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A Comparison of Four Particle Models

A Comparison of DemWaq, DREAM, GNOME, and SIMPAR

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Summary

This reports presents the results of a comparative study of the following four particle/fate models:

- 1. DemWaq, developed by RIKZ
- 2. DREAM, developed by Sintef (Norway)
- 3. GNOME, developed by NOAA (US)
- 4. SIMPAR, developed by RIKZ

The aim was to find a suitable operational fate model to predict the behavior and distribution of calamitous spills of oil and chemicals in the Dutch section of the continental shelf and the Dutch coastal areas. The following aspects of the models have been studied:

- Concepts and characteristics
- Functionalities (general comparison)
- Results for several test scenarios/experiments

The most important conclusion of the report is that comprehensive possibilities and functionalities make DREAM a very promising operational model. Its main attractions are the extensive chemical and oil databases included in the model and the graphical user interface. Although DREAM does not seem to have the highest numerical accuracy, the study shows that its results are comparable with those produced by the other models.

A Comparison of Four Particle Models

Acknowledgement

Besides several colleagues at RIKZ, the NOAA and Sintef institutes have collaborated in this project. NOAA implemented a script to translate the data produced by the RIKZ hydrodynamic SIMONA models into GNOME input data. NOAA provides their model for free (on the Internet). Sintef implemented a script to translate the RIKZ data into DREAM input data, and provided their model to facilitate the evaluation presented in this report. Moreover, Sintef has been very helpful in our efforts to experiment with and understand the model. Martin Geurtz (RIKZ) dusted off DemWaq and ran the DemWaq experiments. Robert Vos (RIKZ) ran the experiments for SIMPAR and advised us on chemical modeling in general.

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A Comparison of Four Particle Models

1 Introduction

Within the scope of the CALPREA project (CALamities Preparation REpression and Advice), the Dutch National Institute for Coastal and Marine Management (RijksInstituut voor Kust & Zee, or RIKZ) intends to use simulation models to predict the behavior and distribution of calamitous spills of oil and chemicals in the Dutch section of the continental shelf and the Dutch coastal areas. For this purpose the operational models using the SIMONA hydrodynamic models WAQUA/TRIWAQ will be used to provide the forecast of currents. To model the distribution of the spills, a fate model has to be coupled with these hydrodynamic models. Currently, the SIMONA model SIMPAR is available for that purpose. SIMPAR is a particle model that is closely related to the WAQUA/TRIWAQ system and is used by the provincial Water Management Directorate of Zeeland (the Netherlands). However, in its present state of development SIMPAR is not very user friendly. It lacks a graphical user interface and a module for oil weathering. These shortcomings also hamper DemWaq, another RIKZ model. DemWaq is slightly outdated but contains many formulations that are typical of the Dutch coastal area.

At other institutes around the world, various alternative fate models are being developed. Many of these models do not seem to have the disadvantages associated with the RIKZ models. It was determined, therefore, that as well as our own particle models, other models should be considered in the search for a suitable solution.

To make a thorough decision, a study was planned to assess and compare several particle models. Since the documentation the developers made available to us did not contain enough detailed information, it was decided to compare the models by assessing the results of several test scenarios. Only two international institutes cooperated in making it possible for us to run these scenarios with their models. Including the two RIKZ models, four particle models have been compared in the study reported in this document:

- DemWaq, developed by RIKZ
- DREAM, develooped by Sintef (Norway)
- GNOME, developed by NOAA (US)
- SIMPAR, developed by RIKZ

At the beginning of the study, the general characteristics of particle models were investigated (Section 2.1). This was followed by an analysis of the concepts and characteristics of the individual models (Section 2.2). Subsequently, the models were compared based on a set of relevant functionalities and features (Section 2.3). For comparing the actual behavior of the particle models, several test scenarios were

defined. Simulations based on these scenarios provided better insight into the behavior of the models (see Chapter 3 and the Appendices). The conclusions and recommendations derived from this study are presented in Chapter 4.

2 Description of the particle models

2.1. Particle models - an introduction

In all four models the spills are modeled as clouds of particles. The particles move due to advective and dispersive processes. Currents and wind stress on the water surface cause advection. In particle models this effect is generally modeled as a Lagrangian movement, which implies that at every step in time each particle is moved by the advective component of that time. In other words, the particles follow the flow.

Dispersion is caused by what is known as small-scale turbulence in water, and is usually modeled as a diffusive process. In some models diffusion is a function of time or size of the spill patch. This is based on the idea that as long as the patch remains small, immediately after a spill, small-scale turbulence causes only slight dispersion. As after some time the patch becomes bigger, larger-scale turbulence causes stronger dispersion. In particle models, the dispersive processes are generally modeled by each time step moving each particle with a random step in a random direction. In most models, the diffusion coefficient determines the magnitude of this random step. An exception to this rule is the Synthetic Eddy Field (SEF) used in DemWaq (see Section 2.2.1).

Mathematical models of material spreading generally use the advection diffusion (or transport) equation. This equation determines the variation of the concentration in time and space, and serves as the basis for particle models (see for example Heemink [8]). In contrast to particle models, there are also models that numerically solve the advection diffusion equation in a conventional way, e.g. finite difference, finite elements or finite volumes. This approach, which results in concentration values in time and space, is often referred to as Eulerian modeling, in contrast with the Lagrangian particle models. Particle models are generally believed to have the following advantages over conventional advection diffusion models:

- Particle models are capable of representing more sub-grid detail. Particles can move around within the grid, 'independent' of grid size, whilst conventional advection diffusion models give one concentration value for each grid cell.
- Particle models are more efficient since only the area of interest (where the spill is) is used in the computation.
- Particle models exclude negative concentrations or numerically introduced material losses.

However, particle models also have a number of disadvantages:

- They need a lot of particles to generate accurate results, especially if the simulation period is long.
- If concentration values are required, the results of the particle model have to be transformed. The simplest way to do this is to count particles in a grid cell. A more advanced way is to consider a particle as a small cloud that also grows in time (by diffusive processes) using, for example, point-spread functions. However, there is no generally accepted method for this.

For more information on particle models, see Fischer [7], Heemink [8] or Stijnen [11].

2.2. Characteristics of the models

The models compared in this study have various characteristics that could not all be mentioned here. This document focuses on the modeling of the particles. As a side path the modeling of oil weathering is briefly discussed. This subsection gives concise descriptions of the models that are compared in this study.

One very important feature shared by all the models is that they can import and use 2D currents produced by WAQUA/TRIWAQ, the hydrodynamic models of RIKZ used operationally in the Netherlands.

For the two non-RIKZ models (DREAM and GNOME), information on the exact numerical formulations was not available. Moreover, the technical domentation of DemWaq is inclomplete. To compensate for this the particle models were compared in actual simulations.

2.2.1. DemWaq

DemWaq, developed years ago by Van Dam at RIKZ, was used primarily for research activities. This model has two formulations for sub-grid eddy diffusivity that were verified with experiments for the Dutch coastal zone. In the first, Scaled Random Walk (SRW), diffusion is a function of patch size (which, in turn, is a function of the standard deviation of the particle positions). The second formulation is a Synthetic Eddy Field, where the eddy diffusion is not described by a diffusion term, but by a field of eddy currents imposed on the particles. The size and direction of the eddies is determined with a random function. For more information about the theory, consult Van Dam [9] and [10].

The magnitude of the dispersion used in DemWaq is based on an energy spectrum determined in experiments in the Dutch coastal zone. The results obtained from DemWaq have been shown to be very close to the measured data resulting from these experiments. Moreover, they are consistent with information from the literature. This is why RIKZ considers the DemWaq dispersion formulations to be very useful. User and system documentation for this model is available. The technical documentation is incomplete. There is no GUI to run the model or to display the results; the program is command-line controlled. The visualization programs for DemWaq is outdated and cannot be used anymore. Therefore, the results have to be post-processed first to obtain a visualization, using Matlab, for example.

2.2.2. DREAM

DREAM (Dose-related Risk and Effects Assessment Model) is a particle model developed by Sintef. It is widely used for environmental studies, for example in the oil industry. DREAM is part of MEMW (Marine Environmental Modeling Workbench) that also contains OSCAR (Oil Spill Contingency and Response for contingency planning) and ParTrack, for drill muds, cuttings, and associated chemicals. The SINTEF OWM (the Oil Weathering Module), available as a separate model, is also used as the weathering engine in OSCAR. 'MEMW is a framework for performing various modeling, simulation, analysis, and presentation tasks related to the marine environment' (quotation from the MEMW User Guide [3]). The possibilities of MEMW are comprehensive. Examples:

- Particle model for oil, chemicals and solid material (such as sediments)
- Extensive chemical and oil database that can be extended or adjusted by the user
- Biological module (effect on fish, plankton, etc.)
- Use of GIS (for example to designate ecologically sensitive areas)
- Definition of mechanical recovery systems (like skimmers, dispersants)
- Extensive graphical output (particles, concentrations, concentrations per component, etc.)
- Graphical presentation of flow, wind, etc.
- Definition of habitat and depth grid
- 3D particle behavior
- Allows import of depth database.

These are probably just a few of the many useful possibilities that MEMW offers.

Sintef has its own laboratories to perform oil and chemicals tests. In addition, the institute regularly runs larger scale tests in the ocean for model verification purposes. The framework is used operationally in Norway when incidents occur, as well as for environmental studies and consultancy.

MEMW uses a rectangular computational grid that is defined by the user and forms part of the area covered by the depth database. It uses this information to define the parameters of the computational grid. It is assumed that the computational grid covers the area of interest, since particles that leave the grid remain 'outside of the model'. The resolution of the spatial grid is also user-defined. MEMW/DREAM is operated by means of a GUI which, due to the large number of functionalities involved, is only suitable for more or less experienced users. Inexperienced users may sometimes find it hard to find specific functions.



Figure 1: example of the MEMW/DREAM user interface A specific quality of DREAM is that oil or chemical products can be fed into the program by specifying the real components. These components are defined in DREAM using a great many chemical and physical specifications. After a spill these components behave differently: some evaporate, some dissolve, etc.

DREAM recognizes three types of particles: surface particles, dissolved particles and solid/droplet particles. Each has a set of characteristics such as mass, size etc. Particles can exchange characteristics, and are introduced or deleted from the computation during a simulation period. For example, when part of the oil disperses, dissolved particles are introduced in the simulation while surface particles might be deleted. In this latter case, the mass of the deleted particles is divided over the remaining surface particles. Due to all these possibilities, DREAM is able to give detailed information on behavior and spread for the different phases and components of the spill.

Note that during the experiments some observations were made that cannot be accounted for. These are presented as issues for further study in Appendix X and have also been passed on to Sintef. These observations include:

- Unaccountable production of particles
- The shift in the current field and
- The dependence of a number of liquid or solid particles in model definition.

By the time this report was finalized, Sintef reported that the first and last item were bugs that had already been solved. The second item probably has to do with the program for converting the Waqua output format to the Sintef input format, and is currently being investigated by Sintef.

2.2.3. GNOME

GNOME, developed by NOAA, is a user-friendly program available for free on the Internet (www.noaa.com). NOAA supports the philosophy that no matter how accurate your numerical model, your outcome will be significantly uncertain as long as you are not sure of the exact spill size, wind fields and currents. In other words, in practice numerical accuracy is not really important. Given that your input is not accurate, it is much more important to know as much as possible about the variations in the solution. This is why GNOME distinguishes between best guess and minimum regret solutions. To that end, GNOME enables the user to account for uncertainty in wind and current information. In the graphical user interface, the best guess solution is presented by black particles, the minimum regret solution by red particles. NOAA claims that the chance of a spill remaining in the area covered by the red splits is in the order of 90 %, provided that a correct degree of uncertainty is used.

GNOME can simulate six types of oil and conservative floating material. It does not support dissolved materials or chemicals, although the conservative material can be misused for this purpose. GNOME simulates the weathering of oil; however, in contrast with DREAM, the results do not show what component of the oil has evaporated or dispersed. If oil weathers in GNOME, the proportional volume of particles is deleted from of the simulation (see Appendix F).

GNOME produces graphical output and can also generate GIS output. Spills can be defined as points, sprays and lines. More information on GNOME is found on the NOAA webpage and, more specifically, in the GNOME user guide [5].

GNOME is used operationally in the US as a tool to determine the probable and possible areas with oil remains. For analyses, other tools are used which are not freely available.



Figure 2: example of the GNOME user interface with best guess (black dots) and minimum regret (red dots) solutions.

2.2.4. SIMPAR

SIMPAR was developed by RIKZ and the Delft University of Technology (TUD) and is part of RIKZ's SIMONA system. It is a 2D model that places great emphasis on mathematical accuracy and offers two diffusion formulations: one with a constant diffusion coefficient and the other with time-dependent diffusion (fractional Brownian motion). SIMPAR has been specifically developed for the Dutch coastal zone where drying and flooding, among others, are important features. The new version of SIMPAR will include an oil module and the Synthetic Eddy Filed (SEF) dispersion formulation of Van Dam et al. (the same as in DemWaq (see Section 2.2.1)), as well as a 3D feature.

The provincial Water Management Directorate of Zeeland (the Netherlands) has implemented SIMPAR in its own operating environment. They use the model operationally to determine the trajectory of spills.

SIMPAR has a module for converting particle location data to concentration data using a histogram method or using point-spread functions. SIMPAR is command-line controlled and does not yet include a ready to use visualization program. Directorate of Zeeland and others developed their own visualization tools. RIKZ is adapting their control plot program WAQVIEW for visualization of SIMPAR results

2.3. General comparison

The functionalities and features of the models have been compared based on a set of features. The results of this comparison are presented in Table 1. Below is a description of each feature that forms part of the comparison.

Operational: indicates whether the model is used for contingency planning and whether it is suitable for use in the case of an oil and chemical spill. This feature should indicate whether the model is considered useful and reliable in operational situations.

3D: indicates whether the model offers possibilities for 3D particle computations using 3D current fields. 3D computations can give more detailed information. TRIWAQ can produce 3D current fields.

Dissolved material: indicates whether the model can simulate the spreading of dissolved material. Some spills concern chemicals. In such cases, dissolved material should be simulated.

Oil (floating material): indicates whether the model simulates the spreading of oil or, more generally, floating material.

Different materials: indicates whether the model distinguishes between different materials. It may be important to simulate the behavior of materials with specific properties, such as density or viscosity.

Constant diffusion: indicates whether the model allows incorporation of a constant diffusion formulation. Even though this is not an advantage per se, it does make a comparison easier since the diffusion formulations generally differ strongly.

Time or patch size dependent diffusion: indicates whether the model has a time or patch size dependent formulation for the diffusion. This is generally considered to be a realistic approach to modeling turbulent dispersion.

North Sea physics in dispersion: indicates whether typical processes for the North Sea (Dutch coastal zone) are included in the dispersion formulation.

Interpolation of currents in time and space: indicates whether the model interpolates the numerical current field in time and space. This would add to the accuracy of the outcome.

Translation into concentrations: indicates whether the system is able to translate the particle variables into concentrations. In many cases the strength of the concentrations is of great importance.

GUI: indicates whether the model has a Graphical User Interface for input and output. A GUI makes a model more user-friendly and improves its acceptance.

Graphical and GIS output: indicates whether the model shows the output in a Graphical User Interface and is able to present the output in GIS applications. This allows quick interpretation of the results.

GIS update: indicates whether the model can update the simulation using measurements presented in GIS format. Using up to date field measurements can improve the predictability of the model.

Wind fields: indicates whether the model imports space and time varying wind fields. Especially during storms the wind factor can vary considerably, which will cause larger dispersion.

Source code: indicates whether the source code of the model is available to RIKZ. For RIKZ it is important to have access to the source code so that it can freely adjust the model as required.

Curvilinear grid: indicates whether the model is able to compute the particle tracks within a curvilinear grid (without transformation to a rectangular grid). Many of RIKZ' hydraulic models are curvilinear. Numerical accuracy benefits when the results are not transformed to a rectangular grid.

Depth: indicates whether the model is able to import a space-varying grid. Variation in depth is an important feature in shallow areas, also for material transport.

Water levels: indicates whether the model is able to use time and space varying water levels in its computations. Concentrations, falling of material, and drying and flooding depend on depth and water levels.

Flooding: indicates whether the model contains functionality for drying and flooding. Drying and flooding are typical features of the Dutch coastal zone and should be modeled specifically.

Extras: indicates whether significantly more functionalities are offered by the model in addition to the ones mentioned in this table.

	Operational	3D	Dissolved material	Oil (surf material)	Oil weathering function	Different materials	Constant diffusion	Time or patch size dependent diffusion	North Sea physics in dispersion	Interpolation currents in time and space	Translation into concentrations	CUI	Graphical and GIS output	GIS Update	Wind fields	Source code	Curvilinear Grid	Depth	Water levels	Flooding	Extras
DemWaq		x	x					х	X*	х						х		х	х		
Dream	х	x	x	х	x	х	X*	х			х	х	x	х	х			x			Χ*
GNOME	х			х	x	х	х					х	x	х							
SIMPAR	х	X*	×	х	X*	X*	x	X*	X*	х	x		X*		х	х	х	x	x	х	

Table 1: Comparison of qualities of the different models

X means availability of the feature.

The meaning of the asterisks in the table is explained below.

DemWaq

North Sea physics in dispersion. See remarks on SRW and SEF in previous section.

DREAM

- Constant diffusion: is not a standard function at this moment. However, Sintef has made available an additional script for computations with constant diffusion to ensure that the experiments can be meaningfully compared.
- Extras: as mentioned in Section 2.2.2, DREAM has many more functionalities than the ones mentioned in this table.

GNOME

No further explanation.

SIMPAR

- 3D: the next version of SIMPAR will be 3D.
- Oil weathering module: the next version of SIMPAR will include an oil module.
- Different material: SIMPAR currently distinguishes between dissolved and floating material. The next version will also be able to recognize different oil types.
- North Sea physics in dispersion: DemWaq's SEF method (van Dam et al.) will be implemented in the next version.
- Graphical and GIS output: post-processing programs are available to produce Graphical and GIS output.

3 The experiments

Several experiments have been performed to compare the different models.

3.1. Aim of the experiments

- Comparing basic model behavior for oils in the short and longer term → Experiment 2
- Comparing model behavior near land and barriers Experiment 3
- Understanding model behavior Additional experiments

3.2. General remarks on the experiments

For all experiments and models one current file was created by WAQUA using the curvilinear ZUNO (Zuidelijke Noordzee, or Southern North Sea) model. This file was used as the basis for the current input. In the simulation with WAQUA the effect of a southwesterly wind of 4 m/s was included. The model was run for one month.

For DemWaq, DREAM and GNOME a sub-area was cut from the ZUNO grid containing the northern part of the Dutch coastal zone. Using the SimSwan program, the sub-area was transformed into a rectilinear grid and the output was written in asci format. Next, for DREAM and GNOME the data was transformed to net-cdf. On request, both Sintef and NOAA adjusted their models so as to be able to read these net-cdf files. GNOME does not use any depth data. The boundary outlines provided by RIKZ are used in GNOME. DREAM uses depth data and boundary outlines, but is not yet able to read the depth data and boundary outlines provided by RIKZ. For this reason a depth database provided by Sintef was used. It should be noted that the Sintef depth database is not as accurate as the RIKZ depth data.

The results of the experiments are briefly described in the paragraphs below. More detailed information on Experiments 1, 2, and 3 can be found in Appendices A, B, and C. Information on the additional experiments can be found in Appendices D, E, and F.

3.3. Experiment No. 1: Tracer on the open sea

In this experiment an instantaneous point spill of tracer material was performed, sufficiently far from land so as not to be influenced by it. No extra wind was imposed, since wind does not directly influence the spreading of dissolved material (which is spread over the water column) as it does the spreading of oil (on the surface). The simulated period was 7 days, where the behavior for t=t0 + 6h, 12h, 18h, and 24h was studied for the short term and the behavior for t=t0 + 1d ... 7d for the longer term.

The models were studied simultaneously; the behavior of the models using different diffusion formulations was also examined.

DemWaq

The experiments were run using the SRW formulation only, since the SEF module ran into some difficulties.

DREAM

The material used was Tracer. Here, three diffusion formulations were used: $Dx = 1 \text{ m}_2/\text{s}$, 10 m2/s and $Dx = D(t) = 1.08 \text{ 10-6 t } 1.34 \text{ m}_2/\text{s}$ (the Okubo relation). As an extra, Dx was set to 0 m2/s so that the advective behavior could be studied.

GNOME

The material used was non-weathering oil. Since there was no extra wind imposed and it is a 2D computation, the oil should behave similarly to dissolved material. The diffusion was set at Dx = 0, 1, and 10 m2/s respectively. Only the best guess results were used.

SIMPAR

For SIMPAR the diffusion was set at Dx = 1 and 10 m2/s respectively. The time-dependent formulation was not tested.

Results

The results of the experiments are shown in detail in Appendix A.

Conclusions:

- A comparison of the models for different diffusion formulations reveals consistent behavior.
- A mutual comparison of the different models produces comparable results:
 - Location of the cloud: The centers of the clouds vary in location. In this experiment the maximum variation is approximately 2.5 km. These deviations may be attributed to:
 - Numerical errors
 - Difference in exact initial time
 - Difference due to different coordinate systems: geographical (GNOME and DREAM) versus RD (SIMPAR and DemWaq)
 - Other causes as yet to be studied
 - Dispersion of the cloud: the similar diffusion formulations cause the different models to produce highly similar dispersion variables.
- The dispersion for DemWaq and DREAM using D(t) shows the most deviant behavior compared with the others. This is no surprise, since DemWaq and DREAM use time-dependent diffusion formulations.

Recommendation for further research:

• Further study is required to establish the cause of discrepancies in location and dispersion, and options to overcome them.

3.4. Experiment No. 2: Oil on the open sea

This experiment is similar to the first, but in this case the substance is oil. Moreover, extra wind on the water surface (4 m/s SW) was included. For all experiments Dx = 10 m2/s was used for the horizontal diffusion.

DemWaq

Not used in this experiment: DemWaq cannot simulate oil, only dissolved material.

DREAM

The material used was Troll (a medium crude oil); see Appendix D.

GNOME

The material used was medium crude oil. In the windage settings persistence was set at standard and infinite respectively. The user documentation does not specify which physical process these settings represent. Windage is 1 % to 4 %. For more information on oil types and weathering in GNOME, consult Appendix E.

SIMPAR

The material used was floating material. Wind drag coefficient = 3.5%.

Results

The results of the experiments are shown in Appendix B. As an extra, GNOME and DREAM have been compared for oil weathering features.

Conclusions:

- The results of the models differ strongly for oil; part of the discrepancy may be caused by different windage and wind stress formulations.
- The deviation can be attributed to a large extent to the fact that DREAM employs a very different and much more extensive description of the material (see also Appendix D). DREAM shows much more detail in material behavior than the other models.

Recommendation:

 The causes of the discrepancies should be studied in more detail to find out whether the detail used in DREAM is necessary for accurate results or whether a rougher representation such as used in GNOME or SIMPAR could also give sufficient information. This study should include consultation of experts on operational contingency planning.

3.5. Experiment No 3: Handling of land and dikes

This experiment comprises two components: a spill near one of the Wadden islands and another spill near the IJsselmeer Dam (Afsluitdijk) (see figures in Appendix C). Both experiments are instantaneous point spills. There is no extra wind. For all experiments $Dx = 10 \text{ m}^2/\text{s}$ was used for the horizontal diffusion.

DemWaq

Not used in this experiment:

DREAM

The material used was Troll (a medium crude oil; see Appendix D), since Troll does and Tracer does not beach. In DREAM, beaching depends on the habitat grid. In the current situation the island is lined with sand beaches, which is probably realistic. Moreover, there is a sandbank northeast of the island of Vlieland (see figures). This feature is treated as land in DREAM, which accounts for the much larger amount of beached material found in DREAM than in GNOME. Further, the IJsselmeer Dam (Afsluitdijk) is not currently defined in the boundary outlines in DREAM and had to be incorporated manually, changing the depth and habitat grid. There was hardly any beaching in DREAM, probably because the seaward section of the dam had been defined as a cobble-gravel beach.

GNOME

The material used was non-weathering oil.

SIMPAR

The material used was floating material. Wind drag coefficient = 3.5%.

Results

The results of the experiments are shown in Appendix C.

Conclusions:

- Visually the results for DREAM and GNOME are alike.
- The results of SIMPAR are essentially different from those of DREAM and GNOME. Subsequent study of the model hinted at the presence of bugs in SIMPAR.
- The amount of beached material differs strongly. This has probably to do with the different definition of land in DREAM and GNOME and the fact that in DREAM different types of habitat can be defined.
- Land and dikes have to be implemented carefully to ensure that the figures on the amount of beached material are meaningful.

Recommendation:

- For SIMPAR to be fit for operational use, the bugs will need to be eliminated.
- Further research and validation on beaching is required.

3.6. Additional experiments

Appendices D, E, and F show the results of several additional experiments.

- Appendix D: DREAM concentration fields for different components. This is an example of how concentration fields for different components of Troll crude oil are visualized in DREAM.
- Appendix E: GNOME study of oil weathering simulation. This shows the weathering curves for the different oil types in GNOME and how this feature is visualized.
- Appendix F: GNOME study of wind simulation. This shows the results of several GNOME experiments for different wind conditions.

4 Conclusions and recommendations

The comparison of the models leads to the following conclusions and recommendations.

4.1. Conclusions

The models have very different origins and are based on different assumptions, which is clearly noticeable in their structure and performance. These differences may obstruct meaningful comparison. Moreover, each model has its own distinct merits and demerits.

The most important advantages are given in Table 1. Below is an overview of additional and very specific qualities:

DemWaq

• This model has two formulations for sub-grid eddy diffusivity that were verified in experiments for the Dutch coastal zone.

MEMW/DREAM

- DREAM offers an extensive set of very interesting functionalities. The possibilities of MEMW, therefore, are substantial.
- An extensive chemical and oil database is included.
- DREAM is able to give detailed information on material behavior and spreading for the different phases and components of the spill.

GNOME

- Very user-friendly.
- GNOME identifies a minimum regret solution in addition to a best guess.

SIMPAR

- A great deal of attention has been paid to mathematical accuracy.
- SIMPAR was developed specifically for the Dutch coastal zone.

The major disadvantages:

DemWaq

- Not very user-friendly.
- Lacks options for oil.

MEMW/DREAM

- Complicated program, due to the large number of functionalities.
- Numerically less accurate than SIMPAR.
- There seem to be some (numerical) inadequacies in the model (which have now reportedly been solved).

GNOME

• The model may be too simple and straightforward. Since we do not have the source code it is hard to adapt it to our wishes.

SIMPAR

- Not very user-friendly.
- The current version lacks a chemical or oil weathering module.
- There seem to be some inadequacies in the model that have not been solved yet.

Taking these differences into account, it would be fortunate if particle behavior were similar. In this regard the experiments show us the following:

- 1. For tracer material the models show comparable results. This is a promising finding.
- 2. For oil the models show quite different results. This is unfortunate and creates a need for further investigation to find out which model or formulation is realistic and valuable.
- 3. The behavior of the models in shallow areas and close to land is different.
 - The definition of land and dikes is very important.
 - There seems to be a significant dissimilarity in the definition of surface material spreading in shallow areas between DREAM/ GNOME versus SIMPAR. The dissimilarity is primarily caused by an error in SIMPAR.

Final conclusion

Considering the possibilities of DREAM and the fact that for the most generic experiment using dissolved material (experiment A) the models do not differ strongly from the others, it can be concluded that from a modeling point of view, DREAM has a large potential. GNOME can be used for quick indications (first guesses), but lacks many of the important features of DREAM.

4.2. Recommendations

Before any of the models is brought into operational use, the following work is necessary:

- More thorough study on the modeling of surface material spreading.
- Further study into functionalities to better understand model behavior.
- Further fine-tuning of the models.
- Continued cooperation with the producers of DREAM (Sintef) to further develop the model so as to make it more suitable for our case.

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Internet sites

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- NOAA (GNOME): http://www.noaa.com/
- TU-Delft: http://ta.twi.tudelft.nl/

A Comparison of Four Particle Models

Appendix A: Comparison of GNOME, DREAM, SIMPAR and DemWaq

In this document the results of the four models are compared.

GNOME: Non-weathering (conservative) oil

- Dx=0 m2/s
- Dx=1 m2/s
- Dx=10 m2/s

DemWaq: Dispersion according to scaled random walk formulation using the real particle age.

DREAM: Material = Tracer; Discharge 1 000 kg.

- Dx=0 m2/s
- Dx=1 m2/s
- Dx=D(t)=1.08 10-6 t(s)1.34 m2/s
- Dx=10 m2/s

SIMPAR: Discharge 20 000 kg.

- Dx=1 m2/s
- Dx=10 m2/s

The discharge was effected at one point (95578, 575834)=(53 10', 4 30') and in one instant (January 6th 1999, 0:00). The simulations ended after 7 days. Wind (4m/s SW) was included in the hydrodynamics. No 'extra wind' was imposed. The same SDS input was used. The time step was 30 min. For GNOME, DREAM and DemWaq 1 000 particles were used, for SIMPAR 5 000.

First some figures are compared, later some data.





No 'extra wind', t=t_0+6 h



No 'extra wind', t=t_0+24 h



No 'extra wind', t=t_0+24 h



No 'extra wind', t=t_0+7 d



No 'extra wind', t=t_0+7 d



The figures below show the course of the center of the particle clouds for $t=t_0 + 6h$, 12h, 18h, 1d, 2d, 3d, 4d, 5d, 6d and 7d in different configurations (where DREAM_1, for example, stands for DREAM with Dx=1 m2/s, and DREAM_Dt for DREAM with Dx=D(t)).



The figures show that within a single model, the centers of the clouds are close for the different diffusion terms. The differences between models are larger, particularly for t = 6 and 18 hours (approximately at the turn of the tide after low tide). After 2 days both SIMPAR and DemWaq begin to show a deviation compared with GNOME and DREAM, whose results are very close. This is also reflected in the next figures, which show the difference between the mean centers in RD_X and RD_Y.



The figures below compare the standard deviations in RD_X and RD_Y. In the first set of figures the standard deviations of GNOME and SIMPAR (Dx=1 m2/s) are compared with the standard deviation in a special, theoretical case. In that theoretical case there are no spatial variations in the currents, which means that the variance in both the x and y directions is equal to 2Dt. In the next set of figures the standard deviations of GNOME (Dx=1 and 10 m2/s), SIMPAR (Dx=1 m2/s) and DemWaq are compared. The lowest figure shows the correlation of the particles in the x and y directions (which, in the theoretical case, would be 0).





The results show that the dispersion is somewhat (though not much) anisotropic, probably due to horizontal velocity shear. The dispersion for DemWaq is smaller in the first 24 hours, but larger than for Dx=1 m2/s after one day. After some time, the difference between DemWaq and GNOME with Dx=10 m2/s decreases.

The correlations have the same order of magnitude for all models. Only for t=6 - 18 h SIMPAR differs, and for larger time frames the difference between the models beings to show.

In the figures below the length and width of the 99% ellipse (an ellipse that would contain approximately 99% of the particle cloud if the spreading were Gaussian) has been determined for GNOME and DEMWAQ. The length and width can be determined using the variances and correlation of the particles. The length and width of the clouds in DREAM have been determined by hand. The error due to the manual work is in the order of 10%.



The figures show that the cloud in DREAM using D(t) grows quickly and becomes much larger than the other clouds. The dispersion for D=1 m2/s and 10 m2/s is similar (DREAM and GNOME).

Conclusions:

- A comparison of the models for different diffusion formulations reveals consistent behavior.
- A comparison of the different models also produces comparable results:
 - Location of the cloud: The centers of the clouds vary in location. In this experiment the maximum variation is approximately 2.5 km. These deviations may be attributed to:
 - Numerical errors
 - Difference in exact initial time
 - Difference due to coordinate system (geographical (GNOME and DREAM) versus RD (SIMPAR and DemWaq)
 Other causes as yet to be studied
 - Other causes as yet to be studied.
 - **Dispersion of the cloud:** the similar diffusion formulations cause the different models to produce highly similar dispersion data.
- The dispersion for DemWaq and DREAM using D(t) shows the most deviant behavior compared with the others. This is no surprise, since DemWaq and DREAM use time-dependent diffusion formulations.

Recommendation

• Further study is required to establish the causes of the discrepancies in location and dispersion, and options to overcome them.

Appendix B: Comparison of GNOME, DREAM and SIMPAR for medium crude oil

In this document the results of three models are compared.

GNOME:	Material = medium crude oil; in the windage settings
	persistence has been set at standard and infinite respectively.
	The user documentation does not specify which physical
	processes these settings represent (!). Windage is 1 $\%$ to 4 $\%.$
DREAM:	Material = Troll
SIMPAR:	Material = floating material; wind drag coefficient = 3.5% .

The discharge was effected at one point (95578, 575834)=(53 10', 4 30') and in one instant (January 6th 1999, 0:00). The simulations ended after 7 days. Wind (4m/s SW) was included in the hydrodynamics and 'extra wind' was imposed. The same SDS input was used. The time step was 30 min. For GNOME and DREAM 2 000 particles were used, for SIMPAR 5 000. The diffusion was $Dx=10 \text{ m}^2/\text{s}$, the discharge 20 000 kg.

First some figures are compared, later some data. As an extra (since it is not part of this study), GNOME and DREAM are compared as regards the weathering of the oil.



t=t_0+6 h

t=t_0+24 h



t=t_0+48 h



Note that DREAM distinguishes between dissolved and surface particles. The movement of surface particles is partly caused by the wind; the movement of dissolved particles is mainly caused by tidal currents. The surface material partly dissolves and 'leaves behind' the cloud of dissolved particles. The small gray circles present the surface material (see figure below). The black particles in the figures are the dissolved particles. This is only a small fraction of the total amount of material. In that sense, therefore, the figure gives a distorted presentation.



The figures show that GNOME with standard persistence compares with SIMPAR, while GNOME with infinite persistence compares with DREAM. How much they compare is shown in the data below.

Data

The figures below show the course of the center of the particle clouds for $t=t_0 + 6h$, 12h, 18h, 1d, and 2d in different configurations. In this context,

- GNOME_10_standard stands for GNOME with Dx=10 m²/s and persistence=standard,
- GNOME_10_infinite stands for GNOME with Dx=10 m²/s and persistence=infinite,
- DREAM_10_dissolved stands for the cloud of dissolved particles in DREAM with Dx=10 m²/s, and
- DREAM_10_surface stands for the cloud of surface particles in DREAM with Dx=10 m²/s.



The diagram shows that for GNOME the means are very close for either formulation of the persistence. The mean of the dissolved cloud of particles in DREAM differs strongly from the other models. The mean of the surface cloud of particles in DREAM is relatively close to the mean found by SIMPAR.

The figures below compare the standard deviations in RD_X and RD_Y. Here, only the standard deviations of GNOME (with standard persistence) and SIMPAR are compared with the standard deviation in a special, theoretical case. In that theoretical case there are no spatial variations in the currents, which means that the variance in both the x and y directions is equal to 2Dt. The lowest figure shows the correlation of the particles in the x and y directions (which, in the theoretical case 2Dt, is 0).



In the figures below the length and width of the 99% ellipse (an ellipse that would contain approximately 99% of the particle cloud if the spreading were Gaussian) has been determined for GNOME (with standard and infinite persistence). The length and width can be determined using the variances and correlation of the particles. The length and width of the clouds in DREAM have been determined by hand. The error due to the manual work is in the order of 10%.



The diagrams show that the spreading in the x direction is similar for all three cases; however, for the y direction the spreading in DREAM is significantly larger than in GNOME.

The oblique angle of the clouds is approximately 45° for both DREAM and GNOME with infinite persistence. This is probably due to the main direction of the currents (northeast at high tide, southwest at low tide).

Weathering

The diagrams below show the weathering of the material according to GNOME and DREAM. SIMPAR is not yet able to give this information. Here, the behavior of Troll is compared with the behavior of both medium crude oil and fuel oil # 6 in GNOME. The results show a slightly deviant behavior.



In the mass balance in DREAM the model distinguishes the following phases of the material:

- Surface
- Evaporated
- Submerged
- Sediment (material taken up by the sediment)
- Cleaned
- Beached
- Decayed
- Out of model (that is, out of computational grid).

GNOME recognizes

- Floating
- Beached
- Evaporated and dispersed
- Off-map

Conclusions:

- The results of the models differ strongly for oil; these differences might be caused in part by different windage/ wind stress etc. formulations.
- A considerable part of the deviation is due to the fact that DREAM offers very different and much more extensive material descriptions (see also Appendix D). Moreover, DREAM shows much more detail in behavioral patterns than the other models.

Recommendation:

The cause of the discrepancies should be studied in more detail to establish whether the detail used in DREAM is necessary for accurate results or whether a rougher representation such as used in GNOME or SIMPAR could provide sufficient information.

Appendix C: Comparison of GNOME, DREAM and SIMPAR for oil near land

In this document the results of three models are compared.

GNOME: Material = Non-weathering oil
DREAM: Material = Troll
SIMPAR: Material = (1) floating material
(2) dissolved material

This experiment consists of two components: one spill (A) near one of the Wadden islands ($(53^{\circ}20',5^{\circ}05')$ _NE = (134669, 594060)_xy), and another spill (B) near the IJsselmeer Dam ($(53^{\circ}02',5^{\circ}10')$ _NE = (140119, 560653)_xy). Both experiments involve instantaneous point spills at t_0=6:00. There is no extra wind. For all experiments Dx =10 m²/s was used for the horizontal diffusion. The time step was 30 min. For GNOME and DREAM 1 000 particles were used, for SIMPAR 5 000.

The results with dissolved materials (only experiment A) have also been considered, given that the results of the SIMPAR simulation differed very strongly from the others.

First some figures are compared, later some data. As an extra (since it is not part of this study), GNOME and DREAM are compared as regards the beaching of the oil.



Experiment A, no 'extra wind'



Experiment A, no 'extra wind'

Experiment B, no 'extra wind'



T=t_0+	GNOME (beache	ed %)	DREAM (ashore %)			
	Ехр А	Ехр В	Ехр А	Ехр В		
6 h	0	7.9	0	0		
12 h	0	7.3	39	0		
18 h	0	23.4	39	0		
24 h	4.4	11	44	0		
48 h	11.8	14.7	47	1		

Notes on the results of experiment A:

- In DREAM, beaching depends on the habitat grid. In the current situation the island is lined with sand beaches, which is probably realistic.
- Northeast of the island of Vlieland (see figures) there is a sandbank. This is regarded as land in DREAM (and SIMPAR), but not in GNOME, which accounts for the much larger amount of beached material in DREAM.
- The results of SIMPAR (floating material) differ strongly from those of DREAM and GNOME, while the results for dissolved material are very similar. This is probably due to a flaw in SIMPAR.

Notes on the results of experiment B:

- The IJsselmeer Dam is not defined as land in DREAM. It had to be input manually, changing the depth and habitat grid. There was hardly any beaching in DREAM, probably because the seaward section had been defined as a cobble-gravel beach.
- The results of SIMPAR differ strongly from those of DREAM and GNOME. Again, this is probably due to a flaw in SIMPAR.

Conclusions:

- Visually the results for SIMPAR (dissolved material), DREAM and GNOME are alike.
- The results of SIMPAR (floating material) are fundamentally different from those of DREAM and GNOME.
- The amount of beached material differs strongly. This has probably to do with the different definitions of land in the two models and the fact that in DREAM different types of habitats can be defined.
- Land and dikes have to be implemented carefully to ensure that the figures on the amount of beached material are meaningful.

Recommendation:

The error in SIMPAR needs to be further looked into.

A Comparison of Four Particle Models

Appendix D: DREAM concentration fields for different components

In DREAM, oil profiles can be defined by means of their constituent components. The components are defined in the components database.

During an experiment the oil weathers and part of the material dissolves in the water column. These phenomena are simulated in a run. The figures below show some of the results for the concentrations of all the components together (the profile) or of an individual component. The figures concern the spreading of Troll medium crude oil.





Concentrations for C3 Benzene

Concentrations for Metabolite 1

Concentrations for Naphthalenes 1



Concentrations for all components of Troll

A Comparison of Four Particle Models

Appendix E: GNOME, study of oil weathering simulation

In GNOME, the following different types of oil can be selected:

- 1. Gasoline
- 2. Kerosene/jet fuels
- 3. Diesel
- 4. Fuel oil #4
- 5. Medium crude oil
- 6. Fuel oil # 6
- 7. Non-weathering

These different types of oil have different weathering behaviors. In the figure below the behavior over 7 days is shown. The figure shows the percentage of floating material; the rest of the material has dispersed and/or evaporated.



The following table shows the results of two experiments (with medium crude oil and with kerosene/jet fuels) using 2 000 particles and adding a 4 m/s SW wind. The results show that the weathering is modeled by deleting 'evaporated and dispersed' particles.



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Appendix F: GNOME, study of the simulation of wind

In GNOME, as in many particle models, wind and currents can be defined separately. However, it is not possible to import spacevarying wind fields. NOAA has suggested that if the wind is strong and involves a great deal of space variation, it can be imported as current fields. This is why the effect of wind is studied briefly here. The following scenarios were used:

- 1. Currents and wind (4 m/s SW), windage setting persistence=standard
- 2. Currents and wind (20 m/s SW), windage setting persistence=standard
- 3. Only wind (20 m/s SW), windage setting persistence=standard
- 4. Currents and wind (4 m/s SW), windage setting persistence=infinite

The wind is uniform and constant. The hydrodynamic model WAQUA determines the currents where a wind speed of 4 m/s SW is included in the simulation. The number of particles is 2 000, the diffusion is 10 m^2/s .







Current and wind 4 m/s

Appendix X: Issues of further study for DREAM

In DREAM we have encountered three problems that require further study:

- 1. The unaccountable production of particles.
- 2. The time shift in the current field.
- 3. The dependence between the number of liquid or solid particles set in the model definition and the number of surface and droplet/ solid particles during the computation.

NOTE: SINTEF has stated that issues 1 and 3 above resulted from bugs that have been eliminated since. Issue No. 2 is probably due to an error in the transformation script from our current data to DREAM input data.

1. Unaccountable production of particles

In this example the number of spills seems to influence the unaccountable production of particles. The second experiment is similar to the first; however, a third spill is added in a deeper location. This seems to cause an unaccountable production of particles in deeper regions elsewhere.

Experiment 1: Two releases, west=balder; east=tracer; releases at z=0

After 5:30:



Experiment 2: Another release, tracer; releases at z=-20









Note 3 particles in deeper locations for the most westerly release (BALDER). Compare this with the figure of experiment 1.





2. Time shift in the current field

A comparison between the current field in DREAM and the current field produced by RIKZ reveals a shift of one hour. Besides, the currents seem to be defined every 59 minutes, while RIKZ gave a field every 30 minutes. The exact cause of these deviations has so far not been identified; SINTEF is currently looking into the matter.

3. The dependence between the number of liquid or solid particles set in the model definition and the number of surface and droplet/solid particles during the computation

With a different number of liquid and solid particles in the simulation run, the distribution over surface particles and droplet/solid particles is very different (as shown in the table). This issue has been presented to SINTEF.

No. of liquid and solid particles	No. of surface particles	No. of droplets/solid particles
100	(after some time) 1	94-99
500	166	8
1 000	333	1
2 000	666	0



This also produces very different graphical results:

A Comparison of Four Particle Models

A Comparison of Four Particle Models