



Toxicity data for modeling impacts of oil components in an Arctic ecosystem



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ABSTRACT

Ecological impact assessment modeling systems are valuable support tools for managing impacts from commercial activities on marine habitats and species. The inclusion of toxic effects modeling in these systems is predicated on the availability and quality of ecotoxicology data. Here we report on a data gathering exercise to obtain toxic effects data on oil compounds for a selection of cold-water marine species of fish and plankton associated with the Barents Sea ecosystem. Effects data were collated from historical and contemporary literature resources for the endpoints mortality, development, growth, bioaccumulation and reproduction. Evaluating the utility and applicability of these data for modeling, we find that data coverage is limited to a sub-set of the required endpoints. There is a need for new experimental studies for zooplankton focused on the endpoints development and bioaccumulation and for larvae and juvenile fish focused on growth and development.

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1. Introduction

The Barents Sea supports a productive and diverse marine ecosystem of major significance for the wider Arctic. It includes a rich benthic fauna including cold-water coral reefs and sponge communities coupled closely with a productive pelagic marine ecosystem of diverse fisheries and marine mammals (Wassmann et al., 2006a). The region supports major fish harvesting activities, particularly for cod, haddock and capelin, and these activities are

the mainstay of coastal communities from Norway to Russia (Olsen et al., 2010). The region is also of major commercial importance for industries that include tourism, shipping, and the extraction of energy resources (Anon, 2003, 2004a,b). The ecosystem approach to management underpins the response to resource extraction in the Arctic with the objective of minimizing impacts, acting within the constraints of the ecosystem and ensuring that environmental quality is maintained. The Barents Sea in particular is managed by the Plan for the Integrated Management of the Marine Environment of the Barents Sea and the Sea Areas off the Lofoten (hereafter IMP) (Anon, 2006, 2011). The IMP was designed as an approach to maintain ecosystem integrity and to achieve sustainable use of ecosystem goods and services. The IMP is to be used to identify and take action on influences which are critical to the health of the marine ecosystem (Anon, 2006).

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While the IMP acknowledges the generally good scientific knowledge for the Barents Sea, it also identifies the need for more knowledge of the ecosystem response to the combined impacts of multiple pressures from different sectors (e.g., oil exploration, fishing and shipping). Further effort is needed to quantify both the realized and potential impacts of commercial activities on habitats and species distributions. To help identify and quantify some of these potential impacts, a new modeling system, based on the ecosystem approach, is being developed for the Barents Sea. This system consists of a suite of existing ecological and toxicological models linked into a single modeling framework (Carroll and Smit, 2011). The system is designed to perform simulations of fish harvesting dynamics and the combined impacts on the populations of key commercial fish species of oil discharges and fisheries biomass extraction.

Briefly, the system includes three ecological models, one to simulate ecological processes up through zooplankton (Wassmann et al., 2006b), a second to simulate the behavior and distribution of fish from larval to juvenile stages (Vikebø et al., 2007) and a third to simulate the behavior and distribution of adult fish (Begley and Howell, 2004). These ecological models are further linked to a fate and transport model that predicts biological exposure levels for individual organisms (Reed et al., 2001). Toxic effects to individual organisms are evaluated for chemical uptake from sea water (water soluble fraction of chemical compounds) and/or food ingestion (De Laender et al., 2010a). At present, the model does not address chemical exposure via oil droplets. Oil droplets form when oil disperses, either naturally by wave action or after application of chemical dispersants. Species are exposed to oil droplets by adhesion to body surfaces or by dietary uptake. Although research has begun producing insight into the effect of oil droplets on marine organisms, at the present time, this area is not sufficiently mature to incorporate into ecological impact assessments (Hansen et al., 2009, 2012; Nordtug et al., 2011).

A key challenge for modeling is to identify and obtain data of sufficient quality that is appropriate for quantifying the potential toxic effects of petroleum discharges (De Laender et al., 2010b). In recent years, there have been a number of efforts to gather and assess existing ecotoxicology data for Arctic species mainly to compare the relative sensitivity of temperate and Arctic organisms to toxic exposures (Olsen et al., 2011; De Hoop et al., 2011). The present paper takes a further step by collecting and extracting data from historical and contemporary literature sources and assembling these into a common database. The present study gathers toxicity studies on a selection of species with habitats extending into the northern areas. These studies include toxicity data on oil substances from several oil groups: benzenes (toluene, xylene, ethyl benzenes), naphthalenes (bicyclic aromatic hydrocarbons), polycyclic aromatic hydrocarbons (PAHs), phenols and C6, C7 saturates. Our specific aim is to identify studies of sufficient quality to meet the needs of ecotoxicology modeling. To achieve this aim, we have organized the obtained toxicity data for implementation into the integrated ecosystem based modeling system described herein. This modeling system provides a valuable test of the utility and applicability of existing data resources for ecotoxicology modeling.

We briefly review the ecotoxicology data requirements for the selected ecotoxicology algorithms and fate/effects model in the ecosystem based modeling system. We then present the process and results of our literature search and data gathering and assessment exercise. We further evaluate the value and limitations of data gathered from existing literature sources and finally, we identify the most critical areas where additional data are likely to lead to improved effects modeling. We believe this new database is of general value for the ecotoxicology community, and that our experiences in organizing these data for use in integrated

ecosystem based modeling provides useful insights for others engaged in similar or related modeling activities.

2. Materials and methods

2.1. Ecotoxicology algorithms

Ecotoxicology algorithms relate an exposure concentration to an effect concentration or alternatively, a biological threshold above which effects are to be expected (De Laender et al., 2010b). Two complimentary ecotoxicology models are incorporated into the Barents Sea ecosystem model. These models quantify changes in rates of survival, growth, reproduction etc., linked to chemical exposures. The data needs connected to the application of these algorithms were used to set priorities for the literature search.

The first algorithm uses a mechanistic bioaccumulation approach to predict toxicant effects on survival, and reproduction (Hendriks et al., 2001, 2005a,b). Internal concentrations (body burden) in biota are estimated based on uptake and elimination rate constants and the exposure concentration of the chemical. Based on classical fugacity theory, the uptake and elimination kinetics are a function of species characteristics (body mass, lipid content and trophic level of the species) and the chemical property octanol-water partition coefficient (K_{ow}) (Hendriks et al., 2001; Hendriks and Heikens, 2001). The estimated body burden and experimental single species toxicity data are used to predict impacts of oil components on the population level. For example, survival and reproduction rates are given as functions of internal concentrations exceeding critical body burdens (CBB) (Hendriks et al., 2005a,b). The algorithm has been calibrated using thousands of accumulation and toxicity values from laboratory experiments with aquatic species. Similar approaches have been used in dynamic ecosystem models to assess variations in bioaccumulation patterns as a result of varying food web relations (De Laender et al., 2010a) and effects on population sizes in ecosystems (De Laender et al., 2008). In the present context, the prediction of effects using this algorithm requires toxicity and bioaccumulation data together with the physicochemical properties of the selected substances.

The second algorithm uses a mechanistic approach to predict toxicant induced changes in individual growth, development, and survival. Mechanistic rules describe the uptake and use of energy by the organism and the consequences for physiological organization throughout the life cycle of the organism (Kooijman, 2000). Uptake and elimination kinetics of a toxicant are a function of the chemical characteristics of a toxicant and body size and lipid content of an organism. When the internal toxicant concentration is above a no effect concentration (NEC) effects evolve as a consequence of disruptions in the energy balance. In the present context, the prediction of effects requires toxicity data for oil components on body size, development and/or survival for the selected species and substances (Jager and Zimmer, 2012; Klok et al., 2012; Kooijman, 2010; Klok, 2007) and the physicochemical properties of these oil components.

Both algorithms have been included in the Barents Sea ecosystem modeling system as they provide complimentary approaches to the assessment of effects of petroleum hydrocarbons on marine organisms. The fugacity based approach (algorithm 1), which is based on the intrinsic properties of chemicals and species characteristics, is useful when the availability of ecotoxicology data is limited. The energy balance approach (algorithm 2) links the toxicity of individual oil components to measured effects derived through experimentation. Both algorithms can be used to determine effect concentrations for all organisms in the core food web complex: phytoplankton-zooplankton-fish, however, at present we only apply algorithm 1 on plankton and algorithm 2 on fish larvae.

At a later stage we intend to apply both algorithms to all organism groups targeted in this modeling system.

2.2. Target organisms

In modeling sub-Arctic – Arctic ecosystems, effect concentrations must be assembled for the core food web complex: phytoplankton-zooplankton-fish. For the present study in which the Barents Sea is the region of interest, the following species were targeted.

2.2.1. Phytoplankton

We focus on cold-water primary producer species for which the impact of petroleum compounds on population growth are available. In northern waters during spring, phytoplankton have a short and intense growth phase (bloom). The resulting energy production is the major pathway whereby energy is transferred from the base of the food web throughout the Arctic marine pelagic system (Wassmann et al., 2006a).

2.2.2. Zooplankton

For zooplankton, studies that contained information on the genus *Calanus* were targeted: *Calanus finmarchicus*, the smallest of the northern residing *Calanus* species, together with *Calanus glacialis* and *Calanus hyperboreus*. The larger and more lipid-rich species *C. glacialis* and *C. hyperboreus*, reside farther north and in deeper waters (Falk-Petersen et al., 2009). These predominantly herbivorous copepods are an important secondary link in the energy transfer to higher trophic level species of northern marine ecosystems (Søreide et al., 2006, 2008). In particular, the lipid stores in these copepods serve as one of the main energy sources for larval and juvenile fish (Falk-Petersen et al., 2007) and hence are critical in sustaining the fisheries connected to the Barents Sea.

2.2.3. Fish

Studies were identified addressing cod (*Gadus morhua*), capelin (*Mallotus villosus*) and Atlantic herring (*Clupea harengus*) as these are the primary fish species in the Barents Sea and hence are also the key species being addressed through ecosystem modeling. In addition, the Pacific herring (*Clupea pallasii*) was included to supplement the amount of data extracted from literature for the Atlantic herring. The stocks of these four species form the basis of large fisheries in the region as well as being vitally important as prey and predators (Runnström, 1936; Bergstad et al., 1987). Juvenile and adult fish migrate throughout the Barents Sea to feed, but return to the coastline to spawn between January and May (Olsen et al., 2010).

2.3. Data extraction from literature resources

The main purpose of this investigation is to identify ecotoxicology studies which may be useful for modeling the effects of petroleum hydrocarbons on our selection of marine organisms. A key requirement for modeling is to be able to simulate both direct and delayed biological effects. For this purpose, the following endpoints were prioritized in this literature search: mortality, growth, reproduction, development, and bioaccumulation (i.e., bioconcentration factors, uptake and elimination rates) (Fig. 1). Literature sources containing toxicity data for the chosen endpoints were selected from the US Environmental Protection Agency (EPA) ECOTOX Release 4.0 database. The database provides references to studies with information on single chemical toxicity for aquatic and terrestrial life (EPA website, <http://cfpub.epa.gov/ecotox/>). Search routines were performed on the ECOTOX database to identify studies providing toxicity endpoints for species with habitats

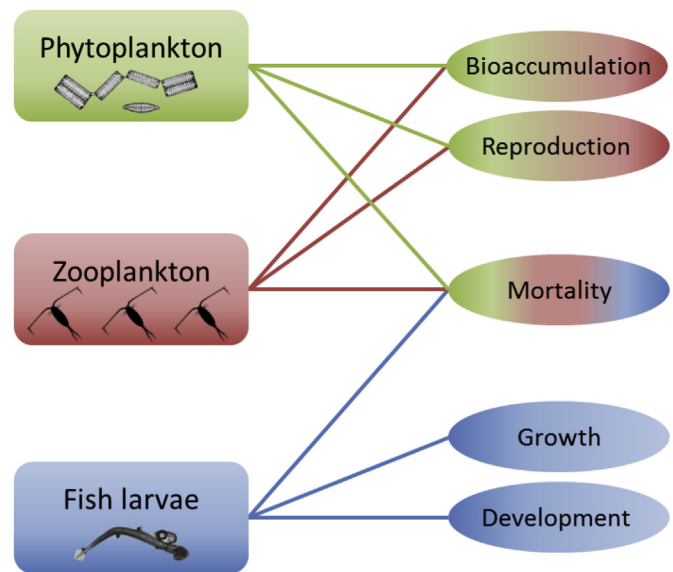


Fig. 1. Effects endpoints for the main organism groups (phytoplankton-zooplankton-fish) addressed in an ecosystem model for the Barents Sea.

extending into cold-water (sub-Arctic to Arctic) ecosystems. In some cases, studies containing the appropriate data (species and endpoints) were either sparse or not found in the ECOTOX database. In these cases, relevant proxy data on related species from temperate waters were collected (Table 2).

For each data record obtained from the database, the following supporting information was also documented: life stage, exposure duration, number of measurements, number of replicates, toxic dose, concentration units, concentration type, chemical description, experimental type, exposure conditions, feeding conditions, temperature, container characteristics, publication reference, and additional experimental notes. For all studies, we noted whether nominal or measured concentrations were reported. We also identified studies where toxic concentrations were at the maximum tested concentration, which oftentimes represented the functional solubility limit for the test. For further supporting details, such as terminology definitions and more detailed explanations of the supporting information, the reader is referred to the EPA website.

A few experiments have been performed in recent years that increase the availability of data on key cold-water living species (Grenvald et al., 2012; Hjorth and Nielsen, 2011; Jensen et al., 2012; Jensen and Carroll, 2010). Where relevant, the data gathered from the ECOTOX database were augmented with data from recent investigations. As was done for the literature resources obtained from the ECOTOX database (Supplemental information), all available supporting information was extracted from the additional literature sources. The endpoint values, together with the previously listed set of supporting information on experimental conditions were organized by species and assembled into three spreadsheets (Tables S1–S3, supplemental information). Information on the abbreviations used in the spreadsheets is provided separately (Table S4, supplemental information). Nearly all the data from the ECOTOX database and the few additional literature resources gathered through this investigation are from studies reported in peer-reviewed publications (Table S5 supplemental information). Therefore no additional data quality screening was performed as the gathered data are considered to meet the accepted scientific standards for peer-reviewed publications. An on-line version of the database is available at <http://akvaplan.niva.no/symbioses/>.

Table 1
The classification system for hydrocarbon compounds (pseudocomponent groups) used by the fate and effects model.

Group no.	Identification	Compounds
1	C1–C4 saturates	C1–C4 gases
2	C5-saturates	n-Pentane, iso-pentane, cyclopentane
3	C6-saturates	n-Hexane, 2-methylpentane, 3-methylpentane, methylcyclopentane, cyclohexane
4	C7-saturates	n-Heptane, 3-methylhexane, 2,3-dimethylpentane, methylcyclohexane
5	C8-saturates	n-Octane
6	C9-saturates	n-Nonane
7	Benzene	Benzene
8	C1-benzenes	Toluene
9	C2-benzenes	Ethylbenzene; o-,m-,p-xylene
10	C3-benzenes	Propylbenzene, 1-methyl-3-ethylbenzene, 1-methyl-4-ethylbenzene, 1-methyl-2-ethylbenzene, 1,3,5-trimethylbenzene, 1,2,4-trimethylbenzene, 1,2,3-trimethylbenzene
11	C4/C5-benzenes	n-Butylbenzene, 1,2,4,5-tetramethylbenzene, n-pentylbenzene
12	C10-sat (GC/FID)	C10 saturates
13	C11–C12	C11–C12 total saturates + aromates
14	C13–C14	C13–C14 total saturates + aromates
15	C15–C16	C15–C16 total saturates + aromates
16	C17–C18	C17–C18 total saturates + aromates
17	C19–C20	C19–C20 total saturates + aromates
18	C21–C25	C21–C25 total saturates + aromates
19	C26–C36	C26–C36 total saturates + aromates
20	Naphthalenes 1	C0- to C1-naphthalenes
21	Naphthalenes 2	C2- to C3-naphthalenes
22	PAH-1	C4-naphthalenes, biphenyl, acenaphthylene, acenaphthene, dibenzofurane, C0- to C1-fluorenes, C0- to C1-phenanthrenes/anthracenes, C0- to C1-dibenzothiophenes
23	PAH-2	C2- to C3-fluorenes, C2- to C4-phenanthrenes/anthracenes, C2- to C4-dibenzothiophenes, fluoranthene, pyrene, C1-to C3-fluoranthenes/pyrenes, benz(a)anthracene, C0- to C4-crysenes, benzo(b,k)fluoranthene, benzo(e,a)pyrene, perylene, dibenzo(a,h)anthracene, benzo(g,h,i)perylene, indeno(1,2,3-c,d)pyrene
24	Phenols C0–C4	C0- to C4-phenols
25	Polars	C10- to C36-polars
26	TEOC	C10- to C36-total extractable organic compounds

2.4. Data requirements for transport modeling

In the present context of ecosystem modeling, an additional challenge is that the parameters and inputs of the ecotoxicology algorithms must correspond to the output provided by transport and fate models. In the case of modeling petroleum discharges, the chemical complexity of petroleum products has led to development of transport and fate models that simulate the distribution in the environment of chemical groups rather than individual compounds. In this approach, compounds having similar properties (e.g., similar structure and size) are assembled in a group, known as a pseudocomponent group. Each pseudocomponent group of oil components is associated with a given set of physical, chemical and toxicological properties (e.g., density, molar weight, solubility, $\log K_{ow}$ and LC50). The approach assumes that hydrocarbons in a given group behave similarly, i.e., have similar distribution and fate in the environment.

The data assembled from literature sources in the current study were sorted into 25 pseudocomponent groups (Table 1). Further description of these pseudocomponent groups is presented in Reed et al. (2001). As a result of this grouping procedure, literature sources describing studies of mixed compounds such as crude oil and chemical dispersants are not usable because the composition of these mixtures is uncertain. Some of the single oil compounds under investigation are also not included in the pseudocomponent classification system (see 'other oil compounds' presented in Table 2). Studies supplying endpoints on chlorinated compounds were included as these are useful for establishing relative toxicity and endpoints. Nonpolar chlorinated organic compounds may have a mode of action that is similar to hydrocarbons (e.g., narcosis).

Toxicity data for these chemicals could be used to support QSAR and read across with the target lipid model (TLM) (Di Toro et al., 2000; McGrath et al., 2004; Redman et al., 2007).

3. Results

The search for information on the selected species groups, phytoplankton, zooplankton and fish, yielded 100 literature sources spanning 72 different oil compounds. They include the complete collection of species specific toxicity endpoints for both single (oil and chlorinated compounds) and mixed compounds (crude oil and dispersants). Of the 519 assembled endpoint values extracted from the assimilated literature (Table 2), 58% are for phytoplankton, 6% are for zooplankton, and 36% are for fish. The majority of endpoint values were extracted from peer reviewed sources. Of these, 319 (61.5%) are derived from studies on single oil compounds. Studies on complex petroleum substances (e.g., crude oil) constitute 109 (21%) of the endpoint values. Dispersants represent 41 (7.7%) of the endpoint values while chlorinated compounds represent an additional 50 (9.4%). Twenty-one of the assimilated 319 endpoint values for oil compounds did not classify into the pseudocomponent groups used in the fate and transport model (Table 2). Hence, of the total number of endpoint values assimilated from literature sources, 298 (57%) were appropriate to be evaluated further for use in modeling. Among these endpoint values, the majority are derived from toxicity tests performed on either fish (25%) or phytoplankton (65%). Among the target endpoints, mortality and growth were the most abundant. For the latter, this refers to population growth for phytoplankton (Table 3).

Table 2

Distribution of endpoint values among species and compound groups studied in the present investigation. Oil compounds/other oil compounds refer to those that Do/Do not map to the list of pseudocomponent groups presented in Table 1.

Species group species names	Type of compounds	Nr. toxicity data recorded
Fish		
<i>Gadus morhua</i>	Oil compounds	67
	Other oil compounds	8
	Chlorinated compounds	0
	Dispersants	38
	Mixed oil compounds	28
<i>Clupea harengus</i>	Oil compounds	2
	Other oil compounds	0
	Chlorinated compounds	0
	Dispersants	3
<i>Clupea pallasii</i>	Mixed oil compounds	11
	Oil compounds	17
	Other oil compounds	0
	Chlorinated compounds	0
<i>Mallotus villosus</i>	Dispersants	0
	Mixed oil compounds	17
	Oil compounds	2
	Other oil compounds	0
Zooplankton		
<i>Calanus finmarchicus</i>	Oil compounds	25
	Other oil compounds	0
	Chlorinated compounds	0
	Dispersants	0
	Mixed oil compounds	0
<i>Calanus glacialis</i>	Oil compounds	5
	Other oil compounds	0
	Chlorinated compounds	0
	Dispersants	0
	Mixed oil compounds	1
<i>Calanus hyperboreus</i>	Oil compounds	0
	Other oil compounds	0
	Chlorinated compounds	0
	Dispersants	0
	Mixed oil compounds	1
Phytoplankton		
Arctic species	Oil compounds	0
	Other oil compounds	0
	Chlorinated compounds	0
	Dispersants	0
	Mixed oil compounds	15
Temperate species	Oil compounds	193
	Other oil compounds	13
	Chlorinated compounds	50
	Dispersants	0
	Mixed oil compounds	33
		530

3.1. Results by species group

3.1.1. Phytoplankton

Only fifteen studies on oil components for Arctic marine phytoplankton were located in the ECOTOX database and these reported on exposures to crude oil. Because the ecosystem model does not address crude oil at the present time we included studies

Table 3

Number of values for each endpoint by organism group.

Number of total toxicity data (value records) for each endpoint			
Endpoints	Fish	Zooplankton	Phytoplankton
Development	9		
Mortality	50	26	
Bioaccumulation	10		2
Growth	6	2	191
Reproduction	4	2	

performed on temperate phytoplankton species. For temperate phytoplankton species, benzene compounds were the most studied (158 endpoint values). In all studies, the selected endpoint was population growth. Among these endpoint values, the most studied pseudocomponent group was group 9 (C2 benzenes; 33%); followed by the pseudocomponent groups (7, 8) which accounted for an additional 22% of the obtained endpoint values. Benzenes are volatile aromatic compounds characterized by high vapor pressures, low-to-medium water solubility, and low molecular weights. These low molecular compounds are typical components in petroleum products (European Environment Agency, 2010). There were also 62 studies on the less soluble and heavier compounds associated with groups 22 (PAH-1) and 23 (Pyrene; Table 1, Fig. 2).

3.1.2. Zooplankton

Among species of the genus *Calanus*, the majority of available data, 25 endpoint values were extracted from studies performed on *C. finmarchicus*. These data map to the following pseudocomponent groups: 3 (C6 saturates), 4 (C7 saturates), 7 (benzene), 8 (C1 benzene), 9 (C2 benzene), 10 (C3 benzene), and 23 (pyrene), and (Table 1, Fig. 2). In these studies the endpoints mortality, individual growth and reproduction were addressed, with no studies addressing bioaccumulation. Mortality was the most studied endpoint (Table 3, Fig. 2). The data obtained for *C. glacialis* for the endpoints mortality and reproduction mapped to pseudocomponent groups 23 (pyrene) and 9 (C2 benzene; Table 3, Fig. 2). A substantial amount of these data was retrieved for water soluble fractions (WSF) of different oils and weathering degrees (Hansen et al., 2013a,b, 2011). As no studies reported on bioaccumulation, there are no pseudocomponent groups which include the entire suite of selected endpoints. No studies on *C. hyperboreus* relate to the defined pseudocomponent groups; while one study was performed on crude oil.

For the largest species within the genus *Calanus*, *C. glacialis*, there were 6 endpoints available (Table 2). Three of these studies address pseudocomponent group 9 (C2 benzene) and an additional 3 address group 23 (pyrene; Fig. 2). For this species, mortality was again the most commonly reported endpoint; reproduction and individual growth were also reported.

3.1.3. Fish

For Cod (*G. morhua*), 130 endpoint values were obtained from the collected literature sources. Of these, only 54 were categorized among pseudocomponent groups. The most studied pseudocomponent group was group 21 (naphthalenes 2) (40.7% of the studies), followed by groups 20 (naphthalenes 1) (20.3%), 24 (C0–C4 phenols), 9 (C2 benzene), 22 (PAH-1) and 23 (C2–C4 pyrene) (Fig. 2). Group 24 (C0–C4 phenols), was the pseudocomponent group with the most data coverage while mortality was the most studied endpoint (Table 3, Fig. 2). In addition to mortality, endpoint values are available for development, and bioaccumulation.

For Capelin (*M. villosus*), only three endpoint values were obtained, both on pseudocomponent group 20 (naphthalenes 1; Table 2, Fig. 2). The associated endpoints were mortality and development. Only two endpoint values are available for Atlantic herring (*C. harengus*): one for group 22 (PAH-1) and one for group 23 (C2–C4 pyrene; Fig. 2). Both are for bioaccumulation; no endpoint values were identified for individual growth, mortality, development, or reproduction. To supplement the limited amount of literature for this species, literature sources on the species Pacific herring (*C. pallasii*) are included. For this species, we identified 17 endpoint values. Of these, 94% were on pseudocomponent group 7 (benzene) and 6% on group 8 (C1 benzene, toluene). For this species toxicity data are available for all endpoints except development. Mortality is the most frequently reported endpoint. Pseudocomponent group 7 (benzene)

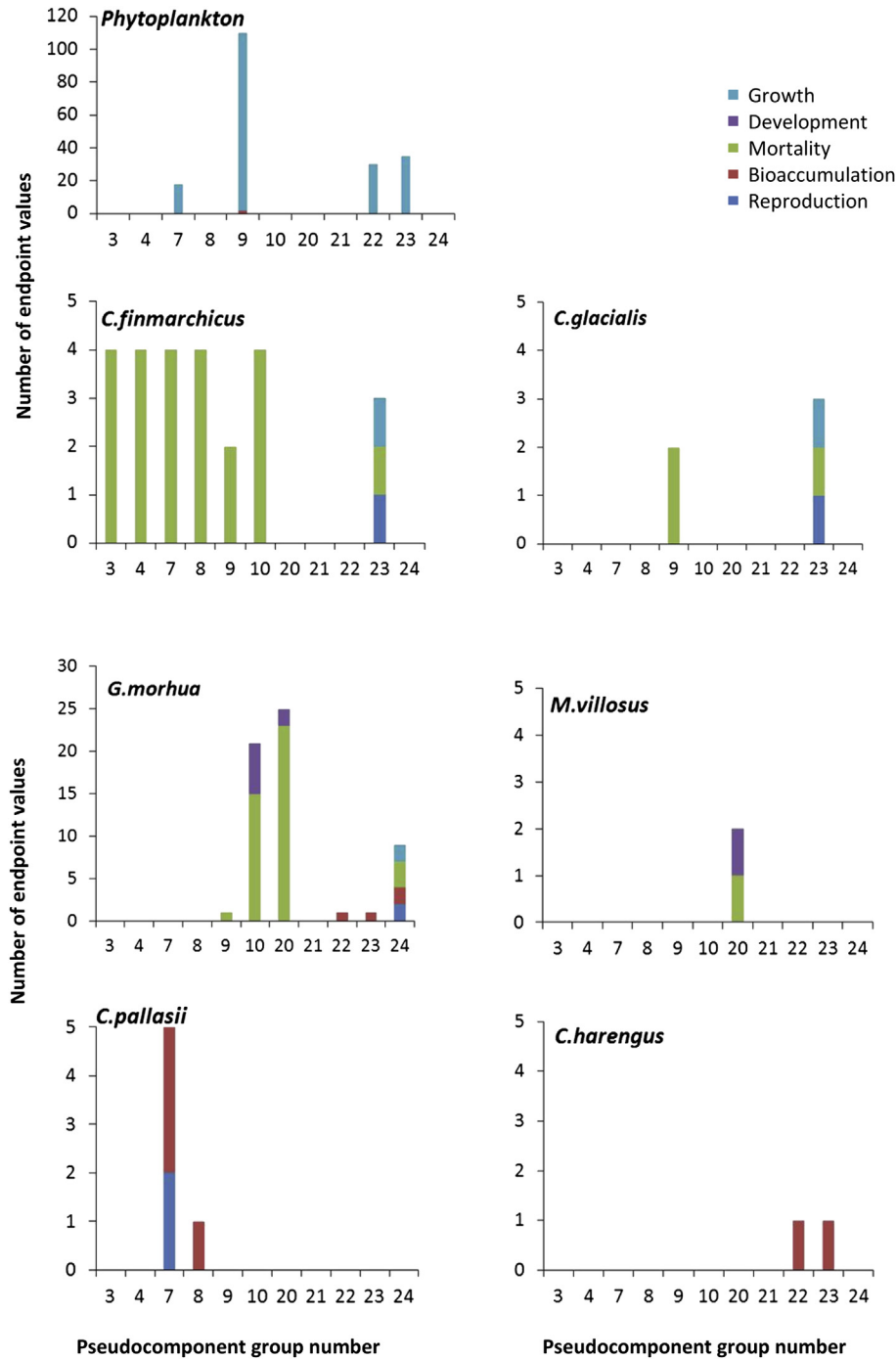


Fig. 2. Number of studies reporting on endpoints distributed among pseudocomponent groups for the selected species of phytoplankton, zooplankton, and fish. The zooplankton species, *C. hyperboreus* is not shown as no studies were available with the relevant data.

included endpoint values for mortality, bioaccumulation, growth, and reproduction (Fig. 2). However, it should be noted that the modeling system for the Barents Sea doesn't currently include fish reproduction. These data were gathered as part of the data synthesis exercise and to make them available for future model development.

4. Discussion

This study synthesized available literature on the effects of petroleum related discharges on selected marine species (plankton and fish) with habitats extending into cold-water ecosystems.

While previous studies have examined the general availability of ecotoxicology data for cold-water, and especially, Arctic species (Chapman and Riddle, 2005; Olsen et al., 2011; De Hoop et al., 2011; Olsen et al., 2007), the present study focuses specifically on the utility of existing ecotoxicology data for modeling purposes. Modeling is today an invaluable tool to extrapolate from individual to population level impacts of toxicants on marine species and, in particular, is essential for ecosystem-based approaches to impact assessment. The data in the present study are to be used by ecotoxicology algorithms included in an ecosystem-based modeling system that combines ecological and toxicological understanding

into a single modeling framework. Through this data synthesis and examination exercise, we have determined both the completeness and applicability of existing toxicity data for modeling effects related to oil discharges by the petroleum industry. We believe this study is of general value to the ecotoxicology community in two ways: first, the assembled data are of use to others engaged in the development and/or application of ecotoxicology models. Second, the results indicate where further ecotoxicology research will be of greatest value for both increasing general knowledge on cold-water ecotoxicology and for designing new ecotoxicology studies for modeling applications.

4.1. Data availability

Our literature assessment indicates that there are data available on oil components for most of the selected species and toxicity endpoints identified as priorities for the selected ecotoxicology algorithms. Of the 100 literature sources used in this study, 93 were listed in the ECOTOX database while the remaining were derived from publications in preparation/review, reports, and recently published studies (Ingvarsdottir et al., 2012; Hjorth and Nielsen, 2011). Our evaluation indicates that the availability of toxicity data is limited for our selected first-priority species of fish, zooplankton, and phytoplankton. This finding supports what has been reported previously on the generally limited availability of ecotoxicology data for cold-water, and especially, Arctic species (Chapman and Riddle, 2005; Olsen et al., 2011; De Hoop et al., 2011).

Of the 519 endpoint values, 57% are associated with single oil compounds that are classifiable within the pseudocomponent groups used for oil transport and fate modeling (Table 2). These were mainly derived from short-term effects studies (<8 days) performed on light and volatile compounds. This was also a finding of De Hoop et al. (2011) in a more limited study of naphthalene, 2-methyl-naphthalene and crude oil (water soluble fraction).

For zooplankton, *C. finmarchicus* is well studied but information is limited for the more northerly species, *C. glacialis*, and there are no relevant studies available for *C. hyperboreus*. While cod is relatively well represented, capelin is under-represented. For herring, although we extracted endpoint data for both Atlantic and Pacific herring, the available toxicity data for oil components is also limited. In general, for fish and zooplankton, mortality is the most studied endpoint while endpoint data for individual growth development, bioaccumulation and reproduction are less available (36% of the data reported in Table 3). For phytoplankton, only 6 studies for cold-water species were identified and these were studies on mixed oil components. Thus, data on temperate species were extracted and used as surrogates for cold-water species in this synthesis. Irrespective of species, few studies report endpoint values for more than one time point (e.g., only at the end of the experiment) and this limits their applicability in ecosystem modeling where time variations are an essential feature (Lee et al., 2002).

The general findings on data availability for the selected species are that there is a limited amount of experimental toxicity studies available in the literature. The data that exist are mainly suited for assessments of acute toxicity, with few data available on endpoints other than mortality. Finally, the majority of data are derived from short-term effects studies performed on light and volatile compounds, regardless of endpoint. These limitations have consequences for the use of these data in ecosystem-based modeling applications.

4.2. Data applicability

We address two issues related to the applicability of the obtained data to modeling: First, we evaluate data coverage for the

endpoints required by the selected ecotoxicology algorithms. Second, we address how well the assembled data map to the pseudocomponent groups required for transport and fate modeling. The combination of these two issues determines how well existing data meets the specifications and requirements for integrated ecosystem modeling. These results further help to identify priorities for new data acquisition activities.

4.2.1. Data coverage for the suite of endpoints and selected species

4.2.1.1. Plankton. To assess the impact of oil components on plankton using algorithm 1, data from literature sources should preferably include both bioaccumulation (bioconcentration factors, uptake and elimination rates) and toxicity endpoints (e.g., LC50, EC50, LOEC, etc.). These parameters, obtained in standard bioaccumulation tests, are used to check whether time-dependent body burdens estimated by the algorithm are correct. Likewise, reduction of survival, reproduction and growth as a function of concentrations in the water or organisms are used to test effect predictions made by the algorithm.

As indicated in Fig. 2 and Table 3, bioaccumulation data are sparse for temperate phytoplankton species and non-existent for cold-water species of both zooplankton and phytoplankton. Data are available on phytoplankton population growth from experiments investigating several oil components. Mortality in zooplankton has also been measured for several oil components, while sub-lethal effects such as reproduction and growth are quite limited. As a result, the model usage today will require the use of data for surrogate species or substitutions of oil components. Such an approach is not uncommon in ecotoxicology, due to existing restrictions on testing for financial, practical and ethical reasons.

4.2.1.2. Fish. The existing literature collected in the current study delivers a reasonable amount of endpoint values on the effects of oil components on juvenile and larval fish, our priority endpoints are mortality, growth and development. Studies of growth or development that report time variations in body size as a function of toxic exposure are of highest relevance (Jager and Zimmer, 2012; Klok et al., 2012).

As noted previously, mortality is the most commonly reported endpoint for fish. Of the 44 records addressing mortality in fish, mostly LC50 values, 28 provide information on the egg stage, 5 on fish larvae, and 8 do not specify life stage. In principle, these data are useful for modeling as long as supporting information is included on the 'number of survivors' for more than one discrete time point during an exposure experiment. When survivors are only reported at the end of the experiment (as is typical in standard acute toxicity test reporting of LC50 values) data are still useful but experience has shown that these data lead to large uncertainties in the obtained parameter estimates (<http://www.debttox.info/book.php>). Among the acquired data records for the endpoint 'growth' in fish, 6 are on larval growth and 2 on juvenile growth in cod and 4 on juvenile growth in herring. Unfortunately these records are less applicable for modeling because none of the studies provide information on body size at more than one time point.

Hence while LC50 (and ECx) values gathered through this data compilation exercise are generally useful, in practice we have determined that few of the published studies are appropriate for the present application due to the lack of necessary supporting information such as animal size, feeding conditions, and temperature. This greatly diminished the number of toxicity endpoints available in the database that are relevant for our aim of modeling effects on fish larvae.

4.2.2. Data mapping to the pseudocomponent groups

None of the pseudocomponent groups are represented by all species; nor do any of the pseudocomponent groups have values associated with the full suite of selected endpoints for either single species or taxonomic groups. The most complete coverage of endpoint values were for pseudocomponent groups 7, 8, 9, and 10. Due to high vapor pressures, these compounds are usually lost to the atmosphere within a few days after being released to the environment (Peterson, 1994). The emphasis on compounds within these particular pseudocomponent groups may be because early studies emphasized the need to determine the acute effects associated with these lighter and more volatile compounds that exert their toxicity mainly through the mode of narcosis (McGrath and Di Toro, 2009; Di Toro and McGrath, 2000; Di Toro et al., 2000).

For phytoplankton, pseudocomponent groups 7, 8, and 9, were covered as well as the heavier compound groups 22 and 23. For the genus *Calanus* as a whole, effects are well covered for both the volatile (7, 8, 9) and heavier compounds associated with group 23. For *C. finmarchicus*, experiments addressing the toxic effects of compounds within pseudocomponent group 23 on bioaccumulation are not available. Similarly, for *C. glacialis*, experiments addressing pseudocomponent groups 9 and 23 are needed for both growth and bioaccumulation. Studies on cod were distributed on groups 9, 21, 20, 22, 23 and 24. However, there are no records on reproduction for pseudocomponent group 24. For capelin, only endpoints associated with compounds within pseudocomponent group 20 are available. And finally, for pacific herring (our surrogate for atlantic herring) nearly all studies relate to pseudocomponent group 7. In general, endpoint values within the lower pseudocomponent groups tend to be available for lower taxonomic groups (phytoplankton and zooplankton) whereas values for the higher pseudocomponent groups are more available for fish. However, as previously indicated, data availability for sub-lethal endpoints are limited within the data set as a whole and as a result, the availability of such data for the pseudocomponent groups is also restricted.

4.3. Priorities for modeling

This compilation of existing data from literature for ecotoxicology algorithms represents an important precursor step to modeling. The exercise has provided key insight into the availability of ecotoxicology data and their utility for modeling the effects petroleum hydrocarbons on cold water species of marine organisms using two different ecotoxicology algorithms. The general outcome of this data synthesis exercise is that the available literature satisfies a limited sub-set of the selected species, endpoints and pseudocomponent groups targeted through this investigation. Given that previous studies indicated similar sensitivity between Arctic and temperate species (Olsen et al., 2011; De Hoop et al., 2011), the compiled data on phytoplankton are applicable for modeling. For zooplankton, *C. finmarchicus* has reasonable coverage of the various pseudocomponent groups and endpoints. For fish, cod has reasonable coverage but not particularly for larvae and juvenile stages which is needed for the modeling system being developed for the Barents Sea. The investigation of pacific herring to obtain additional sub-lethal effects data on herring did not substantially improve data availability and calls into question the value of data discovery efforts using surrogate species.

Additional options for obtaining ecotoxicology data to improve model parameterizations for the species and life stages of interest are:

- 1) Performance of new laboratory experiments to obtain additional endpoint values for selected species, e.g., *C. glacialis*,

C. harengus, *G. morhua* and *M. villosus*. This includes bioaccumulation data for zooplankton and time variant data on growth and development of fish larvae.

- 2) Performance of experiments focused on oil pseudocomponents for which data are not available in the literature but that are of importance in an oil spill context in terms of bioavailability. For example, the availability of toxicity data for naphthalene compounds (group 20–21) is relatively low.
- 3) Greater reliance on numerical estimation procedures such as QSAR approaches.

QSARs for accumulation are about equally accurate for oil components and other chemicals (De Hoop et al., 2013.). Application of toxicity QSARs relies on the assumption that narcosis is the dominant mode of action, a common starting point in oil risk assessment procedures (Di Toro et al., 2000; Verbruggen et al., 2008).

We recommend an initial focus on resolving the lack of development and bioaccumulation studies for zooplankton and the lack of growth and development studies for larvae and juvenile fish. Experimental studies are recommended but until such studies have been reported, the available information will be compared with and augmented by QSAR approaches. By using a combination of options we expect to be able to gather sufficient data to advance the further development of ecotoxicology algorithms for use in ecosystem modeling systems.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at <http://dx.doi.org/10.1016/j.marenvres.2013.05.007>.

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