleman (1998)
$K_{DOC}$	Burkhard (2000), Schwarzenbach et al. (2003)
Enhanced Sorption	
$K_{OC}^{OBS}$	No specific data
Internal energies of phase change	Beyer et al. (2002)
Degradation rates	Mackay et al. (2000)

The major data gap pertains to the enhanced sorption to particulate phases other than natural organic matter (e.g. soot carbon) that is often observed with PAHs in the natural environment (Gustafsson et al., 1997, Næs et al., 1998, Schwarzenbach et al., 2003). The extent to which this phenomenon occurs can have an important influence on the distribution, bioaccumulation and biodegradation of contaminants (Cornelissen et al., 2005). Unfortunately, no site-specific data are available for the Sunndalsfjord system. Consequently, enhanced sorption has initially been accounted for by elevating the observed log  $K_{OC}^{OBS}$  two orders of magnitude above log  $K_{OW}$  as enhanced sorption of this magnitude may not be uncommon for this type of situation (Cornelissen et al., 2005). It is recognized that this decision is arbitrary and highly uncertain and this parameter was therefore included in the sensitivity and uncertainty analysis.

## Initial Concentrations in Environmental Media

### *Sediment*

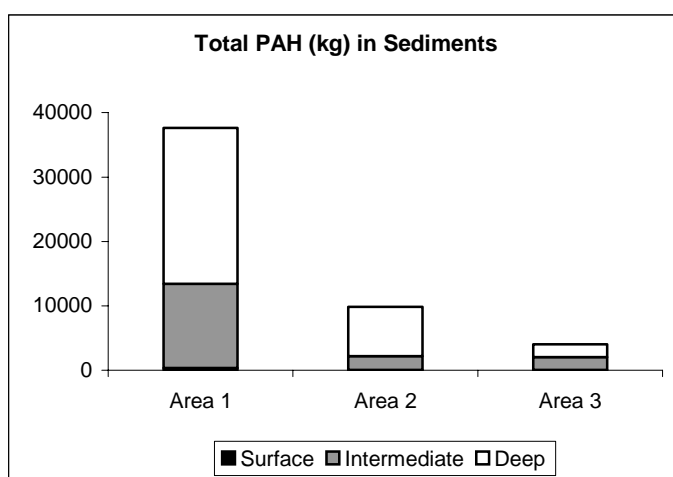
Sediment concentrations of PAHs were taken from a recent study conducted in the Sunndalsfjord (Næs et al., 1999) that reported measurements for two locations in Area 1 ('hot spot') and one location in Area 2 (Inner fjord) and Area 3 (Outer fjord) at a depth of approximately 100 m. This depth, which corresponds to the intermediate sediment layer, was the only depth for which recent measurements are available. Therefore, concentrations were assumed to be equivalent in surface sediments (0 – 5 m) and deep sediments (below sill depth). Based on this assumption, the initial concentrations for total PAHs ( $\Sigma PAH_{16}$ ) were approximately 11 720  $\mu\text{g kg}^{-1}$ , 1035  $\mu\text{g kg}^{-1}$  and 395  $\mu\text{g kg}^{-1}$  for Area 1, Area 2 and Area 3 sediment compartments respectively.

### *Water Column*

No measured concentrations of PAHs in the water column (bulk or truly dissolved) were located. Estimated values were calculated by assuming that particulate organic carbon in the water column initially had the same concentration of PAHs as particulate organic carbon in the sediments.

The total water concentration was then estimated using the assumed concentration of PAHs in particulates ( $\text{g PAH g}^{-1} \text{OC}$ ) multiplied by the concentration of particulates in the water column ( $\text{g OC m}^{-3} \text{water}$ ). From these initial estimates, the model was allowed run for a period of one year after which the final estimated water concentrations were recorded and used as initial values for the 50-year simulations.

Given these initial concentrations, a simple mass inventory of PAHs in the sediments was calculated for the year 2000 and is shown below in Figure 3.



**Figure 3.** Mass Inventory of Total PAHs (kg) Based on Initial Concentrations

Due to the small area of the surface sediments (0 – 5 m), only a small amount of the total mass of PAHs (~ 420 kg) is actually present in this compartment. However, it is important to recall that the total concentration of PAHs in the all sediment layers, assumed equal, was based on measurements taken in the intermediate layer only and these figures simply reflect the relative volumes of the compartments.

#### *Background Levels*

No recent site-specific data on background concentrations in inflowing river, coastal water or ambient air were located. However, Næs et al. (1998) reported concentrations of total PAHs in surface waters from a reference Norwegian coastal site (no direct sources) in the range of  $1 - 10 \text{ ng l}^{-1}$  which corresponds to a study by Palm et al. (2004) from a site in western Sweden ( $2 \text{ ng l}^{-1}$ ) and a compilation by Witt (2000) that presented total PAH concentrations for the open North Sea in the range of  $0.6 - 3.5 \text{ ng l}^{-1}$ . Atmospheric concentrations of PAHs from Palm et al. (2004) and four EMEP monitoring sites in Scandinavia ([www.emep.int](http://www.emep.int)) were then consulted in order to assess the order of magnitude for total air concentrations as well as the relative individual PAH contribution to the total. Although highly variable (seasonally and diurnally), it was observed that average total atmospheric concentrations generally range between  $1 - 10 \text{ ng m}^{-3}$ . Based on this preliminary assessment, background concentrations in Sunndalsfjord were estimated as follows :

*River and Ocean Water:* Average total PAH :  $\sim 1 \text{ ng l}^{-1}$

Individual PAH concentrations were estimated using the relative contribution to total PAH in surface water samples collected from numerous sites around the Baltic Sea (Witt, 2000). This estimation approach yielded individual PAH concentrations ranging from approximately  $3 - 400 \text{ pg l}^{-1}$ .



*Atmosphere:* Average total PAH : ~ 1 ng m<sup>-3</sup>

Individual PAH levels were then calculated using the average contribution to total PAH concentrations as seen at the four EMEP monitoring sites.

Although initial concentrations based on these assumptions are acknowledged as somewhat arbitrary and uncertain, the estimated background levels are likely to be reasonable in terms of the order of magnitude as well as in terms of the relative concentrations of each compound.

### **Emissions**

The aluminium smelter plant in the Sunndalsfjord converted to 100% pre-baked cells over the period 2002 – 2003. In this modelling exercise, direct emissions from the plant are therefore assumed to be zero from 2004 until the end of the simulation period neglecting any possible emissions from waste depots at the site (NIVA 2003).

Total PAH emission estimates for 2000 – 2003 were taken from NIVA (2003) while the individual compound contribution to the total was calculated using effluent monitoring data from two other smelter plants in Norway which were using Söderberg technology at the time (Næs et al., 1995). Total PAH emissions to air and surface water (kg year<sup>-1</sup>) are summarized below.

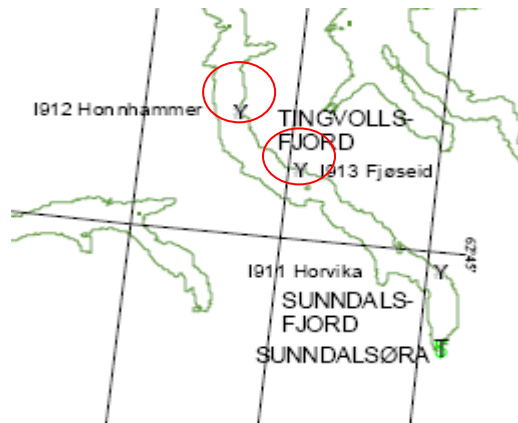
<u>Year</u>	<u>Air</u>	<u>Water</u>
2000	4200	390
2001	5100	390
2002	10000	170
2003	1300	40

## Parameterization of the Biotic Model Component

As discussed in a recent application of the SF-Tool (Saloranta et al., 2006), it is not necessary to apply the biotic model component to generate forecasts of concentrations in target organisms. Time trends in biota can be estimated using initial concentrations in the organism, the fraction of an organism's contaminant burden that originates ultimately from sediment pore-water ( $S_{SED}$ ) and the water column ( $S_{WAT}$ ), and the simulated time trend of concentrations in these two phases. For example, given that an organism derives its contaminant burden entirely from sediment pore-water ( $S_{SED} = 1$ ) and the abiotic model indicates a 20% reduction in sediment pore-water concentrations, we can assume a similar 20% reduction in the biota concentrations (after they have reached the new steady-state given a certain time lag). Note that in this study we have assumed that blue mussels will approach (near)steady-state levels immediately as abiotic concentrations change. This assumption is reasonable for blue mussels, which have been shown to respond quickly to changes in environmental concentrations (Næs et al., 1995).

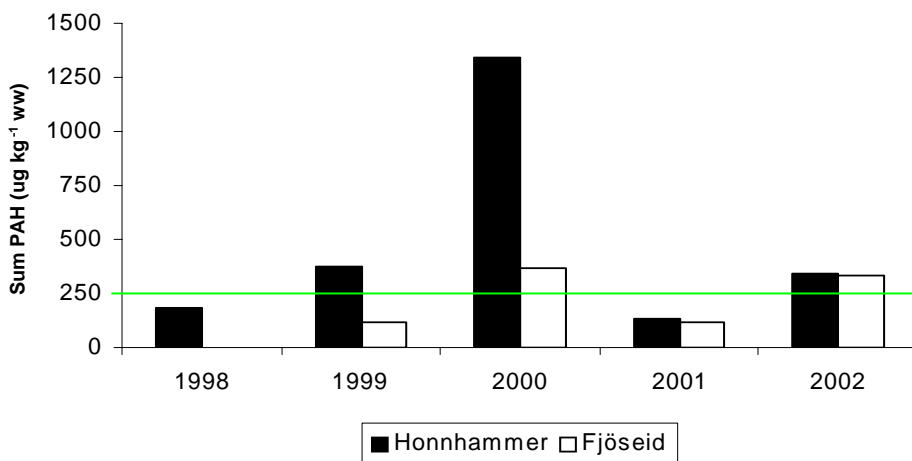
### Initial Concentrations

The locations of two sampling sites for blue mussels in Area 2 (Honnhammer and Fjøseid) are shown below in Figure 4

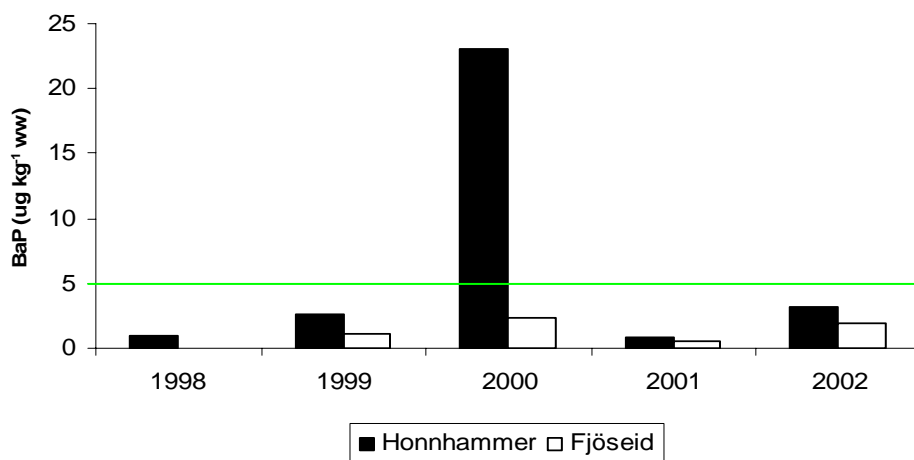


*Figure 4.* Locations of sampling sites

Published monitoring data for blue mussels in the Sunndalsfjord between 1995 – 2000 (Green et al., 2002) from these sites was used to establish initial concentrations for the blue mussels. The data from 1998 – 2002 was considered and is presented for total PAHs (Figure 5) and benzo[a]pyrene (Figure 6).



**Figure 5.** Sum PAH (EPA16) ( $\mu\text{g kg}^{-1}$  ww) in blue mussels at sampling sites (Area 2) in the Sunndalsfjord.



**Figure 6.** Benzo[a]pyrene ( $\mu\text{g kg}^{-1}$  ww) in blue mussels at sampling sites (Area 2) in the Sunndalsfjord.

Note that the dietary advisory thresholds established by the Norwegian Scientific Committee for Food Safety are indicated by the green lines on the graphs. It is interesting that concentrations at Honnhammer appear to be uniformly higher than concentrations at Fjöseid despite the fact that Fjöseid is located closer to the main direct source of PAH contamination. This may indicate secondary sources of importance emanating from Rausand and/or Tingvoll (see Figure 1). The sizeable increase in concentrations observed in 2000 is also difficult to rationalize given the trends in the emission data reported recently (NIVA, 2003). However, such variability is not uncommon and further consideration of these data is beyond the scope of this report.

Initial concentrations in biota were estimated as the geometric mean of all observations from 1998 – 2002. These values are shown below.

Total PAH : 255  $\mu\text{g kg}^{-1}$  ww  
Benzo[a]pyrene : 2  $\mu\text{g kg}^{-1}$  ww

### **Source Contribution of Contaminants**

For the purposes of this modelling exercise, contaminants in blue mussels have been assumed to originate entirely from the water column (i.e.  $S_{\text{WAT}} = 1$ ,  $S_{\text{SED}} = 0$ ). This conclusion was based on studies of blue mussel life history, feeding and gill-ventilation (Newell, 1989 ; van Haren and Kooijman, 1993 ; Kaag et al., 1997 ; Bjork and Gilek, 1999 ; Newell et al., 2005) and also on other bioaccumulation models in aquatic systems (Arnot and Gobas, 2004 ; Stevenson, 2003).

Parameterized in this way, temporal trends in blue mussels will thus reflect the patterns predicted by the abiotic model for concentrations in the water column.

## Results

### Sensitivity Analysis of the Abiotic Model (2000 – 2050)

The sensitivity analysis of the abiotic model was performed using Extended FAST technique (Saltelli et al., 2000). Table 1 lists the min-max ranges that were defined for the 18 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 use of scaling factors means that minimum and maximum parameter values considered are calculated as the default setting multiplied by the *Min* and *Max* scaling factors respectively (see below). Parameter selection and scaling factors were based on Saloranta (2005) and Macleod et al. (2002) in addition to site-specific judgements.

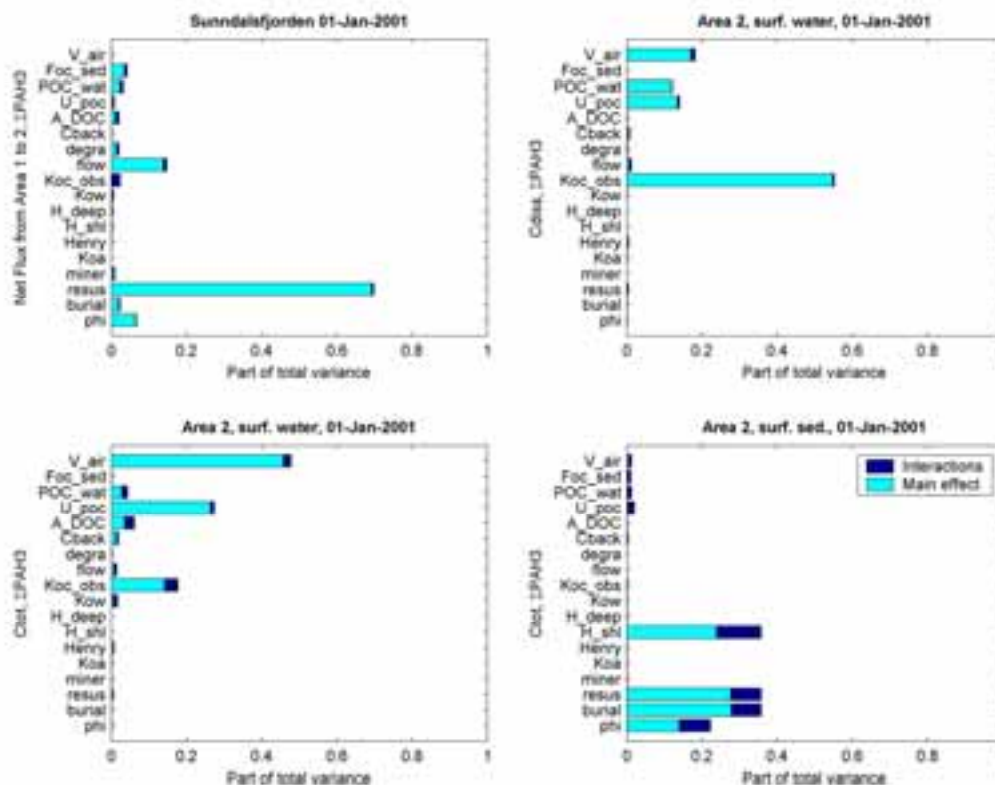
Computing limitations prevented the simultaneous analysis of more than three compounds so three PAHs were selected to represent a broad range in physical-chemical properties and susceptibility to degradation. The model output, for which parameters' sensitivity was monitored, were the net flux from Area 1 to Area 2 (all layers) and the sums of acenaphthene, fluoranthene and dibenzo[ah]anthracene concentrations in surface water and sediment compartments in years 2001, 2006, 2015, and 2050. The model was run from 2000-2050 with initial concentrations based on observation (Næs et al., 1999). 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 ~ 60000.

**Table 1.** Minimum-maximum ranges for the 18 abiotic parameters included in the sensitivity analysis. “(scal.)” denotes cases where the nominal parameter value is scaled within the given range.

<i>Parameter</i>	<i>Min</i>	<i>Max</i>	<i>Unit</i>	<i>Remark</i>
phi	0.7	0.9	-	sediment water content (porosity)
f <sub>OC</sub>	1/3	3	(scal.)	scaling of OC volume fraction in sediment
H <sub>SED</sub>	0.5	2	(scal.)	scaling of sediment active layer depth
Burial	0.2	5	(scal.)	scaling of sediment burial rate
Resus	0.2	5	(scal.)	scaling of sediment resuspension rate
Miner	0.2	5	(scal.)	scaling of sediment mineralization rate
Degrad	1/3	3	(scal.)	scaling of sediment degradation half-life
K <sub>OW</sub>	1/3	3	(scal.)	scaling of K <sub>OW</sub>
H	1/3	3	(scal.)	scaling of Henry's Law coefficient
K <sub>OA</sub>	1/3	3	(scal.)	scaling of K <sub>OA</sub>
K <sub>OC</sub> <sup>OBS</sup>	0.1	10	(scal.)	scaling of K <sub>OC</sub> <sup>OBS</sup>
A <sub>DOC</sub>	0.04	28	(scal.)	scaling of DOC partitioning coeff. <sup>a</sup>
Flow	1/3	3	(scal.)	scaling of water flow regime
C <sub>BACK</sub>	1/3	3	(scal.)	scaling of background conc. in air and river and ocean water outside the model domain
U <sub>POC</sub>	1/3	3	(scal.)	scaling of POC settling velocity
DOC <sub>WATER</sub>	1/3	3	(scal.)	scaling of water DOC concentration
POC <sub>WATER</sub>	1/3	3	(scal.)	scaling of water POC concentration
V <sub>AIR</sub>	0.1	10	(scal.)	scaling of volume of atmosphere

<sup>a</sup> Based on the PAH-specific K<sub>DOC</sub> relationship from Burkhard (2000) :  
 $\log K_{DOC} = 1.18(0.13) \cdot \log K_{OW} - 1.56(0.72)$

The results of the sensitivity analysis in 2001 for the net flux from Area 1 to Area 2, the estimated truly dissolved surface water concentration in Area 2 (C<sub>diss</sub>), the total surface water concentration in Area 2 and the total surface sediment concentration are shown below in Figure 7.



**Figure 7.** Sensitivity analysis of the abiotic model output in the Sunndalsfjord in 2001. “Main effect” denotes the parameter’s contribution alone (first order effect), and “interactions” its contribution due to higher order interactions with other parameters.

#### *Net Flux - 2001*

The net flux from Area 1 to Area 2 (all layers) is most sensitive to the resuspension rate and to a lesser extent, the flow regime (river input and fjord circulation). The flow regime is important because it determines the amount of particle-bound and freely-dissolved chemical transported via advection between the boxes. The resuspension rate is an important parameter determining the flux of deposited chemical back into the water column.

#### *Area 2 Dissolved Water Concentration - 2001*

The freely dissolved water concentrations in Area 2 are most sensitive to the values of  $K_{OC}^{OBS}$ , the particle settling rate ( $U_{POC}$ ), the concentration of particulate organic carbon ( $POC_{WATER}$ ) and the volume of atmospheric compartment. These results can be rationalized by the fact that  $K_{OC}^{OBS}$  determines the ratio of the mass of dissolved to particulate-bound contaminants while  $U_{POC}$  is related to the depuration of contaminants and  $POC_{WATER}$  influences the amount of particles suspended in the water column. The fact that the volume of the atmospheric compartment ( $V_{AIR}$ ) influences the dissolved water concentration indicates the importance of the atmospheric deposition of directly emitted PAHs, the concentration of which depends on the volume of air assumed.

*Area 2 Total Water Concentration - 2001*

The total concentration of PAHs in the water column of the surface layer is most strongly influenced by the atmospheric volume ( $V_{\text{AIR}}$ ) and  $K_{\text{OC}}^{\text{OBS}}$  as well as parameters related to particle dynamics in the water column ( $U_{\text{POC}}$ ). These results follow from the fact that  $K_{\text{OC}}^{\text{OBS}}$  determines the ratio of dissolved to particulate-bound contaminants while particle dynamics determine the depuration of contaminants and the amount of suspended material. Once again, the volume of the atmospheric compartment (and associated PAH deposition) is shown to be significant.

*Area 2 Total Sediment Concentration - 2001*

As expected, the total concentration of PAHs in the surface sediments is most strongly influenced by parameters related to sediment dynamics / depuration of contaminants (burial and resuspension) and well as the parameters characterizing the volume of sediment (porosity and depth of active layer).

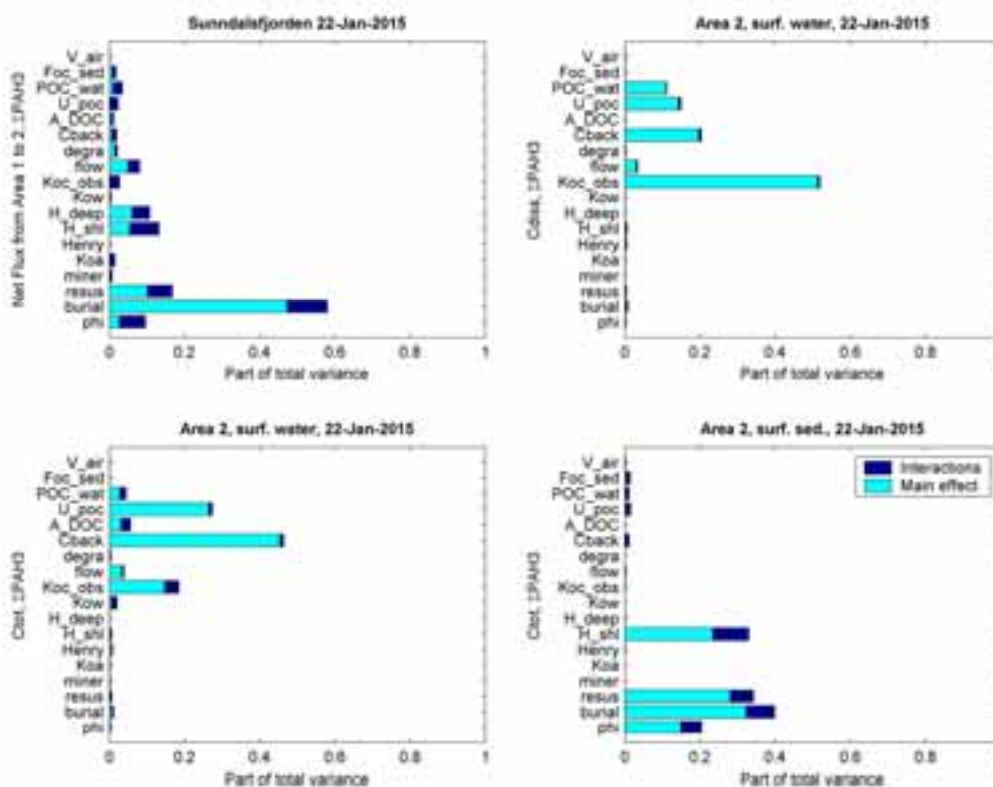
The results of the sensitivity analysis for 2015 are shown in Figure 8. This time was chosen to reflect the situation after the cessation of direct emissions to the system.

*Net Flux - 2015*

In 2015, the net flux between Area 1 and Area 2 is more influenced by burial in the sediments rather than resuspension. This is likely due to the fact that the fugacity gradient between water and sediment has been reduced from the year 2001 and thus resuspension has no large redistributing effect. Burial, however, continues to act as a sink for the sediment concentration, in turn also affecting the concentration in the water column, as this process removes contaminants otherwise available for transport.

*Area 2 Dissolved Water Concentration - 2015*

Predicted PAH concentrations in the dissolved-phase in 2015 are influenced most strongly by the same factors except for the following changes. First, due to the lack of direct emissions, the volume of the atmospheric compartment is no longer as influential. Instead, assumptions regarding the background concentrations in the atmosphere and inflowing water (river and ocean) become important, suggesting that these inputs have become the main determinants of contaminant levels in the system.



**Figure 8.** Sensitivity analysis of the abiotic model output in the Sunndalsfjord in 2015. “Main effect” denotes the parameter’s contribution alone (first order effect), and “interactions” its contribution due to higher order interactions with other parameters.

#### *Area 2 Total Water Concentration - 2015*

Once again, assumptions regarding background concentrations strongly influence the system in addition to the parameters of importance in 2001 with the exception  $V_{AIR}$  (since this parameter is not influential at this time period, as discussed above).

#### *Area 2 Total Sediment Concentration - 2015*

The sensitivity of model predictions in the sediment in 2015 is related to the same factors as in 2001.

The results of the sensitivity analyses for 2025 and 2050 (not shown) also demonstrate the increasing importance of assumptions related to background concentrations.

### **Uncertainty Analysis**

To produce simulation results in terms of probability distributions, rather than single values, an uncertainty analysis of the abiotic model in the SF-tool was performed. Thirteen parameters were selected for this analysis on the basis of the results from the sensitivity analysis and previous investigations (e.g. Macleod et al, 2002 ; Saloranta 2005). In the uncertainty analysis, the model was run 3000 times (for the 16 PAH congeners and for the period 2000-2050) with randomly chosen values for the selected parameters sampled on the basis of the distributions and rank correlation matrix given in Tables 2 and 3 and results were saved on each simulation. 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.

**Table 2.** Probability distribution functions (PDF) for the 13 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 1.

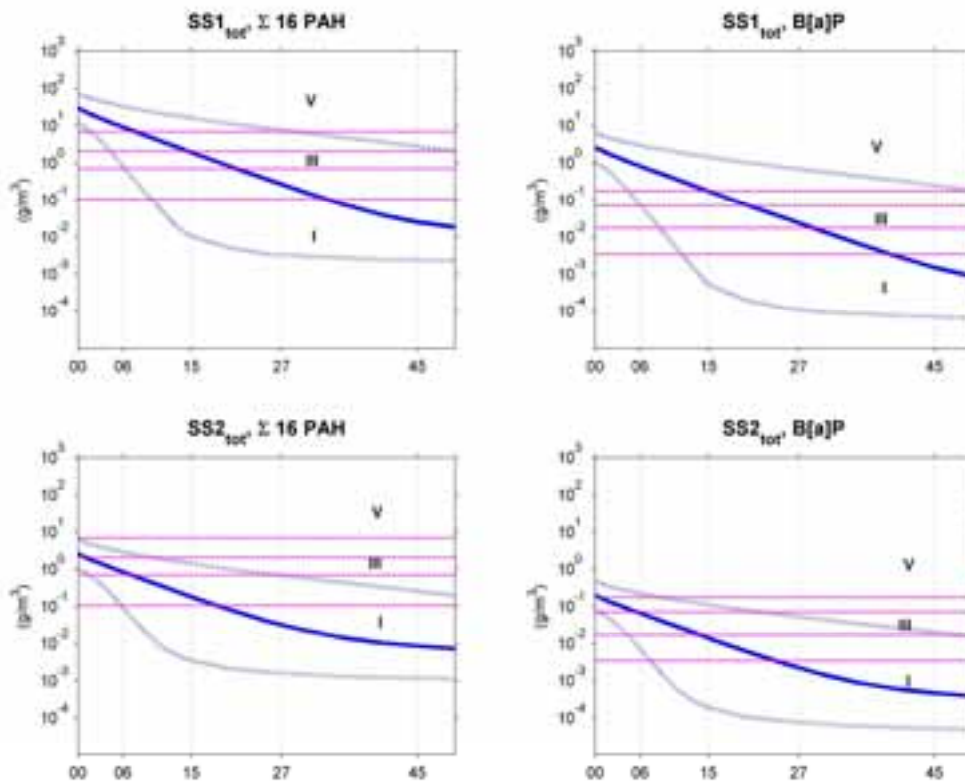
<i>Parameter</i>	<i>PDF</i>	<i>Mean/median/mode</i>	<i>Spread</i>
phi [-]	Triangular	0.85	0.75-0.95 (min-max)
Burial (scal.)	Lognormal	1	5 (CF)
Resus (scal.)	Lognormal	1	5 (CF)
H <sub>SED</sub> [m]	Uniform	0.04	0.02-0.06 (min-max)
K <sub>OC</sub> <sup>OBS</sup> (scal.)	Lognormal	1	10 (CF)
A <sub>DOC</sub> (scal.)	Lognormal	1	28 (CF)
Flow (scal.)	Lognormal	1	1.3 (CF)
C <sub>INIT</sub> (scal.)	Lognormal	1	3 (CF)
C <sub>BACK</sub> (scal.)	Lognormal	1	5 (CF)
U <sub>POC</sub> (scal.)	Lognormal	1	2 (CF)
POC <sub>WATER</sub> (scal.)	Lognormal	1	2 (CF)
V <sub>AIR</sub> (scal.)	Lognormal	1	10 (CF)

**Table 3.** Non-zero rank correlations between the parameters included in the uncertainty analysis. For explanation on parameter abbreviations, see Table 1.

<i>Parameter 1</i>	<i>Parameter 2</i>	<i>Rank correlation</i>
H <sub>SED</sub>	Resus	0.5
phi	H <sub>SED</sub>	-0.5

### Time Development of Sediment Concentrations (2000 – 2050)

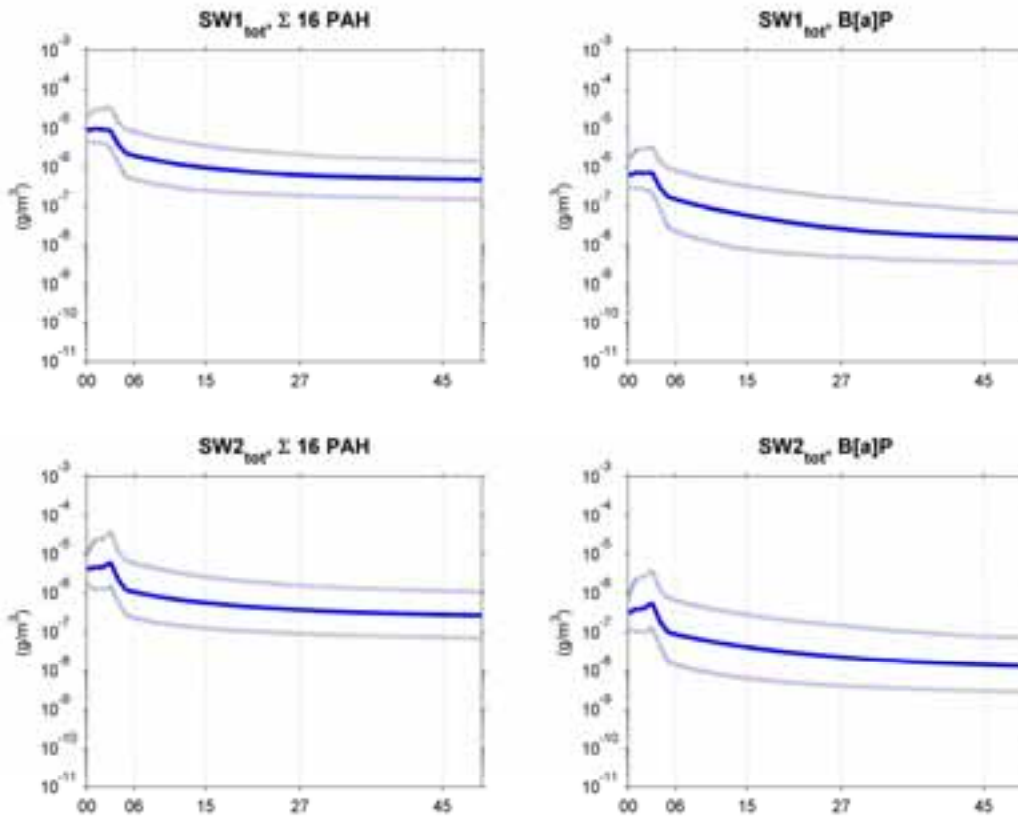
The predicted total PAH and BaP concentrations in surface sediments of Area 1 (SS1) and Area 2 (SS2) over the course of the simulation are shown below in Figure 9.



**Figure 9.** Predicted total PAHs and BaP concentrations in the surface sediments of Area 1 (SS1) and Area 2 (SS2) from 2000 – 2050. The solid line denotes median, and the dashed line denotes 5<sup>th</sup> and 95<sup>th</sup> percentiles of the model simulations of the uncertainty analysis. The horizontal pink lines denote SFT sediment quality class (I-V) boundaries, [ $<300, 2000, 6000, 20000<$ ]  $\mu\text{g}/\text{kg}$  dry weight for total PAH and [ $<10, 50, 200, 500<$ ]  $\mu\text{g}/\text{kg}$  dry weight for BaP.

### Time Development of Water Column Concentrations (2000 – 2050)

The predicted total PAH and BaP concentrations in the surface waters of Area 1 (SW1) and Area 2 (SW2) over the course of the simulation are shown below in Figure 10.



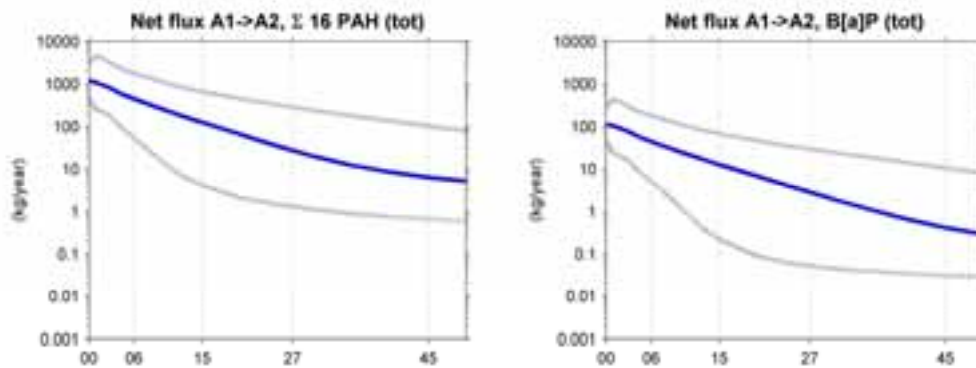
**Figure 10.** Predicted total PAHs and BaP concentrations in the surface waters of Area 1 (SW1) and Area 2 (SW2) from 2000 – 2050. The solid line denotes median, and the dashed line denotes 5<sup>th</sup> and 95<sup>th</sup> percentiles of the model simulations of the uncertainty analysis.

### Net Flux from Area 1 to Area 2 (2000 – 2050)

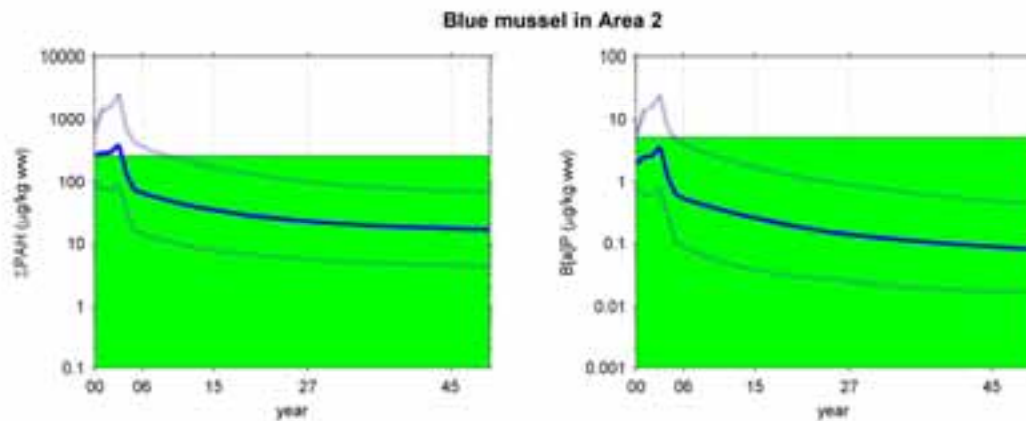
The results for the net flux ( $\text{kg year}^{-1}$ ) of total PAHs and BaP from Area 1 to Area 2 over the course of the simulation period are shown below in Figure 11.

### Predicted Concentrations in Blue Mussels (2000 – 2050)

The predicted concentrations in blue mussels in the surface compartment (0 – 5 m) of Area 2 are shown in Figure 12. The strong decline in predicted concentrations, reflecting the cessation of direct emissions, indicates that surface water column concentrations, and thus blue mussel concentrations, are strongly affected by the input of PAHs from this source.



**Figure 11.** Predicted net flux ( $\text{kg year}^{-1}$ ) of total PAHs and BaP from Area 1 (A1) to Area 2 (A2) from 2000 – 2050. The solid line denotes median, and the dashed line denotes 5<sup>th</sup> and 95<sup>th</sup> percentiles of the model simulations of the uncertainty analysis.



**Figure 12.** Predicted total PAHs and BaP in blue mussels living in Area 2 surface water. The solid line denotes median, and the dashed line denotes 5<sup>th</sup> and 95<sup>th</sup> percentiles of the model simulations of the uncertainty analysis. The area in green represents concentrations below the dietary advisory thresholds established by the Norwegian Scientific Committee for Food Safety ( $\Sigma\text{PAH}_{16} > 250 \mu\text{g kg}^{-1} \text{ ww}$  ;  $\text{B[a]P} > 5 \mu\text{g kg}^{-1} \text{ ww}$ ).

The model output can now be used to address the questions discussed in the section describing the purpose of the modelling exercise.

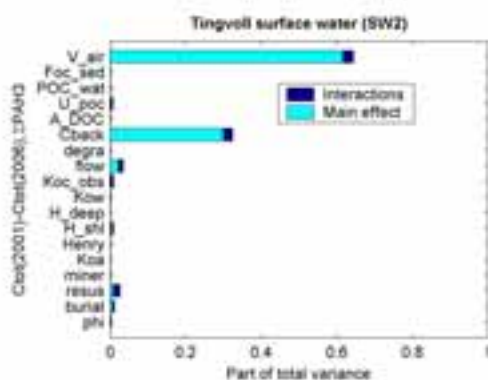
- 1) What is the transport of PAHs from the inner Sunndalsfjord (i.e. near Sunndalsøra) to outer fjord areas (e.g. the Tingvollfjord)?

The initial median net flux of total PAHs from the inner fjord in year 2000 is estimated to be approximately  $1000 \text{ kg year}^{-1}$ , representing approximately 2.5% of the total mass of contaminant present. Although the major contributor to the total flux of PAHs at this time is the sediment compartment, it is important to remember that this flux reflects the sum of the transport of PAHs in the surface, intermediate and deep layers, dominated by the two lower layers which contain the majority of contaminants (see Figure 3). For this reason, the decline in surface water concentrations (see Figure 10) following the cessation of direct emissions does not influence the time development of this measure significantly.

- 2) What concentrations of PAHs will the SF-Tool predict for blue mussels in the Tingvollfjord (Area 2) if future emissions from the Sunndal plant are assumed to be zero?

From initial concentrations of approximately  $255 \mu\text{g kg}^{-1}$  ww total PAH and  $2 \mu\text{g kg}^{-1}$  ww BaP, the concentrations in blue mussels decline rapidly (see Figure 12) following the cessation of direct emissions to the system to levels typically considered high background (Næs et al., 1995) within a few years. As blue mussels are assumed to derive PAH body burdens entirely from the water column, from both dissolved (via ventilation) and particle-bound chemical (via feeding), the decline mirrors the time development of concentrations observed for the water column (see Figure 10). The fact that decreasing sediment concentrations (see Figure 9) are not strongly reflected in the predicted concentrations in the water column of the surface layer in Area 2 is partly due to the small surface area of these sediments ( $\sim 1/165^{\text{th}}$  of the water surface area) and indicates that background inputs (atmospheric, river) determine the long-term PAH levels, rather than fluxes of contaminant out of the sediment bed. This conclusion is also supported by Figure 13, which shows the sensitivity of the change in concentration in Area 2 surface waters between 2001 and 2006 (i.e.  $C_{\text{SW}}^{2001} - C_{\text{SW}}^{2006}$ ).

Figure 13 indicates that the decline in surface water concentrations (and thus blue mussels) is most sensitive to the magnitude of direct air emissions until 2003, which is affected by  $V_{\text{AIR}}$ , and the background concentrations ( $C_{\text{BACK}}$ ) rather than parameters related to sediment or particle dynamics.



**Figure 13.** Sensitivity analysis for the change in Area 2 surface water concentrations between 2001 and 2006

- 3) How will the concentrations of PAHs in the sediments in the Sunndalsfjord and Tingvollfjord change with time and what will be the consequences for the PAH content in blue mussels?

The time development of concentrations in the sediments in the Area 1 and Area 2 is shown in Figure 9. From initial levels, concentrations in the sediments decline by approximately two orders of magnitude over the course of the simulation (2000 – 2050). The removal of PAHs is largely controlled by sediment burial and resuspension (see Figures 7 and 8). As discussed above, the time development of sediment concentrations has less influence on the PAH content in blue mussels in the surface layer because the flux of contaminants in the water column is dominated by inputs from the atmosphere and inflowing waters.

## Conclusions and Recommendations

For blue mussels dwelling in the surface layer of the Tingvollfjord (Area 2, 0 – 5 m), the model indicates that the long-term trends in concentrations of PAHs are more dependent on background inputs from the atmosphere and inflowing water than fluxes from the sediment bed. Any further direct atmospheric emissions will also strongly influence the temporal trends. Based on this exercise, a conservative estimate (i.e. the 95<sup>th</sup> percentile prediction) suggests that levels in blue mussels in this layer should fall below the dietary advisory thresholds rapidly after the complete termination of direct emissions.

It is important to once again stress that the conclusions from this exercise are applicable only to the surface compartment rather than the system in its entirety. The behaviour of PAHs in the intermediate layer, which could also support blue mussels, might be more heavily influenced by PAHs in the sediment bed as exchange between this layer and the atmosphere (via the surface layer) is limited.

It is also important to appreciate the significant uncertainties and sensitivity of the model output related to the lack of specific data for key parameters, such as initial and background concentrations. In light of these data gaps, a first course of action could be to conduct a limited monitoring campaign focusing on at least:

- 1) Background concentrations in air and water in the Sunndalsfjord area.
- 2) Current levels in blue mussels in all surface layers (0 – 5 m) where they exist.

New information on sediment concentrations in surface areas throughout the fjord would also be useful as well as quantitative information on sediment dynamics (e.g. settling, burial and resuspension rates) in the system. With this information, the robustness of the model predictions could be greatly improved.

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# Appendix

## Physical-chemical Properties (I)

Compound	MW (g/mol)	log_Kow (-)	log_Koc_obs (L/kg)	log_Koa (-)	-log_H AT 25oC (kPa m3/mol)
Acenaphthene	154.21	3.92	5.92	6.23	1.91
Acenaphthylene	150.2	3.94	5.94	6.47	2.08
Anthracene	178.2	4.45	6.45	7.34	2.40
Benz[a]anthracene	228.3	5.76	7.76	9.54	3.24
Benzo[a]pyrene	252.3	6.13	8.13	10.86	4.34
Benzo[b]fluoranthrene	252.3	5.78	7.78	10.97	4.80
Benzo[ghi]perylene	268.36	6.5	8.5	11.02	4.12
Benzo[jk]fluoranthrene	252.3	5.78	7.78	10.97	4.80
Chrysene	228.3	5.81	7.81	10.44	4.19
Dibenzo[a,h]anthracene	278.4	6.75	8.75	13.91	6.77
Fluoranthrene	202.3	5.16	7.16	8.60	2.98
Fluorene	166.2	4.18	6.18	7.87	2.10
Indeno[1,2,3cd]pyrene	276.31	6.72	8.72	11.57	4.45
Phenanthrene	178.2	4.46	6.46	7.45	2.49
Pyrene	202.3	4.88	6.88	8.61	3.04
Naphthalene	128.19	3.37	5.37	5.14	1.37

## Physical-chemical Properties (II)

Compound	Degrad. half-life	Degrad. half-life	dU_oa	dU_ow	dU_aw
	water (d)	sediment (d)	(kJ mol-1)	(kJ mol-1)	(kJ mol-1)
Acenaphthene	22.92	708.33	-80.61	-28.71	51.90
Acenaphthylene	22.92	708.33	-80.61	-28.71	51.90
Anthracene	22.92	708.33	-68.50	-19.70	48.80
Benz[a]anthracene	70.83	2291.67	-89.70	-23.30	66.40
Benzo[a]pyrene	70.83	2291.67	-62.29	-25.40	36.89
Benzo[b]fluoranthrene	22.92	708.33	-92.60	-18.00	74.00
Benzo[ghi]perylene	70.83	2291.67	-92.60	-18.00	74.00
Benzo[jk]fluoranthrene	22.92	708.33	-92.60	-18.00	74.00
Chrysene	70.83	2291.67	-123.60	-22.70	100.90
Dibenzo[a,h]anthracene	70.83	2291.67	-92.60	-18.00	74.00
Fluoranthrene	70.83	2291.67	-81.61	-23.75	57.86
Fluorene	22.92	708.33	-77.89	-24.05	53.85
Indeno[1,2,3cd]pyrene	70.83	2291.67	-92.60	-18.00	74.00
Phenanthrene	70.83	2291.67	-73.95	-20.52	53.42
Pyrene	70.83	2291.67	-71.56	-23.93	47.63
Naphthalene	7.08	229.17	-60.35	-15.70	44.65

Fjord Circulation and River Input

Water Flow (m <sup>3</sup> /s)	To:											
From:	TW1	IW1	DW1	TW2	IW2	DW2	TW3	IW3	DW3	R	O	
TW1	0	20	0	89.65	0	0	0	0	0	0	0	
IW1	20	0	100	0	715	0	0	0	0	0	0	
DW1	0	100	0	0	0	50	0	0	0	0	0	
TW2	8.15	0	0	0	60	0	89.65	0	0	0	0	
IW2	0	715	0	60	0	300	0	715	0	0	0	
DW2	0	0	50	0	300	0	0	0	50	0	0	
TW3	0	0	0	8.15	0	0	0	60	0	0	81.5	
IW3	0	0	0	0	715	0	60	0	300	0	715	
DW3	0	0	0	0	0	50	0	300	0	0	50	
R	81.5	0	0	0	0	0	0	0	0	0	0	
O	0	0	0	0	0	0	0	715	50	0	0	

Physical Properties of Water Compartments

Compartment	Area (m <sup>2</sup> )	C_POC (mg/m <sup>3</sup> )	C_DOC (mg/m <sup>3</sup> )	Temp (deg C)
SW1	25672500	300	3000	10
IW1	25447500	300	3000	8
DW1	16535000	300	3000	6
SW2	75735000	300	3000	10
IW2	75712500	300	3000	8
DW2	59382500	300	3000	6
SW3	81632500	300	3000	10
IW3	81055000	300	3000	8
DW3	40477500	300	3000	6

Physical Properties of Sediment Compartments

Compartment	Area (m <sup>2</sup> )	H (m)	f <sub>oc</sub>	C_DOC (mg/m <sup>3</sup> )	phi	Temp (deg C)	U_BUR (m/d)	U_RES (m/d)	k <sub>sw</sub> (m/d)	Thalf_MIN (d)
SS1	225000	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
IS1	8912500	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
DS1	16535000	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
SS2	460000	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
IS2	16330000	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
DS2	59382500	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
SS3	577500	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
IS3	40577500	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000
DS3	40477500	0.05	0.0365	30000	0.86	6	1.146E-06	1.146E-06	0.0024	35000