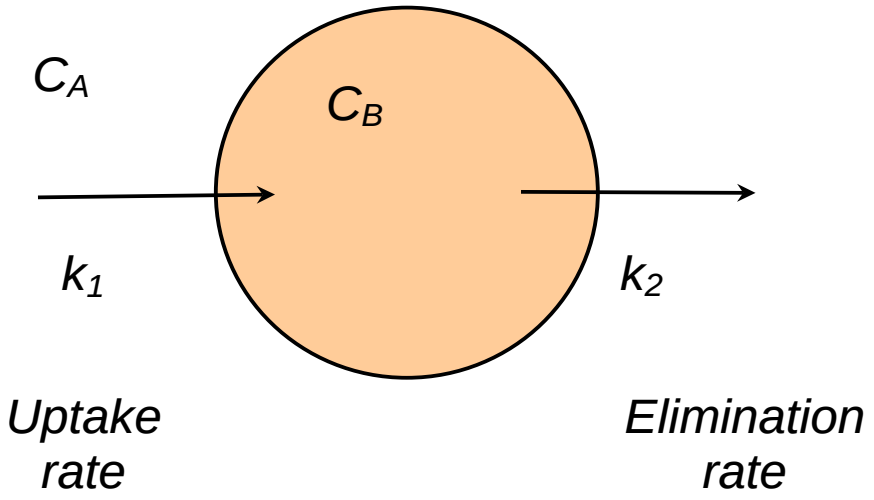
Report

QSAR methodology for calculating impact on organisms exposed to dissolved oil in the water column

ERA Acute for water column exposed organisms

Author(s)
Ute Brönner
Trond Nordtug



SINTEF Materials and Chemistry
Environmental Monitoring and Modelling
2020-03-06

SINTEF

SINTEF Materialer og kjemi
SINTEF Materials and Chemistry

Address:
Postboks 4760 Sluppen
NO-7465 Trondheim
NORWAY

Telephone:+47 73593000
Telefax:+47 73597043

info.mk@sintef.no
www.sintef.no/mk
Enterprise /VAT No:
NO 948007029 MVA

KEYWORDS:
ERA Acute
Risk Assessment
QSAR
CBR
TLM
OMEGA

Report

QSAR methodology for calculating impact on organisms exposed to dissolved oil in the water column

VERSION
2.0

DATE
2020-03-06

AUTHOR(S)
Ute Brönner
Trond Nordtug

CLIENT(S)
Total EP
Statoil

CLIENT'S REF.
Grethe Kjeilen-Eilertsen
Tonje Waterloo-Rogstad

PROJECT NO.
102001410

NUMBER OF PAGES/APPENDICES:
23 + Appendices

ABSTRACT

ERA Acute – water column compartment

ERA Acute uses results from an oil spill model to calculate impact from exposure to the spilled oil in the four compartments: sea surface, shoreline, water column and sea floor. The oil spill model is run in stochastic mode to combine the impact with a probability for the impact to calculate environmental risk.

This report describes exposure calculations in the water column as available with the OSCAR model per today in stochastic mode. Since the model is calibrated with toxicity data for zooplankton, the report describes how it may be applied to other organisms in the water column including phytoplankton, fish egg / larvae, fish as well as corals and sponges.

In the last chapter we describe how to use OSCAR together with the ERA Acute software and suggest improvements for future solutions.

PREPARED BY
Ute Brönner, Trond Nordtug

SIGNATURE

CHECKED BY
Mark Reed, Petter Rønningen

SIGNATURE

APPROVED BY
Atle Kleven

SIGNATURE

REPORT NO.	ISBN	CLASSIFICATION	CLASSIFICATION THIS PAGE
OC2020 A-030	978-82-7174-376-5	Unrestricted	Unrestricted

Document history

VERSION	DATE	VERSION DESCRIPTION
0.1	2014-11-25	Version for QA
0.2	2014-11-27	Version after QA, added ERA Acute methodology
0.3	2014-11-28	Added VEC description and literature list
0.4	2014-11-28	DRAFT version for project deliverable
1.0	2015-01-20	Final version
2.0	2020-03-06	Downgrading of SINTEF report F26517: same content as before, unrestricted

SINTEF

Table of contents

APPENDICES

SINTEF F26670 QSAR in Environmental Risk Assessment.pdf

1 Introduction

ERA Acute uses results from an oil spill model to calculate impact from exposure to the spilled oil in the compartments sea surface, shoreline, water column and sea floor. The oil spill model is run in stochastic mode to combine the impact with a probability for the impact to calculate environmental risk.

The main challenges in computing the impact of crude oil on organisms in water in addition to the complex composition of oil is the temporal variation in both chemical and physical properties of the oil as well as temporal variation in concentrations due to dilution. In the following we describe how population loss can be predicted with the application of OSCAR based on Critical Body Residue calculations with QSARs for toxicity.

In order to cope with the extremely high number of individual oil compounds SINTEF's Oil Spill Contingency and Response (OSCAR) model uses 25 pseudo-components that represent groups of chemicals with similar properties. The partitioning of components between oil and water in time and space is calculated based on the physical and chemical properties of each pseudo-component and the effects of the physical environment.

The basis for the mortality predictions is the interaction between organisms and oil, and in the current version of OSCAR the exposure to oil in the water column is associated to the dissolved fraction only. The calculation of toxicity is based on acute effects assuming non-specific narcosis as the mode of action.

The LC_{50} for individual compounds contained in crude oil are derived from empirical data or extrapolated to compounds with unknown toxicity using a simple QSAR based on the octanol/water partitioning coefficient (K_{OW}) which may either be experimentally determined or estimated from chemical structure. LC_{50} are documented in [1]. K_{OW} are derived from K_{OC} values stored in the oil properties database [2][1].

2 OSCAR methodology for estimating loss of individuals (lethality)

Exposure in the water column is highly variable due to dilution and weathering processes, as well as uneven or patchy distributions of organisms in space and time. For this reason, the methodology described here calculates a time-dependent body residue based on time-varying exposure. Body residue is a parameter well suited for impact- and risk assessment of marine oil spills in the water column

- Changing exposure can be calculated via realistic time integration (uptake kinetics)
- Body residue can be verified *in nature* through chemical analysis of biota and therefore verify model calculations (LC/EC_{50} cannot)
- Body residue is linked to EC/LC-curves through known relationships

SINTEF's OSCAR model in its current version (per today: MEMW6.6.1) can calculate body residue in organisms exposed to dissolved oil components in the water column in stochastic mode and relate it to a critical body burden for computing lethality.

2.1 QSARs for calculating EC/LC50

The proposed methodology requires that the oil spill model represent oil in the water column with a chemical profile that is sufficiently detailed so as to reflect changes in toxicology associated with changes in the composition of the water-accommodated fraction (WAF) over time. OSCAR, for example, represents oil using 25 pseudo-components, each representing a number of distinct but related chemical components in the

[1] We are aware that this might add complications. The new version of the exposure model implements K_{OW} values consistent with the used LC_{50} values from the database.

oil (see [1]). The present version of OSCAR (6.6.1) predicts the lethality of the average temperate pelagic crustacean. Toxicity is based on regressions based on empirical data for single non-polar oil components (non-polar narcosis) and phenols (polar narcosis). The origin of the data is from established databases and publications and the criteria for selection and subdivision is discussed elsewhere [3], [4]. In general, a regression is made for a defined group of animals (e.g. pelagic crustaceans or fish). Thus, the line describing the regressions represents the median LC_{50} as a function of K_{ow}. According to the basic theory of non-specific narcosis the LC_{50} values should be expressed as molar concentrations. Groups considered relevant for acute toxicity are those having a log K_{ow} below approx. 6 and are expected to be dissolved in the water phase to some extent. The currently used values are a dataset of quality assured and time corrected LC_{50} values extracted from available databases and literature [1].

2.2 Establishing critical body residue CBR

For narcotic chemicals the body concentration of an individual is related to acute effects and the Critical Body Residue (CBR). CBR is the body concentration that corresponds to 50% mortality. Thus, *CBR* is given from steady state equilibrium condition as

$$CBR_i = BCF_i \bullet LC_{50i} \qquad (2\text{-}1)$$

for each pseudo-component i. The bio concentration factor (BCF) is related to K_{OW} and is found from established QSARs.

2.3 Temperature compensation

There is currently no compensation for temperature in the toxicity calculations. However, a compensation for temperature may be included in a sensitivity factor that is used to compensate for the sensitivity of different species (see below).

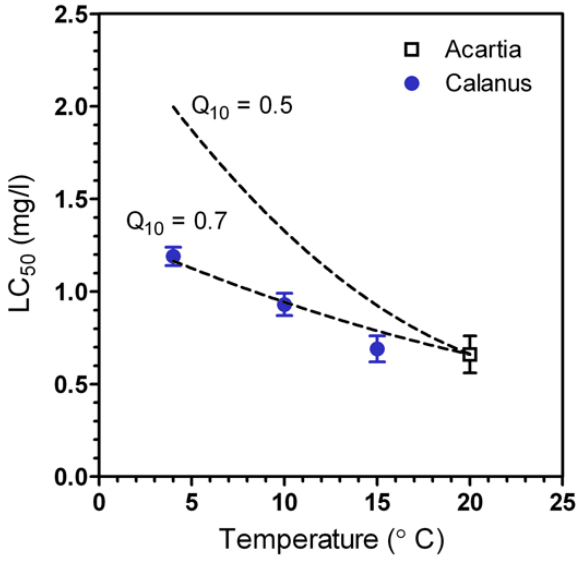


Fig. 1. Toxicity of 3,5-dichlorophenol (DCP) using the standard *Acartia tonsa* test (ISO 14669:1999) and corresponding tests with *C. finmarchicus* acclimated and tested at different temperatures. Dashed line corresponds to different Q_{10} value of 0.5 as an example. Vertical bars indicate the 95% confidence interval (adapted from [5]**).**

The Q_{10} temperature coefficient is a measure of the rate of change of a biological or chemical system as a consequence of increasing the temperature by 10^0 C. We have previously shown that the sensitivity of the related arctic species *Calanus glacialis* tested at 2^0 C is lower than for *Calanus finmarchicus* tested at 10^0 C for selected oil component mixtures [6]. Some studies have used a Q_{10} compensation for LC_{50} of 0.33 [7]. This corresponds to a 3-fold increase in LC_{50} at 10^0 C temperature reduction. When comparing the LC_{50} of *C. finmarchicus* acclimated and tested with 3,5-dichlorophenol at three temperatures in the range 4 to 15^0 C with the LC_{50} of *Acartia tonsa* tested at 20^0 C [5] the Q_{10} for LC_{50} (48 hours) in C. finmarchicus in the range 4 to 15^0 C was about 0.7. In Figure 1 these data are compared to *A. tonsa* LC_{50} assuming a Q_{10} of 0.5.

2.4 Body residue calculations

OSCAR represents oil as 25 pseudo components. For each of the 25 components and each computational time step OSCAR solves the equation

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \qquad (2\text{-}2)$$

or

$$\Delta C_B = (k_1 C_A - k_2 C_B)\Delta t \qquad (2\text{-}3)$$

with

Δt = time step

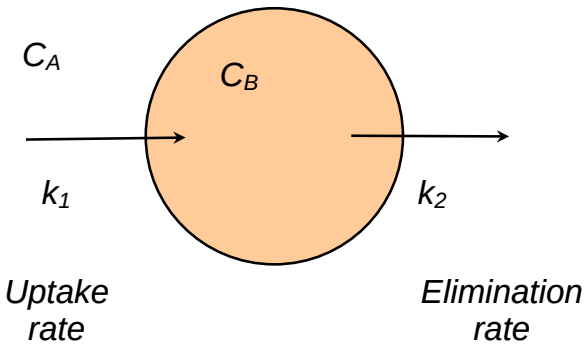
C_A = ambient concentration of the component

C_B = concentration in tissue (body residue) of the component

k_1 = uptake rate

k_2 = depuration rate

Fig 2. Principle for body residue. The body concentration C_B is result of uptake and elimination. The uptake rate is proportional to the environmental concentration C_A, while the elimination rate is proportional to the body concentration C_B. The uptake rate is related to the size of the organism and the lipophilic properties of the compounds which are related to the octanol/water partitioning constant (Log Kow) [10], [21], [22].

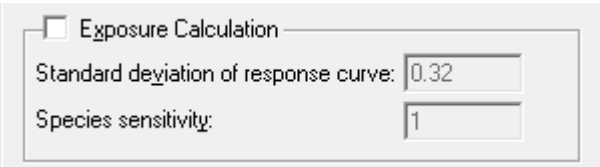


From French-McCay [8] the rate coefficients are given as:

$k_2 = a(K_{ow})^b$ with a = 29.5, b = -0.414 with k_2 in units 1/day. k_1 is calculated from the bio-concentration factor for the component

$$k_1 = BCF \cdot k_2 \qquad (2\text{-}4)$$

with a QSAR for the BCF, $BCF = \alpha(K_{ow})^{\beta}$ and α = 0.048, β = 1 (from Mackay, 1982 [9], quoted by [8]).



The exposure calculations are species independent; LC_{50i} values are based on data for zooplankton. The stochastic simulation setup for Exposure Calculations therefore includes a sensitivity factor ("Species sensitivity"). The database LC_{50i} values will be divided by this factor, accounting for more (factor > 1) or less (factor < 1) sensitive organisms.

This sensitivity factor might also be used to account for temperature effects as described above or chronic effects by reducing the $LC_{50}^{i}$to an e.g. $\overline{LC_5^i}$ for the components. Conservative approaches often use 10 as a sensitivity factor to calculate NOEC levels.

The *CBR* for the current composition of pseudo-components i is given by

$$CBR_{mix} = \frac{C_B}{\sum \frac{C_{Bi}}{CBR_i}} \qquad (2\text{-}5)$$

with C_B being the total body burden of all components and C_{Bi}, CBR_i the body burden and critical body burden for each component, respectively.

2.5 Mortality via concentration-effect relationships (dose response curves)

With a known critical body residue, the mortality at any given body residue (BR) may be calculated from a concentration - effect or dose - response curve. In OSCAR it is assumed that the dose - response curve follows a log-normal distribution with a standard deviation equal to that of the dose response curve for lethal concentration [10][4].

The mortality *P* ("fraction killed") corresponding to the given body residue C_B is derived from a concentration - effect curve which is implemented as

$$P = \Phi(x, 0, \sigma)$$

where Φ is the cumulative normal distribution with argument *x*, mean value 0 and standard deviation (slope) σ, $x = \log\left({C_B}/{CBR}\right) or \log\left(\sum \frac{C_{Bi}}{CBR_i}\right)$ and $\sigma = 0.32$.

Smit et. al [11] discussed standard deviations for dose-response curves in environmental risk assessment. Slopes for effect - concentration curves were determined for more than 300 test populations and showed an average of 0.65 corresponding to an EC_{50}/EC_5 ratio of 2.9. Median slopes for 96h test were significant steeper for fish and molluscs compared to those for algae and crustaceans.

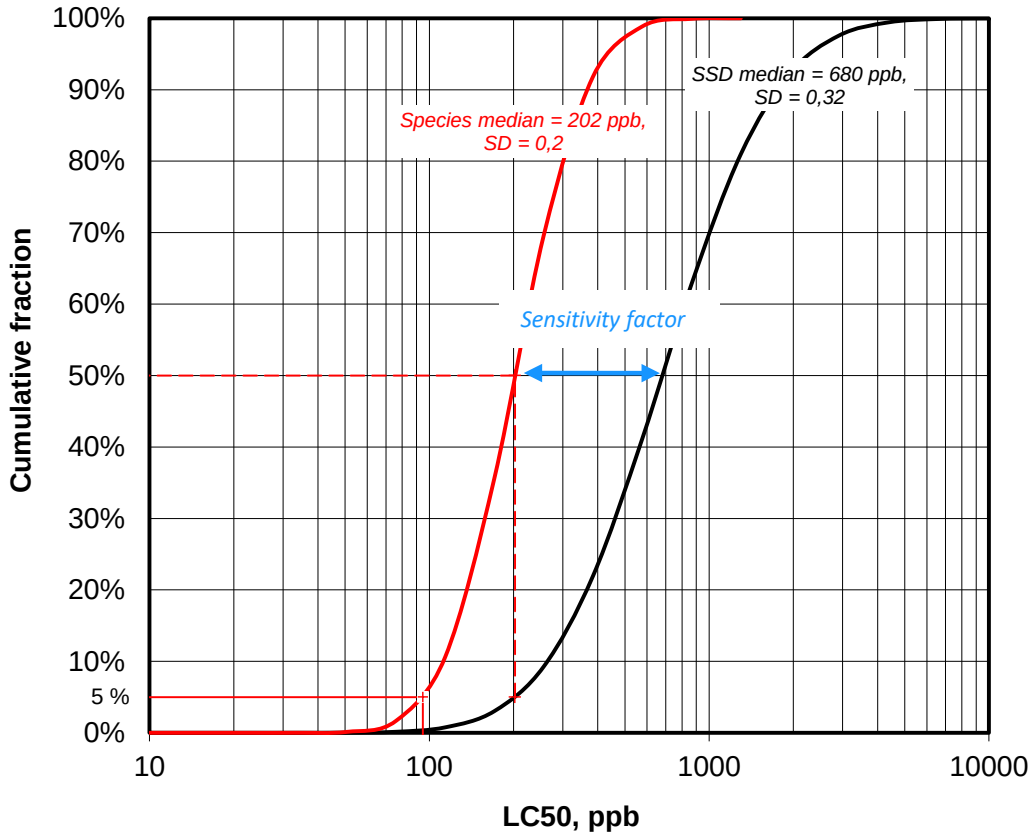


Figure 1 Theoretical example of a species sensitivity distribution (SSD) curve (black) and the dose response curve for a sensitive species (red) at the 5% level of the SSD-curve equalling a sensitivity factor of 3.4 (680/202).

Mortality in the exposure calculations can only increase or be constant, i.e. after each time step t we have $P = Max\ (P(t), P(t-1))$.

3 Valued ecosystem components (VEC)

3.1 Sensitivity of VECs

In order to target specific VECs a minimum of information about the species sensitivity to petroleum hydrocarbons is needed. If data are available that can relate the sensitivity of a certain VEC to other species - for instance using SSD-curves - the deviation from the median value of the SSD curve can be directly used to establish a sensitivity factor for that particular VEC. At the current state, however, we suggest looking at the more general tends related to compartment and trophic level in addition to geographical regions separated by temperature conditions.

We divide the defined geographic areas for ERA Acute into cold areas (water temperature < 5°C), temperate (5-20°C) and warm areas (>20°C) since toxicity testing experiments are done under standard conditions representative for a specific area, among others temperature and daylight. *Cold areas* will comprise Canada, *Temperate areas* will comprise Northern Europe and Argentina, and *Warm areas* will comprise Mediterranean Sea, West Africa (Angola) and South Africa, Gulf of Mexico South China Sea (Indonesia), Australia and Persian Gulf.

Calculating toxicity in the body residue model is based on acute toxicity data for different species exposed to single oil components. The most extensive data available are of zooplankton (pelagic crustaceans). These are the basis for the calculations made in OSCAR (LC_{50} values available in oil properties database). Zooplankton also shows the highest sensitivity to oil components.

Since the exposure model used in OSCAR is species independent, less sensitive species might be accounted for by applying a sensitivity factor. The above implies that the sensitivity factor for the "average zooplankton" is 1.0. In order to calculate the sensitivity of the other VEC groups we have related available toxicity data on single components to zooplankton to establish an average sensitivity factor for algae, benthic species and fish, fish egg and larvae.

3.2 Sensitivity factors for algae, fish, benthos

In a previous study data were collected from the ECOTOX database (U.S. Environmental protection Agency). Only data where LC_{50} (zooplankton, benthos and fish) or EC_{50} on growth (plant) were specified, were used. These data were sorted according to group after the following scheme

Phytoplankton: green algae

Zooplankton: copepods, shrimps, mysids

Benthos: benthic crustaceans, molluscs, echinoderms, polychaete worms

Fish: all fish species regardless of life stage.

Search was conducted for specified chemicals analysed for the OSCAR model input. Only the chemicals with a log(K_{ow}) less than 5.8 were included and all data were corrected for test duration according to French McCay, 2002 [7].

It`s well known that LC_{50}-values show a considerable variation within groups of organisms as well as between groups. This is part of the variation seen in the reported LC_{50}-values. Major factors are the condition of the tested organisms, experimental design and the verification of the exposure concentration. Significant outliers[2] were therefore removed and the averages of the remaining EC50/LC50 values (607 data points) were calculated for each chemical. For chemicals with toxicity data for at least two groups including zooplankton, the sensitivity factor relative to zooplankton was calculated. The average of all sensitivity

[2] Outliers were defined by criteria for accepting data from the original publications; most of them were removed due to lack of documentation of exposure concentrations etc.

factors is shown in table 1. Due to recent studies on fish embryos and first-feeding larvae (e.g. [12], [13], [14]) showing effects at quite low concentrations of oil there may be a need to introduce a separate sensitivity factor for fish egg and larvae.

Table 1 Relative sensitivity (= sensitivity factors) of groups of marine organisms based on 607 LC/EC50 values for oil compounds in the ECOTOX database.

	Algae EC_{50}	Zooplankton LC_{50}	Benthos LC_{50}	Fish LC_{50}*
Sensitivity factor relative to zooplankton	0,41	1	0,38	0,93
Standard slope of SSD curve	0,10		0,09	0,20

* including fish eggs and larvae. Higher sensitivity for eggs and larvae can be accounted for by the sensitivity factor. While eggs and larvae show acute effects, will fish be prone to delayed and chronic effects.

3.3 Temperature-dependent sensitivity

The basic toxicity data used in creating the QSAR for LC_{50} is almost exclusively from experiments performed at 20˚ C. As discussed above toxicity is affected by temperature and in order to account for different temperature regions a temperature compensation should be included in the calculations.

In the present version of OSCAR this has to be included as part of the sensitivity factor. Most data indicate that the change in LC_{50} per 10˚ C increase in temperature (Q10 for LC_{50}) of temperature acclimated individuals is in the range 0.3 – 0.5; however a SINTEF study showed a Q10 of 0.7 for *C. finmarchicus* (see 2.3).

4 Corals and sponges as organisms exposed through the water column

4.1 Corals

There is a large amount of literature on effects on corals and discharges from petroleum activity. Most of this literature is related to impacts from sedimentation of drilling discharges. Reports from previous oil spill incidents are mostly related to warm water corals in shallow water. Thus, we have not been able to find consistent data to evaluate the acute sensitivity to water soluble oil components relative to other species groups. According to NOAA (US National Ocean and Atmospheric Administration [15]) the effects from acute oil spills are more likely to appear as sub-lethal effects that may later cause bleaching[3] and reduced reproduction rather than acute mortality.

The effects of an oil spill are highly dependent on the conditions of the spill (oil type, depth, habitat), observed effects from large oil spills might be severe (e.g. [16]), but on the contrary the extent of coral reef damage directly attributable to the world's largest oil spill in the Persian Gulf in January 1991, has been remarkably minor according to NOAA. There are indications of effects on deep water corals after the Deepwater Horizon blow-out in the Gulf of Mexico at distances up to 22 kilometers from the spill site ([17]). However, due to the many potential sources of oil releases (natural and anthropogenic) in the area it is

[3] Corals that are exposed to toxicant causing stress by changes in conditions such as temperature, light, or nutrients, expel the symbiotic algae living in their tissues, causing them to turn white. (http://oceanservice.noaa.gov/facts/coral_bleach.html)

difficult to estimate the extent of damage caused by the Deepwater Horizon blow-out and even more difficult to estimate the concentrations of oil that caused the effects.

Corals have detoxification systems for organic chemicals ([18]) similar to other marine species and there are no indications that corals are more sensitive to acute oil exposure than other species. The reverse is also true; there are indications that some corals may be quite resistant to acute oil exposure, possibly because of their ability retract into the calcified tube structures. However, due to the apparent scarcity of acute toxicity data we suggest that the sensitivity to dissolved oil components for corals is set equal to marine zooplankton.

4.2 Sponges

Just like corals there is an apparent lack of acute toxicity data on specific oil components or the water-soluble fraction (WSF) for sponges. Cebrian and Uriz [19] studied the effects on larval settlement during a 10 day exposure of two widespread Mediterranean sponges (*Crambe crambe* and *Scopalina lophyropoda*) to a mixture of heavy PAHs (log K_{OW} between 5.8 and 6.7). At the highest concentration of 1µg/L a slight delay in settlement was observed for one of the species. However, there was no significant increase in mortality. Given the high K_{OW} and thus potentially high acute toxicity of the PAHs used compared to PAHs found in the WSF of oil the results indicate that these larvae were not significantly more sensitive than other planktonic organisms.

Assuming that adult sponges are no more sensitive than larvae we therefore suggest using the same average sensitivity for sponges as corals (and use the same sensitivity as for zooplankton).

5 Suggested ERA Acute methodology for water column exposed organisms

ERA Acute uses results from an oil spill model like OSCAR to calculate impact from exposure to the dissolved fraction of the oil in the water column. As per today, OSCAR is run in stochastic mode which combines the impact with a probability for the impact to calculate environmental risk.

The impact from exposure to dissolved oil in the water column is reported as "fraction killed" and "body burden". "Fraction killed" is calculated from "body burden" via a concentration-effect (dose-response) curve as described above where the critical body burden is determined via LC_{50} values.

Approaches for the lag phase (time until restitution starts) and the calculation of time for restitution will be addressed in future deliverables.

The methodology is described in three versions since we assess the current available option as non-optimal. In the previous phase of the project SINTEF suggested improvements to OSCAR which were mostly related to the compartment *sea floor* but would improve available results for the compartment *water column* as well. Newer development of OSCAR and changed availability and costs of computer power and storage enable us to suggest a third version, which would be the preferred one as per today.

The objective of the three versions is to improve the available results without major changes in the ERA Acute methodology.

5.1 ERA Acute with OSCAR as available per today

OSCAR

The current version of OSCAR is 6.6.1. OSCAR will be run in stochastic mode, including "Exposure Calculations".

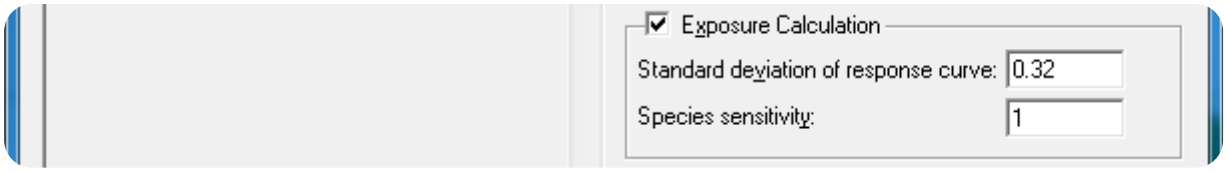


Figure 2 OSCAR dialogue for specification of Exposure Calculations

Standard deviation and sensitivity have to be specified for the organism of interest. Other than in the other compartments, where the oil spill model results are applied to a population *after* the model runs, the water column methodology will require the specification of the population's sensitivity *before* OSCAR is run. This has the disadvantage that only one organism group (sensitivity) can be defined which will have to represent the most sensitive species one wants to consider. For all other populations with organisms less sensitive the results will be somewhat conservative. The alternative is to apply a higher standard deviation of the response curve (slopes of the concentration-effect curves for several species are more gently inclined).

Recommended values are given in Table 2. However, these two parameters are used to define the response curve which relates the computed body burden to mortality. Since the maximum body burden itself is available as well, concentration-effect curves may be applied in the ERA Acute software as well, see below.

Table 2: Recommended values for exposure calculations with OSCAR6.6.1 (and before), switching between areas as required (e.g. winter in Northern Europe)

Cold Areas (Eastern Canada) (<5° C) (Q10 of 0.4 and 0.7 applied assuming standard toxicity testing between 13° and 20° C)		
VEC	Standard deviation of response curve	Species sensitivity
Phytoplankton	0.1	0.41 * 0.4 (=0.164)
Zooplankton	**0.32**	**1 * 0.7 (=0.7)**
Fish egg/larvae	0.32	1 * 0.4 (=0.4)
Fish (adult)	0.2	0.93 * 0.4 (=0.372)
Corals & Sponges (from zooplankton)	*0.32*	*1 * 0.4 (=0.4)*

Temperate Areas (Northern Europe and Argentina) (5° to 20° C) (assuming standard toxicity testing between 13° and 20° C)		
VEC	Standard deviation of response curve	Species sensitivity
Phytoplankton	0.1	0.41
Zooplankton	**0.32**	**1**
Fish egg/larvae	0.32	1
Fish (adult)	0.2	0.93
Corals & Sponges (from zooplankton)	*0.32*	*1*

Warm Areas (Mediterranean Sea, West Africa (Angola) and South Africa, Gulf of Mexico, South China Sea (Indonesia), Australia, Persian Gulf) (Q10 of 0.4 and 0.7 applied assuming standard toxicity testing between 13° and 20° C)		
VEC	Standard deviation of response curve	Species sensitivity
Phytoplankton	0.1	0.41 / 0.4 (=1.025)
Zooplankton	**0.32**	**1 / 0.7 (=1.43)**
Fish egg/larvae	0.32	1 / 0.4 (=2.5)
Fish (adult)	0.2	0.93 / 0.4 (=2,325)
Corals & Sponges (from zooplankton)	*0.32*	*1 / 0.4 (=2.5)*

Post-processing - Water Column / Concentration Grid

OSCAR computes results in the water column in the four dimensions time, depth, latitude and longitude (t, z, y, and x). Under stochastic simulations these dimensions are reduced from four to three to two dimensions for the final risk maps. This means that a lot of valuable data from the calculations is not available for the ERA Acute software, which is one reason that the exposure calculations in the water column should be executed under run time and not under post-processing.

The following file formats are described for the sake of completeness; they are not used directly for ERA Acute.

Stochastic Run Result (STT Format, OSCAR model engine)

The STT file contains for each simulation a list of all affected concentration grid cells. This file contains four-dimensional data, viz. the time dimension has been removed by calculating averages and maxima but there is the simulation as a "dimension" (simulation, z, y, and x). Averages are calculated by adding up the concentrations for a cell each time the cell contains oil. This sum is then divided by the number of hits[4]. Each entry contains

1. Dissolved concentration (average, i.e. for each cell the simulation sum divided by number of hits)
2. THC[5] concentration (average)
3. Mixing depth (average)
4. Arrival time (first time step this cell contained oil)
5. Exposure time (number of time steps times time step length this cell contained oil)
6. Last arrival time (last time step this cell contained oil)
7. Fraction killed (maximum)
8. Body residue (maximum)

Accumulated Stochastic Run Result (STAT Format)

This file contains three-dimensional data; the simulation "dimension" has been removed by applying maxima over all simulations (with exception to arrival time which is the minimum of all simulations) (z, y x).

The file contains

1. Maximum of STT values for the dissolved concentration (maximum of the averages)
2. Maximum of STT values for the THC concentration (maximum of the averages)
3. Maximum of STT values for the mixing depth
4. Minimum of STT values for the arrival time
5. Maximum of STT values for the exposure time
6. Maximum of STT values for the last arrival time
7. Maximum of STT values for the fraction killed
8. Maximum of STT values for the body residue

UTM grid export (ERA Acute software)

Also, the UTM export is generated from the STT file. This file is used in the ERA Acute software. Each line in the text file is a unique combination of scenario number, compartment (Surface, Shoreline, Water-

[4] A "hit" is defined as a time step in which a concentration grid cell contained oil during a simulation as oil might enter and leave a cell during the scope of a simulation.
[5] Note that "Total" in THC does not refer to all components in contrast to specific components but to dissolved fraction and droplet fraction together. Both fractions contain all 25 pseudo components.

column), and UTM grid cell id. A UTM grid cell comprises all water cells having their (horizontal) centre within that UTM cell, the water column cell quantities in a vertical column being reduced to a cell in a plane by applying maxima (with exception to arrival time where minimum is used).

For the water column this results in the following data:

1. Vertical maximum of all average dissolved concentrations
2. Vertical maximum of all average total hydrocarbon concentrations
3. Vertical maximum of all mixing depths
4. Vertical minimum of all arrival times
5. Vertical maximum of all exposure times
6. Vertical maximum of all last times
7. Vertical maximum of all maxima of fraction killed
8. Vertical maximum of all maxima of body residue

ERA Acute software

The ERA Acute software matches the exported UTM grid with resource data in GIS format and optionally performs additional calculations for the impact and risk respectively. Since the suggested approach here calculates the impact for the chosen sensitivity directly, these results ("fraction killed") may be used directly and further calculations within the ERA Acute software (ERA-SW) are not necessary.

1. OSCAR is run in stochastic mode.
2. Oil spill output and exposure are exported to UTM grid.
3. p_{let} = fraction killed for each cell can be used directly in the ERA-SW.
4. p_{let} * N can be calculated for each UTM cell with N from resource data.

Advantages and shortcomings of this approach

The advantage of using this approach is that there is not too much change to the methodology that was established in the ERA Acute project until now.

However, as mentioned above, it is only possible to calculate impact for one sensitivity-slope pair of values which is why one could argue that the effect-concentration calculations (see 2.5 and Table 2) should be performed within ERA-SW. It should be noted that only the vertical maximum of all maxima of all simulations is available from the UTM export, which would be conservative in the same way or even more than using one sensitivity value for all organisms.

The biggest shortcoming of the current methodology for the water column is the use of vertical maxima, which means that a maximum located in the upper water column might be used for risk assessment in the lower water column or vice versa. This means that organisms like corals and sponges might be "exposed" to concentrations in the upper water column leading to too conservative results when matching resource and oil drift data in ERA-SW.

Another disadvantage is that the implemented CBR model that is used for stochastic exposure calculations is a simplified version of the CBR model that is available for deterministic simulations (see QSAR report, Brönner, 2014). K_{OW} values are calculated from K_{OC} data and have a slight deviation from K_{OW} values reported elsewhere. The model is almost unused; activation of the exposure calculations is expected to increase the computational time (which might not be an issue, though). Due to this fact it might be deprecated in the future and / or replaced by other exposure models.

5.2 ERA Acute with OSCAR as suggested in phase II, 2012

In phase II of this project SINTEF suggested enhancements for OSCAR for better environmental risk assessment, among others to address the disadvantage with using the vertical maximum of the water column in the UTM export (Brönner, 2012). The proposal resulted in two files for the UTM grid export, one for the upper and one for the lower water column, where the depth for the two layers would be specified by the user.

OSCAR

OSCAR is run analogue to 5.1. The same recommendations for exposure calculations will apply here.

Post-processing - Water Column / Concentration Grid

The UTM export will produce two files for the water column, one for the upper and one for the lower water column. The vertical maxima will apply for the respective part of the water column only. Calculated risk for the water column is reported as before via "fraction killed" and "body residue".

ERA Acute software

The ERA-SW will match the UTM grids for the upper and lower water column with the respective resource data. The lower water column risk will be matches with resource data for corals and sponges, the upper water column data can either be combined with the lower water column data for resources like fish, while resources like zooplankton (copepods) might be matched against one of the files depending on season and their behaviour depending on that season (autumn, winter: lower water column, spring, summer: upper water column).

The same methodology applies as with using OSCAR in its current version: if the "fraction killed" data are used directly there will be no need for additional calculations in ERA-SW.

1. OSCAR is run in stochastic mode.
2. Oil spill output and exposure are exported to UTM grid.
3. p_{let} = fraction killed for each cell can be used directly in the ERA-SW.
4. p_{let} * N can be calculated for each UTM cell with N from resource data.

Advantages and shortcomings of this approach

While the biggest shortcoming of the first version (5.1) is addressed in this alternative the other shortcomings do still apply (simplified implementation, species independent, unused).

5.3 ERA Acute with OSCAR as suggested in phase III, 2015

Future versions of OSCAR will probably not employ stochastic simulations in their current form anymore. Standardisation of input and output data formats will allow for more sophisticated statistics that will be run as ensembles of deterministic runs. This means that the complete set of four (five) dimensional results will be available for statistic post-processing.

Per today simulations for stochastic runs are sampled by start time and rate/duration matrices only. The ease of modification of the input data for OSCAR simulations will allow for other sampling as well. In addition, uncertainty will be possible to quantify in the results.

OSCAR

OSCAR is run as a set ("ensemble") of scenarios. Each scenario is run in deterministic mode and will produce a full four (five) dimensional result set (simulation, time, z, y x).

Bio exposure modelling

The CBR model is currently under development and will be implemented as a particle based model for individuals with uptake and depuration kinetics as described in SINTEF report F26670 "QSAR in Environmental Risk Assessment" (Brönner et al., 2014**)** using the more advanced kinetics from OMEGA [20].

The particle based CBR model will accounts for organism behaviour (planktonic, stationary benthic, swimming) as well as spatial distribution at the beginning of each simulation. The pilot version of this model is planned to be implemented in spring next year.

A more detailed description of OSCAR in this suggested future version and the available output for all four compartments can be found in SINTEF report F26671 "Suggested OSCAR design for future application with ERA Acute" (in preparation), another deliverable within the scope of this project.

Post processing

Since the complete result set is available after simulation, statistics like average, floating average, distributions or maxima can be calculated from the output and be tailored to the requirements of ERA-SW. *It will be possible to generate the same results as before, i.e. body burden and fraction killed will be available results*.

In addition, data can be filtered by pseudo-component, by layer or whatever is necessary to match the organism data available. The main difference will be that it will be possible to run the exposure calculations for several organisms at the same time with different particles representing different species.

Since the exposure calculations are dependent on the time variable results from the oil drift model but not vice versa it is theoretically possible to calculate exposure for different species as post-processing. This approach would have the same disadvantage as the current version, i.e. the spatial distribution of the organisms over time is not accounted for.

Data can be exported as UTM grid as before or post-processed to directly common GIS compatible formats like shape files (Esri ArcGIS), KML (google earth), GML (OGC) or NetCDF (OGC).

ERA Acute software

ERA-SW will need to be adapted if the output format from OSCAR is changed.

The new bio exposure model can compute "fraction killed" and "body burden" as previous versions. Ideally these data will be transferred to ERA-SW as three-dimensional data set to avoid averaging or calculation of maxima over parts of the water column.

The data can then be matched with available resource data which would ideally be three dimensional as well. Population model like SINMOD calculate zooplankton like C. finmarchicus in 3D.

1. OSCAR is run in ensemble mode.
2. Oil spill output and exposure are post-processed to the required format.
3. p_{let} = fraction killed for each 3D cell can be used directly in the ERA-SW.
4. p_{let} * N can be calculated for each 3D cell with N from resource data. If resource data is not available in 3D, p_{let} will be accumulated to 2D (p_{let}') and matched with the 2D resource data via p_{let}' * N

A more detailed description of ERA-SW with this suggested future version and the available output for all four compartments can be found in SINTEF report F26671 "Suggested OSCAR design for future application with ERA Acute" (in preparation), another deliverable within the scope of this project.

6 Acknowledgements

This work was financed by Total and Statoil within the joint industry project ERA Acute – Environmental Risk Assessment for acute oil spills. SINTEF received valuable feedback from all project participants.

7 References

[1] Ø. Johansen, “EIF Acute 2005 - SINTEF contribution,” 2005.

[2] D. P. French, M. Reed, and K. Javko, “The CERCLA Type A Natural Resource Damage Assessment Model for Coastal and Marine Environments (NRDAM/CME) Technical Documentation Volume I - Part 2 M odel Description,” 1996.

[3] H. G. Johnsen, T. Nordtug, and H. Nilsen, “Calculation of PNEC values for the water column applied in environmental risk management for accidental discharges.,” 2005.

[4] H. Nilsen, H. Greiff Johnsen, T. Nordtug, and Ø. Johansen, “Threshold values and exposure to risk functions for oil components in the water column to be used for risk assessment of acute discharges (EIF Acute),” 2006.

[5] T. Nordtug, D. Altin, L. Einarson, and L. Ystanes, “Relevance of the Acartia tonsa acute toxicity test for classifying the toxicity of chemicals used in arctic regions.” The 18th International Oil Field Chemistry Symposium, Geilo, Norway, 2007.

[6] B. H. Hansen, D. Altin, S. F. Rørvik, and I. B. Øverjordet, “Comparative study on acute effects of water accommodated fractions of an artificially weathered crude oil on Calanus finmarchicus and Calanus glacialis (Crustacea: Copepoda),” *Sci. Total Environement*, vol. 409, pp. 704–709, 2011.

[7] D. French-McCay, “Development and application of an oil toxicity and exposure model, OilToxEx,” *Environ. Toxicol. Chem.*, 2002.

[8] D. P. French-McCay, “Development and application of an oil toxicity and exposure model, OilToxEx.,” *Environ. Toxicol. Chem.*, vol. 21, no. 10, pp. 2080–94, Oct. 2002.

[9] D. Mackay, “Correlation of bioconcentration factors.,” *Environ. Sci. Technol.*, vol. 16, no. 5, pp. 274–8, May 1982.

[10] L. McCarty and D. Mackay, “Enhancing ecotoxicological modeling and assessment. Body residues and modes of toxic action,” *Environ. Sci. Technol.*, 1993.

[11] M. G. D. Smit, A. J. Hendriks, J. H. M. Schobben, C. C. Karman, and H. P. Schobben, “The Variation in Slope of Concentration-Effect Relationships,” *Ecotoxicol. Environ. Saf.*, vol. 48, pp. 43–50, 2001.

[12] J. P. Incardona, C. A. Vines, B. F. Anulacion, D. H. Baldwin, H. L. Day, B. L. French, J. S. Labenia, T. L. Linbo, M. S. Myers, O. P. Olson, C. A. Sloan, S. Sol, F. J. Griffin, K. Menard, S. G. Morgan, J. E. West, T. K. Collier, G. M. Ylitalo, G. N. Cherr, and N. L. Scholz, “PNAS Plus: Unexpectedly high mortality in Pacific herring embryos exposed to the 2007 Cosco Busan oil spill in San Francisco Bay,” *Proceedings of the National Academy of Sciences*, vol. 109, no. 2. pp. E51–E58, 2012.

[13] J. P. Incardona, T. L. Swarts, R. C. Edmunds, T. L. Linbo, A. Aquilina-Beck, C. A. Sloan, L. D. Gardner, B. A. Block, and N. L. Scholz, “Exxon Valdez to Deepwater Horizon: Comparable toxicity of both crude oils to fish early life stages,” *Aquat. Toxicol.*, vol. 142–143, pp. 303–316, 2013.

[14] T. Nordtug, A. J. Olsen, D. Altin, I. Overrein, W. Storøy, B. H. Hansen, and F. De Laender, "Oil droplets do not affect assimilation and survival probability of first feeding larvae of North-East Arctic cod.," *Sci. Total Environ.*, vol. 412–413, pp. 148–53, Dec. 2011.

[15] NOAA, "How does an oil spill affect coral reefs?" [Online]. Available: http://coralreef.noaa.gov/aboutcorals/facts/coral_oilspill.html).

[16] J. B. C. Jackson, J. D. Cubit, B. D. Keller, V. Batista, K. Burns, H. M. Caffey, R. L. Caldwell, S. D. Garrity, C. D. Getter, C. Gonzales, H. M. Guzman, K. W. Kaufman, A. H. Knap, S. C. Levings, M. K. Marshall, R. Steger, R. C. Thompson, and E. Weil, "Ecological effects of a major oil spill on Panamanian coastal marine communities: Science, v. 243, p. 37-44.," *Science (80-.).*, vol. 243, no. 4887, pp. 37–44, 1989.

[17] C. R. Fisher, P.-Y. Hsing, C. L. Kaiser, D. R. Yoerger, H. H. Roberts, W. W. Shedd, E. E. Cordes, T. M. Shank, S. P. Berlet, M. G. Saunders, E. A. Larcom, and J. M. Brooks, "Footprint of Deepwater Horizon blowout impact to deep-water coral communities," *Proc. Natl. Acad. Sci.*, vol. 111, no. 32, pp. 11744–11749, Jul. 2014.

[18] J. M. Rotchell and G. K. Ostrander, "Molecular Toxicology of Corals: A Review," *Journal of Toxicology and Environmental Health, Part B*, vol. 14, no. 8. pp. 571–592, 2011.

[19] E. Cebrian and M. J. Uriz, "Contrasting effects of heavy metals and hydrocarbons on larval settlement and juvenile survival in sponges," *Aquat. Toxicol.*, vol. 81, no. 2, pp. 137–143, 2007.

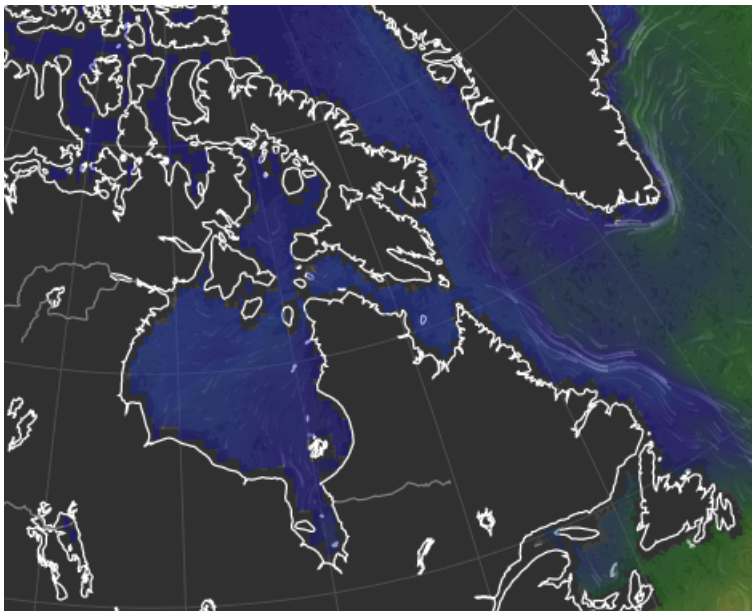
[20] L. De Hoop, M. a J. Huijbregts, A. M. Schipper, K. Veltman, F. De Laender, K. P. J. Viaene, C. Klok, a J. Hendriks, L. De Hoop, and F. De, "Modelling bioaccumulation of oil constituents in aquatic species.," *Mar. Pollut. Bull.*, vol. 76, no. 1–2, pp. 178–86, Nov. 2013.

[21] A. J. Hendriks, A. van der Linde, G. Cornelissen, and D. T. Sijm, "The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight.," *Environ. Toxicol. Chem.*, vol. 20, no. 7, pp. 1399–420, Jul. 2001.

[22] D. P. French-McCay, "Oil spill impact modelling," *Environ. Toxicol. Chem.*, vol. 23, no. 10, 2003.

A Sea Surface temperature for the geographic locations in ERA Acute as basis for categories

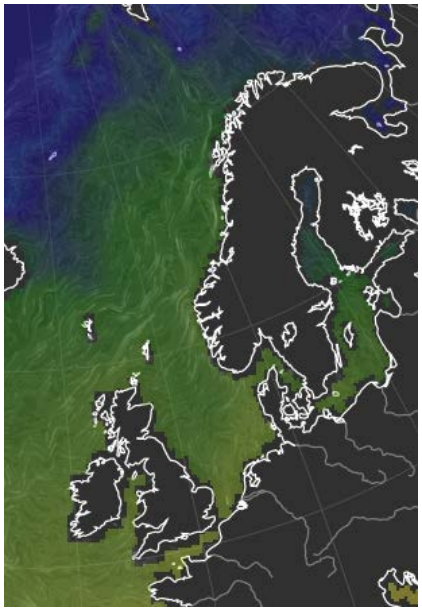
East Coast Canada:



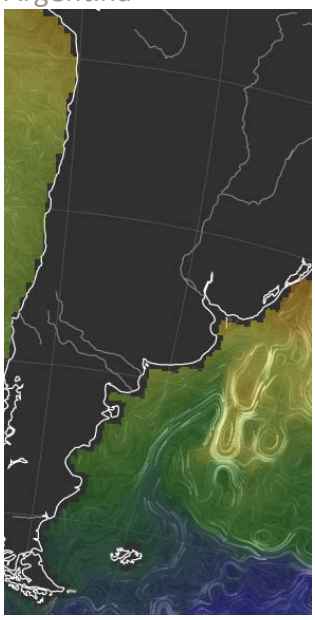
(ocean surface temperatures from
http://earth.nullschool.net/#current/ocean/surface/currents/overlay=sea_surface_temp/orthographic)

blue: < 5°C, green to yellow: 5-20°C, orange to red: >20°C

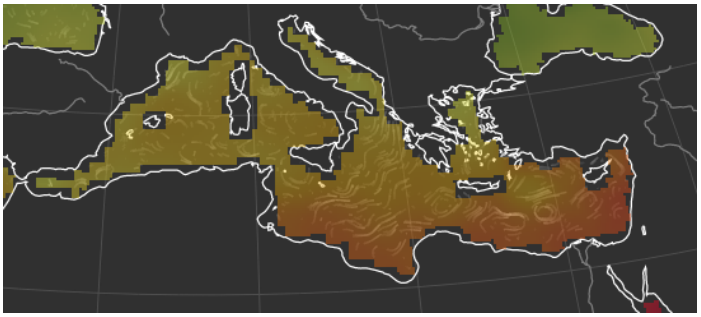
Northern Europe



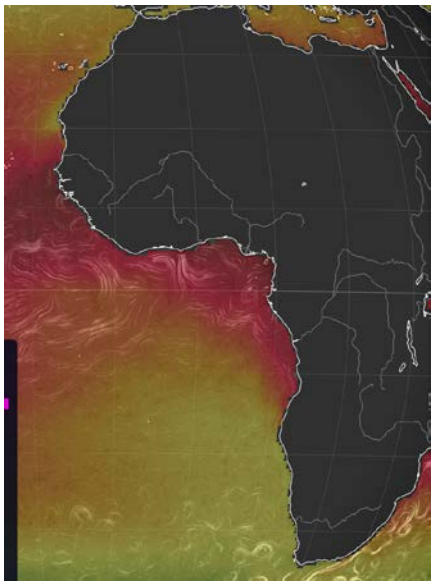
Argentina

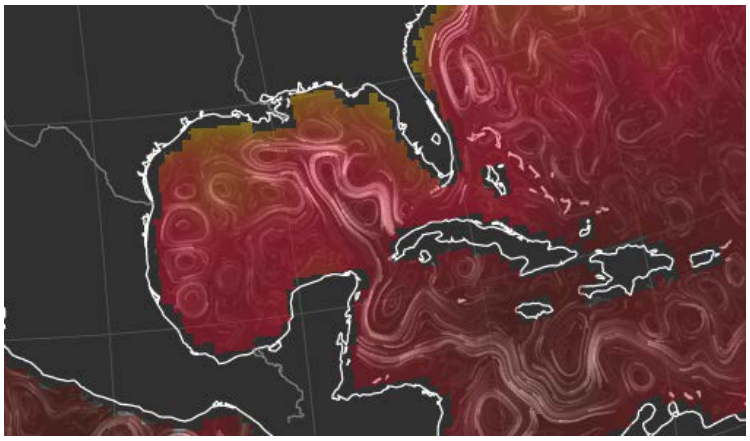


Mediterranean Sea

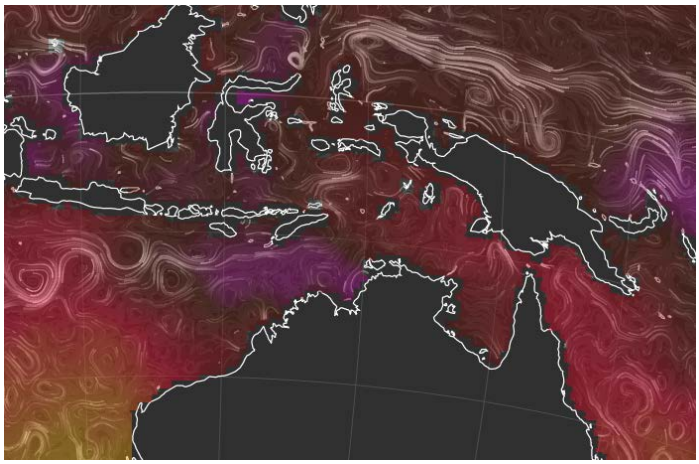


West Africa (Angola) and South Africa, Gulf of Mexico

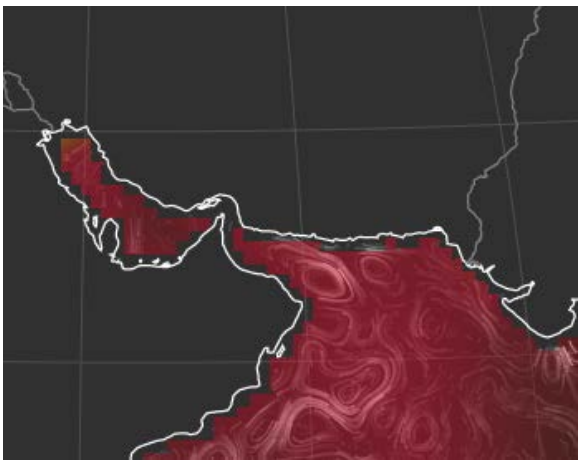




South China Sea (Indonesia), Australia



Persian Gulf



Technology for a better society

www.sintef.no