

# **084 – NORWEGIAN OIL AND GAS RECOMMENDED GUIDELINES**

## **EIF COMPUTATIONAL GUIDELINES**

A Manual for Standardised Modelling and Determination of  
the Environmental Impact Factor (EIF)



Norsk olje & gass

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## 1 Introduction

The purpose of the EIF computational guidelines is to provide a standard method for modelling and determination of the Environmental Impact Factor as a basis for the “zero discharge” work and reporting for offshore discharges of produced water in the Norwegian sector of the North Sea and the Norwegian Sea. The document shall form the basis for all EIF determinations related to “zero discharge” reporting from the oil and gas production operators in the Norwegian sector in 2003, and for further annual risk assessment reporting in this area. The objective is to secure standardised EIF determination from all operators, thus facilitating comparison of EIF values among various oil and gas fields.

This description and standardisation of the modelling and EIF calculation is based on the DREAM model version 2.0. The user’s manual from DREAM 2.0 (SINTEF 2002), the PNEC report (Frost 2002) and the description of the EIF methodology given by Johnsen et al. (2000) serve as a basis for this document.

This guideline document is divided into sections describing procedures for calculating and presenting an EIF:

- Overview of steps in computing an EIF
- Input data – chemical, physical, biological and meteorological parameters needed to run the model
- Model parameters and computational considerations – definitions of concepts and terms, standardised set-up of internal governing model parameters
- Model output and EIF calculation methodology
- Reporting of the EIF

Using these standardised data and methods, the EIF should be determined for all discharge points of produced water for specific years and for the lifetime of an installation or production field.

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## 2 Model input data

### 2.1 Chemical compound groups

#### 2.1.1 Natural compounds

Natural compounds present in produced water are divided into several compound groups. Physical/chemical and biological properties of each group are represented by one of the compounds in the group. For some groups different compounds are chosen to represent physical/chemical and biological properties, respectively. Compound groups and associated representatives are listed in Table 2.1. A more detailed list of the compounds included in each group is found in Appendix 1.

**Table 2.1: Produced water compound groups representing naturally occurring components in produced water discharge**

Group	Main group	Compounds	Representative Physical/chemical	Representative Biological
1	EIF-BTEX	Benzene, toluene, ethylbenzene, xylene	Ethylbenzene	Benzene
2	EIF-Naphthalenes	Naphthalene + C1-C3 alkyl homologues	Naphthalene	Naphthalene
3	EIF-PAH 2-3 ring	Compounds on the EPA 16 PAH list with 2-3 rings, including C1-C3 alkylhomologues of phenanthrene and dibenzothiophene, but excluding naphthalenes	Phenanthrene	Phenanthrene
4	EIF-PAH 4-5 ring	Compounds on the EPA 16 PAH list with 4 rings or more	Chrysene	Benzo(a)pyrene
5	EIF-Phenols C0-C3	Phenol + C1-C3 alkyl-homologues	p-Cresol	Phenol
6	EIF-Phenols C4-C5	C4-C5 alkylphenol homologues	pentylphenol	
7	EIF-Phenols C6-C9	C6-C9 alkylphenol homologues	Nonylphenol	Nonylphenol
8	EIF-Hepthane	Aliphatic hydrocarbons (oil in water)	Hepthane	Hepthane
9	EIF-Copper	Cu	Cu	Cu
10	EIF-Zinc	Zn	Zn	Zn
11	EIF-Nickel	Ni	Ni	Ni
12	EIF-Lead	Pb	Pb	Pb
13	EIF-Cadmium	Cd	Cd	Cd
14	EIF-Mercury	Hg	Hg	Hg

Concentration of natural compounds in produced water should be taken from the latest results from chemical characterisation of produced water, according to the Norwegian Oil and Gas Guidelines.

### **2.1.2 Anthropogenic chemicals**

Process chemicals or other anthropogenic (man-added) compounds are included on a field-specific basis. Physical/chemical data for the process chemicals are taken from the HOCNF forms. When modelling man-added chemicals, the amount of the total chemical product in the water phase is used as model input, if component-specific data are not available. When selecting a representative compound for the chemical, the same compound is chosen to represent both physical/chemical and biological properties (see Table 2.2).

If no documented or estimated oil/water distribution data are available, 100% of the chemical is assumed to follow the water phase.

Chemicals can be added continuously or over a limited period of time (batch-wise). Continuously added chemicals are included in the EIF calculation together with the natural compounds. Chemicals used over a limited period of time (e.g. biocides, scale squeeze chemicals) are included in a separate EIF-calculation together with continuously added chemicals and the natural compounds, and are reported separately (see Chapter 5). Discharges of oil in connection with jet-operations are also to be calculated as batch-wise discharges as for chemicals used over a limited period of time.

## **2.2 Data on physical and chemical properties**

Data on physical and chemical properties of natural compounds in produced water are standardised for EIF calculation (see Appendix A). For man-added chemicals each chemical, or single component of the chemical, needs to be added to the chemical component database. The physical-chemical properties of the chemical or component shall be taken from the HOCNF of the product. The last sheet of Appendix A shows the minimum data input for new chemicals or components. Be aware that a new chemical or component should be added to the “Chemicals” database, not the “Oil database” (Use “Set Source” in the Component Editor in DREAM).

**Table 2.2: Production chemicals in produced water included in the EIF calculation.**

Group	Main group	Compounds	Representative Physico-chemical and Biological
15	Scale inhibitor	Product specific	Most conservative value from HOCNF
16	Anti foam	Product specific	Most conservative value from HOCNF
17	Emulsion breaker	Product specific	Most conservative value from HOCNF
18	Corrosion inhibitor	Product specific	Most conservative value from HOCNF
19	Biocide	Product specific	Most conservative value from HOCNF
20	H <sub>2</sub> S-scavenger	Product specific	Most conservative value from HOCNF
21	Other	...	....

#### **Add process chemicals to the database**

- Use standard EIF chemicals for naturally occurring components
  - Define process chemicals from HOCNF (OSPAR) forms
  - Process chemicals are assumed soluble (solubility > 500 mg/l) if other data is not available
  - **Degradation (water and sediment):** assume first order rate, based on the 28 day results in the HOCNF report (see section below on Biodegradation)
  - **K<sub>oc</sub>** (or K<sub>ow</sub>) is not important because the suspended particulate concentration is set to 0 in the simulation (all dissolved components are assumed bio-available)
  - **PNEC** = lowest EC<sub>50</sub> or LC<sub>50</sub> in the HOCNF report multiplied by the appropriate assessment factor based on number and quality of data available (see chapter 2.3.2)
  - **Density** from HOCNF
  - **Vapour pressure** is set to 0.001 atmospheres (to minimize evaporative losses)
- other parameters in the DREAM component database can be set to unity (1.0)

## **2.3 Biological data**

### **2.3.1 Biodegradation**

Table 2.3 shows the biodegradation rates, described as half-lives (days) and k-values, of the different produced water compound groups selected to represent the "naturally" occurring

components in the produced water. The table also presents the compound selected to represent the different groups with respect to physical and chemical properties and biodegradation in the recipient.

**TABLE 2.3: Standard biodegradation rates for produced water compound groups**

<u>Group</u>	<u>Main group</u>	<u>Representative compound</u>	<u>Biodegradation rate</u> <u>½ life (days)</u>	<u>k-values</u>
1	EIF-BTEX	Ethyl-benzene	0,5	1,39
2	EIF-Naphthalenes	Naphthalene	1,5	0,462
3	EIF-PAH 2-3 ring	Phenanthrene	17	0,041
4	EIF-PAH 4-5 ring	Chrysene	350	0,002
5	EIF-Phenol-C0-C3	p-cresol	1,2	0,578
6	EIF-Phenol-C4-C5	pentylphenol	10	0,069
7	EIF-Phenol-C6-C9	Nonylphenol		0,002
8	EIF-Heptan*	Heptan	60	0,012
9	EIF-Copper (Cu)	Field-specific	No degradation	0,0000001
10	EIF-Zinc (Zn)	Field-specific	No degradation	0,0000001
11	EIF-Nickel (Ni)	Field-specific	No degradation	0,0000001
12	EIF-Lead (Pb)	Field-specific	No degradation	0,0000001
13	EIF-Cadmium (Cd)	Field-specific	No degradation	0,0000001
14	EIF-Mercury (Hg)	Field-specific	No degradation	0,0000001
11-n	Production chemicals		HOCNF (BOD 28 d) specific data	

\* Aliphatic hydrocarbons (oil in water)

The biodegradation rates in DREAM are described as k-values from Equation 1:

$$k = -(1/\text{time}) * \ln ((100 - \% \text{ BOD}) / 100) \quad \text{Equation 1}$$

where; time is usually 28 days (standard test conditions)

Biodegradation rates for process or man-added chemicals are taken from the BOD test available in the HOCNF (Harmonised Offshore Chemical Notification Format) form. The k-value is determined from the percentage biodegradation within 28 days (BOD) with marine bacteria (OECD 203). If physical/chemical and toxicity data for a process chemical are available on a single component level, all components in the actual process chemical can be included in the modelling and the biodegradation rate of the individual constituents is applied, entered both cells for water and sediment biodegradation (component database editor).

For production chemicals representing a mixture of compounds, the lowest biodegradation rate measured in the required OSPAR test for the single selected constituent of the actual chemical is applied. Other field specific compounds, natural or man-added may also be added to the list, providing necessary physical/chemical and toxicity data are available.

### 2.3.2 PNEC (Predicted No Effect Concentration)

In principle, the PNEC is calculated by dividing the lowest short-term L(E)C50 or long-term NOEC value from species represented at one of three trophic levels with an appropriate assessment factor in accordance with the TGD (EC, 1996). The assessment factor is determined by the availability of reliable chronic data.

PNEC values have been calculated for a number of naturally occurring components within the defined compound groups (Frost, 2002). The components selected to represent the PNEC of the various groups characterising the produced water composition are shown in Table 2.4.

**Table 2.4: The PNEC values of the various groups of naturally occurring compounds representing produced water**

<u>Group</u>	<u>Main group</u>	<u>Representative compound</u>	<u>PNEC values (ppb)</u>
1	EIF-BTEX	Benzene	17
2	EIF-Naphthalenes	Naphthalene	2,1
3	EIF-PAH 2-3 ring	Phenanthrene	0,15
4	EIF-PAH 4-5 ring	Benz(a)pyrene	0,05
5	EIF-Phenol-C0-C3	Phenol	10
6	EIF-Phenol-C4-C5	Pentylphenol	0,36
7	EIF-Phenol-C6-C9	Nonylphenol	0,04
8	EIF-Heptan*	heptan	40,4
9	EIF-Copper (Cu)	Copper	0,02
10	EIF-Zinc (Zn)	Zinc	0,46
11	EIF-Nickel (Ni)	Nickel	1,22

12	EIF-Lead (Pb)	Lead	0,182
13	EIF-Cadmium (Cd)	Cadmium	0,028
14	EIF-Mercury (Hg)	Mercury	0,008
11-n	Production chemicals		HOCNF specific data

\* Dispersed oil

In the standardised HOCNF forms only acute toxicity data are available for offshore chemicals (whole product). According to OSPAR standards (OSPAR, 1995), toxicity testing on offshore chemicals should be performed on marine organisms, including an alga (*Skeletonema costatum*), a crustacean (*Acartia tonsa*), and a fish larvae (*Scophthalmus maximus.*), representing species living in the water column. According to TGD guidance (EU, 1996), a PNEC is derived by dividing the lowest acute LC<sub>50</sub> or EC<sub>50</sub> concentration by the maximum assessment factor of 1000, when only acute toxicity data are available.

Toxicity data for calculating PNEC values of the individual components of the chemical product are only rarely available. If toxicity data are available only on a whole product basis, the PNEC will be determined from the toxicity of the whole product, identical to the PNEC method applied for chemicals composed of a single component.

When toxicity data are available on the component level, PNEC values of the individual components representing the chemical preparation are preferably applied.

## 2.4 Met-Ocean data

Standardised current fields and wind time series for EIF calculations for different regions of the Norwegian Sector of the North Sea are given in Table 2.5. The current and wind fields are represented in the table by the file-names used in the DREAM model. The standardised modelling period is 1.5 – 30.5.1990.

**Table 2.5: Current- and wind files to be used in EIF calculation in different regions of the Norwegian sector**

Region	Current file	Wind file
The North Sea	May90.dir	Gullfaks.wnd
The Ekofisk area	May90.dir	Ekofisk.wnd
The Norwegian Sea	NHAV-mai.dir	NHAV65_7.wnd

### 3 Model parameters and computational considerations

Chapter 3 addresses the standardisation of internal model input parameters that affect the EIF quantitatively. The proposed values for these variables are all based on comprehensive sensitivity testing of the DREAM model.

#### 3.1 Definitions

Key concepts discussed in this chapter are defined here:

- **Grid:** a grid is a 2- or 3-dimensional lattice or mesh used to discretize space into individual cells for purposes of numerical computation. For underwater releases in DREAM, all grids are rectilinear and all cells are of the same size.
- **Grid resolution:** the resolution of a grid refers to the size of individual cells in the grid: smaller cells provide higher **spatial resolution**.
- **Habitat grid:** defines the physical domain in which the model operates. This domain is divided up into rectangular cells, in which land, water, and water depth are defined. The user controls the resolution of the habitat grid when the grid is created. This resolution is generally non-critical to the EIF computation in offshore areas, since there is no need to define coastlines in detail, and because the resolution of the concentration grid is defined independently by the user. On the other hand, the outer extent of the habitat grid defines the maximum geographic area within which water concentrations will be calculated.
- **Concentration grid:** the model computes and reports concentrations in the water column using the concentration grid. This grid is fixed in space and time when an EIF is to be calculated. The “Expanding grid” option is de-selected in the Model Parameters dialogue. The resolution of the concentration grid is controlled by the user through specification of the number of cells in the horizontal and vertical directions of the concentration grid, also in the Model Parameters dialogue.
- **Lower Concentration Limit:** the lowest concentration that will be recorded in the output files. In the Model Parameters dialogue box, set the Lower Concentration Limit to about 10% of the lowest PNEC value in the release. This will ensure that all concentrations with the potential for non-zero risk values will be retained.

**Time step:** specifies the time interval between subsequent calculations in the simulation. Smaller time steps are required when rates of change are more rapid. A smaller timestep produces increased **time resolution**.

- **Number of particles:** DREAM is a particle-based dilution model. Increasing the number of particles used in a simulation generally increases the statistical stability of the results by increasing the potential **spatial resolution** of the transport process. Experience suggests that 1000 active particles will produce stable results given a 100m x 100m concentration grid and a 5-minute timestep.
- **Output interval:** determines at which frequency the concentration fields and risk results are written to the output data files.
- **EIF:** an EIF of unity ( $EIF = 1$ ) is defined as a volume of water with horizontal dimensions of 100m x 100m and 10m in depth in which the total risk, including contributions from all chemical components in a release with a PEC/PNEC ratio higher than one.

### **3.2 Setting up DREAM for an EIF calculation**

The establishment of the geographic boundary for an EIF calculation is in general an iterative process. One seeks to balance the need for spatial and temporal resolution against the practical constraint of computational time. The resolution necessary to produce a reasonably accurate EIF for a given release scenario is a function of the:

- Composition of the release,
- Release rate, and
- Current velocities in the area for the duration of the simulation.

The spatial resolution can be increased (i.e. the size of the cells in the concentration grid can be decreased) by

- Decreasing the size of the habitat grid (and thereby the concentration grid), or
- Increasing the number of cells in the concentration grid.

Either method will require a decrease in the timestep in accordance with the new grid size, as specified in Equation 2 and Table 4.1. Increasing the resolution of the concentration grid will increase the running time for the simulation because:

- A smaller timestep results in more calculations being carried out by the model for a given simulation duration;
- More cells will contain concentration values, increasing the amount of computation to be carried out by the risk tool, and
- More particles will be needed in the simulation to adequately resolve details in the concentration field.

Reducing the size of the habitat grid is desirable in that one can increase the resolution of the concentration grid without increasing the number of cells in the grid. This helps keep computation time down. The limit to decreasing the size of the habitat grid is associated with the need to keep

relevant risk areas (i.e. those with PEC/PNEC > 1) away from the boundaries, where the loss of particles may artificially reduce the concentration field.

One can establish the final habitat grid in two stages. The first stage, referred to here as screening, uses a large grid to establish the approximate extent of the area within which PEC/PNEC exceeds one. The second stage is the actual computation of the risk map upon which the EIF will be based, and may itself require a few iterations. A standard procedure for computing an EIF is described below, including potential problems that may be encountered.

### **3.2.1 Stage 1: Screening**

First a relatively large habitat grid is created centred on the release site(s). This grid should retain most (> 90%) of the chemical mass released during the simulation. Experience shows that for a large single release (e.g. > 50,000 tonnes of produced water per day), a habitat grid of approximately 100 km North-South and East-West may be necessary. For smaller releases, a somewhat smaller initial screening area may suffice. The user should check the mass balance at the end of the screening simulation to verify that no more than 10% of the mass is in the “Outside” compartment of the mass balance. A second check should be performed after running the Risk Map tool, to assure that PEC/PNEC higher than one does not appear too near the boundary, as discussed further under Stage 2.

The resolution of the habitat grid is non-critical in most offshore areas, but should be fine enough to capture any rapid changes in bathymetry. In the North Sea and Norwegian Sea offshore, 1 km resolution is more than adequate.

The concentration grid for screening can be set to 200 x 200 x 10 cells. This will result in a spatial resolution for a 100 km habitat grid of 100 km / 200 cells = 500 m per cell. For relatively small release rates or low chemical concentrations in the release, either a smaller habitat grid or a greater number of horizontal cells in the concentration grid will increase the spatial resolution.

Run the simulation, and the “Create Risk Map” tool.

**Table 3.1: Suggested model parameters for screening, assuming a 100 km x 100 km habitat grid**

<b>Model parameter</b>		<b>Comments</b>
Number of surface particles	400	Non-critical for EIF computations; given that all components are designated with high solubilities, droplets will have short lifetimes
Number of subsurface particles	400	“More is better” here, but 400 gives short simulation times
Number of cells in concentration grid (xzy)	200 x 200 x 10	Gives 500 m cells in a 100 km grid. The overall size of the concentration grid is the same as the habitat grid, since the Expanding Grid option is de-selected in the model parameters dialogue. The number of cells can be increased or decreased to change the resolution of the screening run. Individual cells must be small enough to register concentration values exceeding PNEC, at least very near the source.
Lower concentration limit (ppb)	10% of lowest PNEC value in the release	Assures good representation of the concentration field near the outer edges
Depth of concentration grid (m)	Min: 0, Max: 100 m	Results in 10 m vertical layers
Output interval (hours)	6	Results in 4 samples of model results per day

<b>Time step considerations</b>				
<b>Stepwise procedure</b>	<b>Size of habitat grid area</b>	<b>Number of cells in concentration grid</b>	<b>Model resolution</b>	<b>Recommended Maximum Timestep (minutes; assumes max. current velocity ~ 0.25 m/s)</b>
Screening	100km x 100km	200 x 200 x 10	500m x 500m x 10m	25
Iteration 1	20km x 20 km	200 x 200 x 10	100m x 100m x 10m	5
Iteration 2	50km x 50 km	200 x 200 x 10	250m x 250m x 10m	15

### **3.2.2 Stage 2: EIF computation**

Stage 2 proceeds based on the results of the screening simulation. Three possible outcomes of the screening scenario are:

- 1 The risk field is less than one or zero everywhere;
- 2 The risk field nears or intersects the boundary of the grid. The risk area with PEC/PNEC higher than one is clearly defined within the grid.

Case 1 results from cells being too large to resolve the concentration from the release point(s) in the grid. A finer meshed grid with 100 m resolution should be applied. If 100 m resolution was used in the screening, then EIF shall be reported as zero.

Case 2 is resolved by implementing a larger habitat grid encompassing the entire area with  $PEC/PNEC > 1$ , plus additional area beyond where the risk field intersected the screening habitat grid boundary. This process is repeated iteratively until the resulting risk field values of PEC/PNEC higher than one are retained well within the habitat grid.

Case 3 is the ideal result, in that fewer iterations are generally required to arrive at a satisfactory result. Both Cases 1 and 2 require correction to become a “Case 3”.

### **3.3 Computational considerations**

Dimensions of the concentration grid, the number of particles used to simulate a release scenario, and the computational timestep influence the time to run a simulation and the space required for storage of results. <sup>1</sup> Setting these parameters at standardised values thus represents a compromise between ideally preferred values (i.e. very high resolution in both space and time) and practical possibilities for running large numbers of simulations assuming the use of today’s “high-end” personal computers.

Recommended specifications for a personal computer to be used for operational EIF calculations are:

- 2+ GHz CPU
- 512 MB RAM
- 80 GB hard disk

The calculations may be carried out on less powerful machines, but will take more time to complete. A CD-ROM drive with read-write capabilities is useful for exchanging data with other off-site users.

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<sup>1</sup> The number of components in the release is also a factor that affects processing time, but is not considered here since the user has little control in this regard.

## 4 DREAM model output and EIF calculation

An EIF calculation is based on data produced by the Risk Calculation tool in DREAM.:

1. The water volume in which the PEC/PNEC ratio is greater than one, and
2. The percent contribution to the environmental risk from each of the components in the simulated release.

The data above are entered into the EIF work sheet (see Appendix 2) as explained below:

- DREAM model output volume (PEC/PNEC >1) is entered at the top of the sheet.
- Produced water volume (basis and new): shall be the same number, and is the volume of produced water (tonnes/day) used in the DREAM modelling
- Chemical compound (basis and new): shall be the same number, and is the concentration of natural compounds or chemicals that are used in the DREAM modelling
- PNEC (basis and new): shall be the same number, and is the PNEC of natural compounds or chemicals that are used in the DREAM modelling (as standardised in Chapter 2.3 of this manual).

## 5 Reporting

This Chapter outlines the reporting of an EIF as determined based on the specifications given in this guideline manual.

### 5.1 *EIF work sheet*

EIF work sheet (ref. Chapter 4 and Appendix 2) should be reported. In addition the produced water volume prognosis as used for the lifetime EIF calculations should be reported. Concentration of man-added chemicals added over a limited time period, should also be reported. For chemicals added over limited time periods, the corresponding time of use should be given. Man added chemicals should be reported with product name. Detailed composition should not be included in the manual, but the applied PNEC value and actual weights for the EIF calculation should be given. However, the operators should save the detailed information related to composition and choice of representative compound for the EIF modelling internally, for potential future applications.

Model parameters: The input data to the *scenario.prv* file from the Dream-model should be reported in an appendix to document the model input parameters.

### 5.2 *Environmental impact factor*

EIF for the actual reporting year should be reported as maximum EIF for the standardised modelling period. In case EIF has been determined for a scenario in which specific chemicals are added for a limited time (Scale squeeze, biocide treatment, jetting operations), the maximum EIF value for the standardised modelled time period where these chemicals are included should be reported separately. In this case the annual EIF should be adjusted by the contribution from these chemicals by the time-weighting equation:

$$\text{EIF} = (\text{T}_1 \times \text{EIF}_1) / 365 + (\text{T}_2 \times \text{EIF}_2) / 365$$

Where  $\text{T}_1$  and  $\text{EIF}_1$  represents the scenario where a certain chemical is discharged over a limited time window and  $\text{T}_2$  and  $\text{EIF}_2$  reflects the “normal” continuous discharge situation.

### 5.3 *Contribution to risk*

Contribution to risk from the different natural and man added chemical compounds in the discharged water should be reported as a “pie-chart” where the percent contribution to EIF (risk) is shown for the different produced water constituents. These results should be related to the total, annual EIF.

## 6 References

Frost, T.K. (2002). Calculation of PNEC values applied in environmental risk management of produced water discharges. Report no. F&T 200212100003, Statoil, Trondheim.

Johnsen, S., T.K. Frost, M. Hjelvold, T.I.R. Utvik (2000). The environmental impact factor – a proposed tool for produced water impact reduction, management, and regulation. SPE paper no. 61178, Stavanger 2000.

Norwegian Oil and Gas (2003): Guidelines for chemical characterisation of produced water., Norwegian Oil and Gas, Stavanger, In press.

SINTEF (2002): Reed, M., B. Hetland, M.K. Ditlevsen, and N. Ekrol. 2001. DREAM Version 2.0. Dose related Risk Effect Assessment Model. Users Manual. SINTEF Applied Chemistry, Environmental Engineering, Trondheim, Norway

## Appendix 1: Hydrocarbon components in each EIF group

<b>Naphthalene (mg/L)</b>	<ul style="list-style-type: none"> <li>• Naphthalene</li> <li>• C1-Naphthalenes</li> <li>• C2-Naphthalenes</li> <li>• C3-Naphthalenes</li> </ul>
<b>PAH 2-3 ring (mg/L)</b>	<ul style="list-style-type: none"> <li>• Total 2/3-ring e.g. <ul style="list-style-type: none"> <li>○ Acenaphthylene</li> <li>○ Acenaphthene</li> <li>○ Fluorene</li> <li>○ Phenanthrene, including C1-C3 alkylhomologues</li> <li>○ Anthracene</li> <li>○ Dibenzothiophenes, including C1-C3 alkylhomologues</li> </ul> </li> </ul>
<b>PAH 4+ ring (mg/L)</b>	<ul style="list-style-type: none"> <li>• Total 4/5-ring e.g. <ul style="list-style-type: none"> <li>○ Fluoranthene</li> <li>○ Pyrene</li> <li>○ Chrysene</li> <li>○ bens(a)antrasen</li> <li>○ Benzo(b)fluoranthene</li> <li>○ Benzo(k)fluoranthene</li> <li>○ Benzo(a)pyrene</li> <li>○ Indeno(123,cd)pyrene</li> <li>○ Dibenzo(ah)anthracene</li> <li>○ Benzo(ghi)perylene</li> </ul> </li> </ul>
<b>Phenol C0-C3 (mg/L)</b>	<ul style="list-style-type: none"> <li>• Phenol</li> <li>• C1-Phenols <ul style="list-style-type: none"> <li>○ o-cresol</li> <li>○ m-cresol</li> <li>○ p-cresol</li> </ul> </li> <li>• C2-Phenols <ul style="list-style-type: none"> <li>○ 2,5-Xylenol</li> <li>○ 3,5-Xylenol</li> <li>○ 2,4-Xylenol</li> <li>○ 4-Ethylphenol</li> <li>○ other C2-phenol alkylhomologues defined by analytical method*</li> </ul> </li> <li>• C3-Phenols</li> </ul>

	<ul style="list-style-type: none"> <li>○ 2-n-Propylphenol</li> <li>○ 2,3,5-Trimethylphenol</li> <li>○ 4-n-Propylphenol</li> <li>○ 2,4,6-Trimethylphenol</li> <li>○ other C3-phenol alkylhomologues defined by analytical method*</li> </ul>
<b>Phenol C4-5 (mg/L)</b>	<ul style="list-style-type: none"> <li>• C4-Phenols <ul style="list-style-type: none"> <li>○ 4-tert-Butylphenol</li> <li>○ 4-iso-Propyl-3-Methylphenol</li> <li>○ 4-n-Butylphenol</li> <li>○ other C4-phenol alkylhomologues defined by analytical method*</li> </ul> </li> <li>• C5-Phenols <ul style="list-style-type: none"> <li>○ 2-tert-Butyl-4-Methylphenol</li> <li>○ 4-tert-Butyl-2-Methylphenol</li> <li>○ 4-n-Pentylphenol</li> <li>○ other C5-phenol alkylhomologues defined by analytical method*</li> </ul> </li> </ul>
<b>Phenol C6+ (mg/L)</b>	<ul style="list-style-type: none"> <li>• Sum C6-Phenols <ul style="list-style-type: none"> <li>○ 2,6-Di-iso-Propylphenol</li> <li>○ 2,5-Di-iso-Propylphenol</li> <li>○ 4-n-Pentylphenol</li> <li>○ 2-tert-Butyl-4-Ethylphenol</li> <li>○ 6-tert-Butyl-2,4-Dimethylphenol</li> </ul> </li> <li>• Sum C7-Phenols <ul style="list-style-type: none"> <li>○ 4-n-Heptylphenol</li> </ul> </li> <li>• Sum C8-Phenols <ul style="list-style-type: none"> <li>○ 2,4-Di-sec-Butylphenol</li> <li>○ 4-tert-Octylphenol</li> <li>○ 2,6-Di-tert-Butylphenol</li> <li>○ 2,6-Di-tert-Butyl-4-Methylphenol</li> <li>○ 4-n-Octylphenol</li> </ul> </li> <li>• Sum C9-Phenols <ul style="list-style-type: none"> <li>○ 2-Methyl-4-tert-Octylphenol</li> <li>○ 4-n-Nonylphenol</li> <li>○ 4,6-Di-tert-Butyl-2-Methylphenol</li> <li>○ 2,6-dimethyl-4-(1,1-dimethylpropyl)phenol</li> <li>○ 4-(1-ethyl-1-methylpropyl)-2-methylphenol</li> </ul> </li> </ul>

\*See Norwegian Oil and Gas Guidelines for chemical characterisation of produced water for further details on alkylated phenols (Norwegian Oil and Gas, 2003).

**Appendix 2:**  
**EIF Example**

**Simulated  
EIF (from  
DREAM)**

**113,52**

Compound group	Discharge, tonnes/day		Concentration, mg/l		PNEC ppb		Contribution to risk (%)	Contribution to EIF	Weight	Contribution incl. Weight	EIF
	Basis	New	Basis	New	Basis	New					
Total	27315	27315									
BTEX			1,38	1,38	17	17	1,23	1,40	1	1,40	
Naphtalenes			1,177	1,177	2,1	2,1	20,09	22,81	1	22,81	
2-3 ring PAH			0,055	0,055	0,15	0,15	20,31	23,06	1	23,06	
4-ring+ PAH			0,002	0,002	0,05	0,05	1,77	2,01	2	4,02	
Phenols C0-C3			0,179	0,179	10	10	0,37	0,42	1	0,42	
Phenols C4-C5			0,1	0,1	0,36	0,36	14,25	16,18	1	16,18	
Phenols 6+			0,002	0,002	0,04	0,04	2,28	2,59	2	5,18	
Aliphatics			21	21	40,4	40,4	29,54	33,53	2	67,07	
Zink			3,06E-02	3,06E-02	2,4	2,4	0,49	0,56	1	0,56	
Mercury			1,30E-05	1,30E-05	0,01	0,01	0,05	0,06	1	0,06	
Lead			8,50E-04	8,50E-04	0,34	0,34	0,08	0,09	1	0,09	
Copper			7,87E-02	7,87E-02	0,76	0,76	5,18	5,88	1	5,88	
Nickel			2,46E-03	2,46E-03	1,22	1,22	0,06	0,07	1	0,07	
Cadmium			5,90E-04	5,90E-04	0,1	0,1	0,2	0,23	1	0,23	
Scale inhibitor			11,81	11,81	1000	1000	0,44	0,50	1	0,50	
Flocculant			1,09	1,09	500	500	0,07	0,08	1	0,08	
Emulsion breaker			2,38	2,38	163	163	0,55	0,62	2	1,25	
Defoamer			0,09	0,09	134	134	0,02	0,02	2	0,05	
Biocide 1			0,34	0,34	5	5	3,02	3,43	1	3,43	
Biocide 2			0,0008	0,0008	0,76	0,76	0,03	0,03	1	0,03	
Corrosion inhibitor			0,002	0,002	617	617	0	0,00	1	0,00	
							<b>100,0</b>	<b>113,55</b>		<b>152,33</b>	<b>152</b>

## Appendix 3: Example applications

### 1.1 Example 1: Small release

This first example is for a small release, and reports results for three different time steps to underscore the relevance and importance of this parameter.

Produced water release rate: 1000 tonnes/day.

Final habitat grid: 11x 11 km

Concentration grid: 100 x 100 x 10 cells

Concentration cell size: about 112 m x 112 m x 10 m, or about 1.3 EIF units per cell

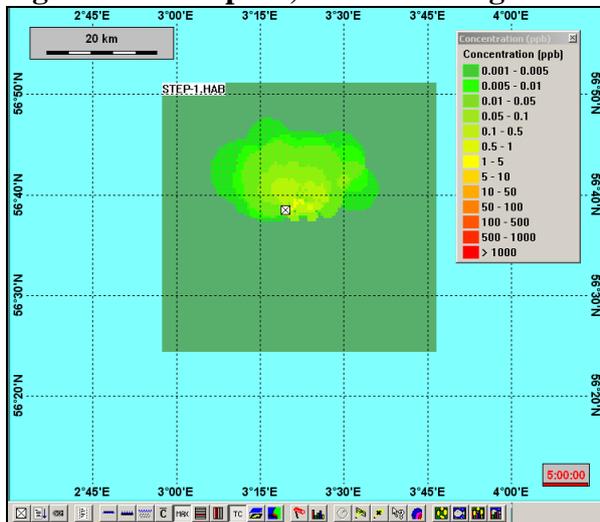
Timesteps used:

- Screening (Figure 1.1): 25 min
- First iteration (Figure 1.2): 15 min
- Final iteration (Figure 1.3): 5 min

Sub-surface particles: 1000

Lower concentration limit: 0.004 ppb

Figure 1.1 Example 1, Grid-screening #1



Step 1: Habitat grid: 50x50 km, to map the overall concentration-field

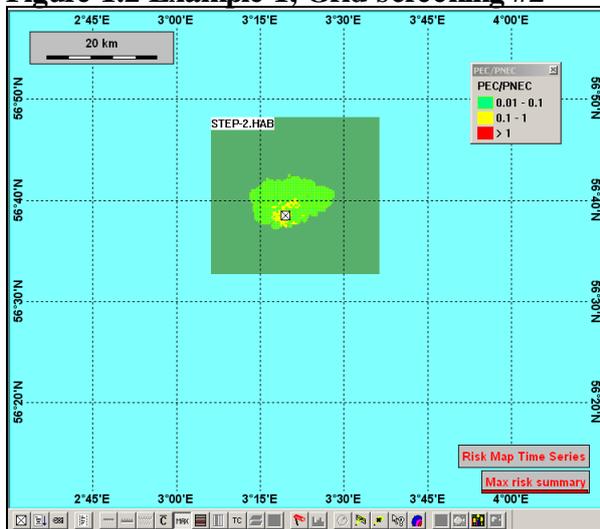
Concentration grid: 100 x 100 x 10 cells (500 m per cell)

Timestep: 25 min.

EIF computed: 0.0

Conclusion: need better resolution

**Figure 1.2 Example 1, Grid-screening #2**



Step 2: Habitat grid 30x30 km covers the concentration-field produced in Step 1.

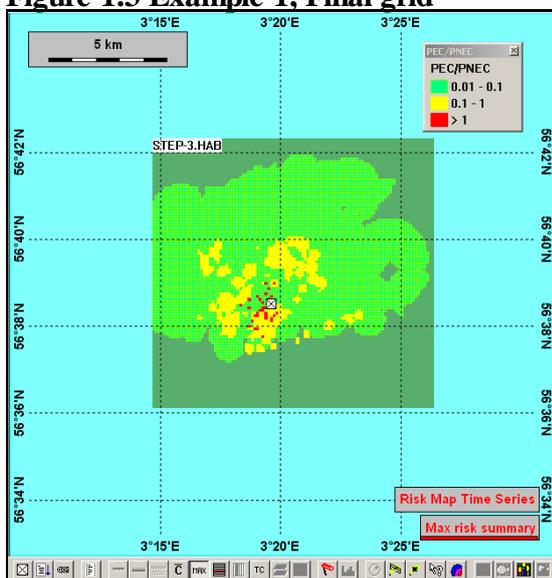
Concentration grid: 100 x 100 x 10 cells (300 m per cell)

Timestep: 15 min

EIF computed: 0.0

Conclusion: still better resolution needed

**Figure 1.3 Example 1, Final grid**



Step 3: Habitat grid 10x10 km, covers the risk-area

Concentration grid 100x100x10 cells (100 m per cell)

Timestep: 5 minutes

EIF computed: 5.18

Conclusion: appears marginally satisfactory; re-compute concentration field and risk field several times to test for stability of the result, which depends on 3 – 4 cells exceeding  $PEC/PNEC = 1$ ; smaller cells and timestep will be necessary to further reduce variability  
Mean value for 5 runs: 4.67 (accepted for reporting)

**Table 1.2: EIF units calculated by DREAM for Example 1, with 5 repeated simulations for 2 different timesteps.**

<b>Timestep (minutes)</b>	<b>10</b>	<b>5</b>
Test 1	5.1835	5.1835
Test 2	3.8876	5.1835
Test 3	5.1835	5.1835
Test 4	5.1835	3.8876
Test 5	3.8876	3.8876
<b>Mean</b>	<b>4.665</b>	<b>4.665</b>
Standard deviation	0.709	0.709
Std Dev/Mean	0.15	0.15
Range	1.3	1.3
Range/Mean	0.3	0.3

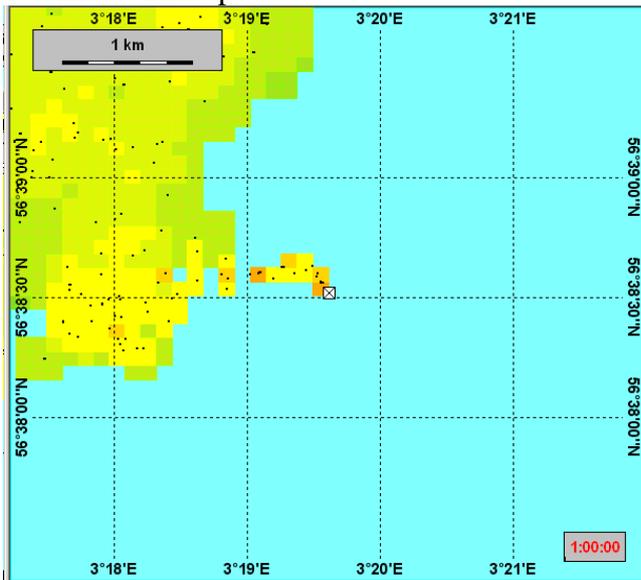
The final iteration (Figure 1.3) has been simulated 5 times using both a 5-minute and a 10-minute timestep. The 5-minute timestep is the theoretically “safe” value; the 10-minute step allows the computation to proceed twice as fast, but may introduce instabilities in the results in some cases. Here we see that the results are essentially the same for the two sets of cases, so the 10-minute step could be used for subsequent variations involving the composition of release in the scenario.

This example demonstrates that the model is not overly sensitive to the timestep, and that if one is to run a large number of similar scenarios for a given release, a little experimentation with the timestep may save some computational time.

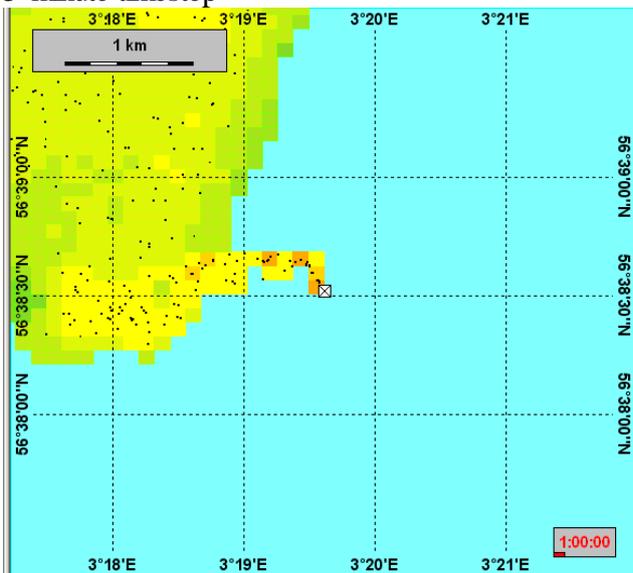
It is also useful to be aware of the number of cells involved in producing an EIF. In this case, an EIF of 3.88 units corresponds to 3 cells in the concentration grid. Plus/minus one cell results in a 33% change in the EIF, so that smaller cells and a smaller timestep would stabilize the result, if the variation is too large for the purposes of the calculation. On the other hand, if one is comparing this release with another one with an EIF of 500, then the difference between 3.88 and 5.18 is not really important.

Figure 1.4 shows a snapshot of one simulation for 10-, 5-, and 1-minute timesteps after 1 day of simulation. Reducing the timestep to one minute results in better definition of the concentration field around the edges, but since the PEC/PNEC ratio only exceeds unity very near the source, this added definition is irrelevant to the results.

10-minute timestep



5-minute timestep



1-minute timestep

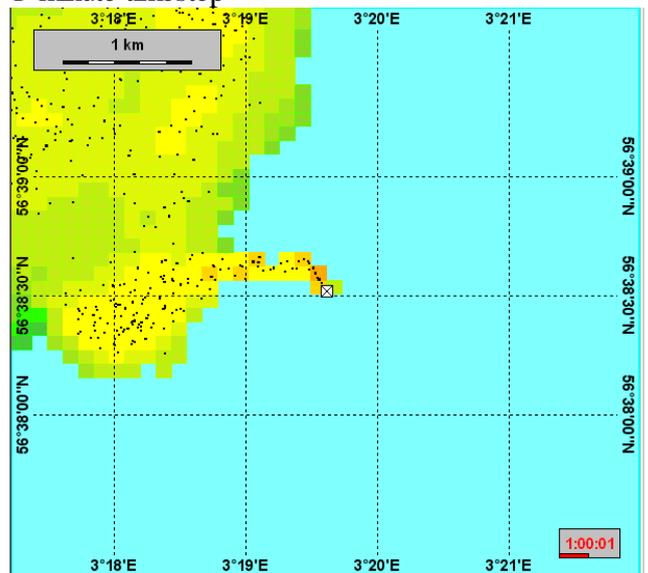


Figure 1.4: Snapshots of concentration field for Example 1, using 10-, 5-, and 1-minute timesteps for the calculation.

## 1.2 Large release

Produced water release rate: 50,000 tonnes/day.

Habitat grid: 55 x 55 km

Concentration grid: 100 x 100 x 10 cells

Concentration cell size: about 550x550 m, or about 30 EIF units per cell.

Timestep: 60 and 10 min (for comparison purposes; 10 minutes is the better choice here)

Sub-surface particles: 1000

Lower concentration limit: 0.004 ppb

Five test cases at each timestep were run, with the random number generator initialised with a random seed. The table below shows the variation in the EIF for these cases:

Table 1.3 EIF units calculated by DREAM for Example 2, with 5 repeated simulations for 2 different timesteps.

<b>Timestep (minutes)</b>	<b>60</b>	<b>10</b>
Simulation # 1	8118	8351
# 2	7621	8147
# 3	7651	8147
# 4	8088	8176
# 5	8351	8059
<b>Mean</b>	<b>7970</b>	<b>8180</b>
Standard deviation	320	110
Std Dev/Mean	0.04	0.01
Range	729	192
Range / Mean	0.09	0.02

The 60-minute timestep results in a particle displacement of 900 m in a current of 0.25 m/s. Reviewing the current field shows that the actual current is often below this value, but is sometimes as high as 40 cm/sec. This means that the release process in the model often does not fill all the cells near the source. If one new particle is created each timestep, each particle will have 6 times as much mass as a particle released every 10 minutes. Minimum transport time from the middle of the 55 km habitat grid to the boundary is about  $27 \text{ km} / 0.25 \text{ m s}^{-1} = 30$  hours. Actual transport time is greater than this because the current is not always in the same direction. The maximum number of particles in the grid is about 300 for this case with the 60-minute timestep. When this many particles have been released, particles are being transported out of the boundaries about as fast as they are being released from the source. The low particle density combined with the extremely large timestep (large in proportion to the cell size and current velocities) result in a relatively unstable EIF calculation.

The 10-minute timestep results in a relatively continuous release, in the sense that particles fill all cells between the source and cells containing particles previously released. In addition, the increased frequency of particle release results in use of the full 1000 particles allocated by the user, which in turn produces a less variable EIF calculation, with a range that is only 2% of the mean value.