

FLEXSEM: A NEW METHOD FOR OFFLINE OCEAN MODELLING

Technical Report from DCE – Danish Centre for Environment and Energy

No. 105

2017



AARHUS
UNIVERSITY

DCE – DANISH CENTRE FOR ENVIRONMENT AND ENERGY

[Blank page]

FLEXSEM: A NEW METHOD FOR OFFLINE OCEAN MODELLING

Technical Report from DCE – Danish Centre for Environment and Energy

No. 105

2017

Janus Larsen¹
Marie Maar¹
Thorger Brüning²
Jun She³
Christian Mohn¹

¹Aarhus University, Department of Bioscience

²Bundesamt für Seeschifffahrt und Hydrographie (BSH)

³Danish Meteorological Institute



AARHUS
UNIVERSITY

DCE – DANISH CENTRE FOR ENVIRONMENT AND ENERGY

Data sheet

Series title and no.:	Technical Report from DCE – Danish Centre for Environment and Energy No. 105
Title:	Flexsem: A new method for offline ocean modelling
Authors:	Janus Larsen ¹ , Marie Maar ¹ , Thorger Brüning ² , Jun She ³ , Christian Mohn ¹
Institutions:	¹ Aarhus University, Department of Bioscience, ² Bundesamt für Seeschifffahrt und Hydrographie (BSH), ³ Danish Meteorological Institute
Publisher:	Aarhus University, DCE – Danish Centre for Environment and Energy ©
URL:	http://dce.au.dk/en
Year of publication:	October 2017
Editing completed:	September 2017
Referee:	Karen Timmermann
Quality assurance, DCE:	Poul Nordemann Jensen
Financial support:	This work was part of the BNI (Baltic Nest Institute) funded by Aarhus University (AU). Additional funding was provided by the EU FP7-SPACE-2011 project MyOcean2 (grant no. 283367) and by the Danish Council for Strategic Research project “Integrated Management of Agriculture, Fishery, Environment and Economy” (IMAGE, grant no. 09-067259)
Please cite as:	Larsen J, Maar M, Brüning T, She J, Mohn C. 2017. Flexsem: A new method for offline ocean modelling. Aarhus University, DCE – Danish Centre for Environment and Energy, 28 pp. Technical Report from DCE – Danish Centre for Environment and Energy No. 105. http://dce2.au.dk/pub/TR105.pdf
	Reproduction permitted provided the source is explicitly acknowledged
Abstract:	3D marine biogeochemical models require forcing from a hydrodynamic model in order to move nutrients and algae (state variables) around by advection. Often the biogeochemical model is run online (at the same time) as the hydrodynamic model. Some model systems offers offline capability, where the hydrodynamic forcing is stored in files and read in while running the biogeochemical model. However, the models are still run on the same computational mesh. Here we present a novel method implemented in the Flexsem model framework that allows running the biogeochemical model on an unstructured computational mesh forced by a structured grid hydrodynamic model. This method offers much greater flexibility in choosing a computational mesh more suitable to the biogeochemical problem.
Keywords:	Model software; marine modelling; ecological modelling; offline advection-diffusion; unstructured mesh; flux interpolation.
Layout:	Anne van Acker
Drawings:	The authors
Front page illustration:	Kattegat bathymetry with a Flexsem unstructured mesh on top by Janus Larsen
ISBN:	978-87-7156-285-9
ISSN (electronic):	2245-019X
Number of pages:	28
Internet version:	The report is available in electronic format (pdf) at http://dce2.au.dk/pub/TR105.pdf

Contents

Preface	5
Summary	6
Sammenfatning	7
1 Introduction	8
2 Method	10
2.1 Flexsem framework	10
2.2 Flexsem computational mesh	11
2.3 Calculating the fluxes	12
2.4 Adjusting unstructured fluxes to ensure conservation of mass	13
2.5 Advection scheme on the structured mesh	14
3 Computational experiments	15
3.1 Test cases	15
4 Results	17
4.1 Mesh types	17
4.2 Accuracy of the method	18
4.3 Conservation of mass	18
4.4 Time-steps	20
5 Discussion	21
6 Conclusions	23
7 References	24
Appendix A	28

[Blank page]

Preface

In this report, we present a new method that enables running unstructured 3D marine biogeochemical models in the Flexsem framework forced by velocity fields from an external structured grid hydrodynamic model. This development of an offline capability to Flexsem was a part of work carried out under the Baltic Nest Institute (BNI), MyOcean2 and the Image projects.

Summary

Assessment of complex marine ecosystems requires a detailed understanding of processes, drivers and their interactions across multiple scales. This information is exceedingly provided by complex three-dimensional (3D), often simultaneously online coupled physical and ecosystem models, setting great demands on computing and operating resources and skills. The present study demonstrates a novel model system for fully 3D offline flexible mesh advection forced by velocities from structured grid models. The offline method is here described in detail and validated by assessing the errors of an analytical solution. Different case studies with passive tracers evaluated the model performance and effects of different computational meshes and time-steps. The method was shown to be accurate with a low error term for both mass balance and transformation of an analytical velocity field. The offline unstructured model yielded general distribution patterns of passive tracers comparable to the original structured grid tracer distribution. Further, it was demonstrated that the flow field can be interpolated to create a higher spatial resolution in the offline unstructured model although without additional information of flow patterns, which will enable high resolution modelling of e.g. nutrients and pollutants leaking from open water aquacultures or particle tracking. Hence, the method was shown suitable for future implementation of offline models in various areas including fjords, estuaries, coastal and open marine waters with any available hydrodynamic forcing.

Sammenfatning

Vurdering af marine økosystemer kræver en detaljeret forståelse af processer, presfaktorer og deres interaktioner i tid og rum. Denne forståelse opnås i stigende grad via komplekse tredimensionale (3D) økosystemmodeller. Disse modeller bruger oftest en 'online' kobling mellem den fysiske model og den økologiske model, dvs. at begge modeller kører samtidigt på den samme rumlige modelopløsning (beregningsnet). Denne metode er dog ofte beregningstung, tidskrævende og kræver en supercomputer. I denne rapport demonstreres en ny, hurtigere og mere fleksibel metode (Flexsem), hvor den økologiske model kan køre 'offline' dvs. alene ved indlæsning af gemte fysikfiler. Samtidig kan Flexsem køre på en anden rumlig opløsning end den fysiske model. Dvs. det nye ved denne metode er, at Flexsem kan bruge et mere fleksibelt ustruktureret beregningsnet (polygoner), selvom fysikken stammer fra et struktureret beregningsnet (kvadrater). Vi validerede Flexsem ved at teste massebalancen og se på den modellerede fordeling af passive sporstoffer på forskellige beregningsnet. Flexsem viste sig at bevare massebalancen og dermed give en nøjagtig beskrivelse af fysikken. Desuden gav Flexsem det generelle fordelingsmønstre af passive sporstoffer som for den fysiske model. Vi demonstrerede også muligheden for at interpolere hastighedsfelterne i et mindre område, således at den rumlige opløsning forøges. Dette muliggør en mere nøjagtig beskrivelse af spredningen af fx næringsstoffer og forurenende stoffer fra et havbrug, ferskvandskilde eller lignende. Flexsems brugervenlighed gør det endvidere nemt at udvikle nye økologiske modelkomponenter, som fx kan beskrive miljøtilstanden (Chl *a*, iltvind, bunddyr, m.m.). Metoden kan bruges til implementering af økosystemmodeller i forskellige områder (herunder fjorde, flodmundinger, kystnære samt åbne havområder), hvor der er adgang til en fysisk model, og man ønsker en fleksibel, brugervenlig og hurtig løsning, der kan køre på en almindelig pc. Denne enkelhed gør Flexsem egnet som et fremtidigt forvaltningsværktøj.

1 Introduction

The development and application of fast and flexible marine modelling tools is an increasingly important and recommended approach to support integrated assessments, adaptive management e.g. implementation of the Marine Strategy Framework Directive and conservation of vulnerable marine and coastal ecosystems (Fulton et al. 2011; OSPAR 2012). In addition, hydrodynamic and ecological modelling has become an important tool in marine research (Piroddi et al. 2015).

Improved understanding of many aspects of marine ecosystem dynamics and functioning, together with the availability of powerful computing resources, have created a wealth of ecosystem models over the past three decades including simplified box models (Raillard & Menesguen 1994; Grant et al. 2007; Savchuk & Wulff 2009), spatial explicit end-2-end models (Fulton 2010; Shin et al. 2010; Smith et al. 2011), and complex 3D high-resolution models (Baretta et al. 1995; Neumann 2000; Skogen et al. 2004; Daewel & Schrum 2013). The predictive and analytical capacity of ecosystem models is largely determined by their capability to resolve the dynamical scales of key processes, drivers and feedbacks (North et al. 2008; Paris et al. 2013). Whilst analysis of complex ecosystem dynamics on high spatial and temporal resolutions often stimulates the use of equally complex and online (coupled) 3D physical-biogeochemical dynamical models, where all physical and biogeochemical equations are solved simultaneously for each time step. The advantage of online coupling is that allows support for 2-way coupling, e.g. where the shading effect of algae affects the water temperature. Drawbacks are large computational effort and specialist manpower requirements (Fulton et al. 2004; Filgueira et al. 2012). A practicable solution to this challenge is to use offline coupling or other multi-scale nesting techniques (Fulton et al. 2004; Mason et al. 2010). In offline coupling, the physics are solved first and stored and the biogeochemical model is run subsequently by using the physical fields at different time steps. This will lead to significant reduction of large computational overheads generated by simultaneously running multiple models to facilitate exchange of boundary conditions and forcing (Umgiesser et al. 2003; Cailleau et al. 2008). Another advantage is the resolving of small spatial scales in single or multiple areas of special interest with high flexibility in the design of the computational mesh (Mason et al. 2010).

Recent alternative advances in the development of physical-biogeochemical ocean models focused on combining full model capabilities and flexible offline coupling options with ease of use, thus offering non-specialists and early stage researchers easier access to ecosystem modelling tools without the need of expert knowledge in computer programming (Filgueira et al. 2012; Ferreira et al. 2014; Blauw et al. 2009; Pereira et al. 2006). *Table 1.1* provides an overview of the main characteristics of the most popular and widely distributed modelling tools offering optional or fully functional offline coupling. However, the existing offline solutions are often dependent on the mesh type (unstructured or structured) of the hydrodynamic forcing, thus providing little flexibility in the model set-up. The present study demonstrates a new 3D offline advection method that allows both unstructured and structured mesh types irrespective of the hydrodynamic forcing as a feature of the Flexsem model system (Larsen et al. 2013). This method provides extra benefits in terms of i) flexibility in the choice of hydrodynamic forcing

and ii) the possibility to use an unstructured mesh to model the geometrically complex regional topography, rather than try to model the complex region within a larger-scale structured Cartesian grid system.

Table 1.1. Examples of popular 3D ocean model systems that can run offline with ecological modules. HD = hydrodynamic.

Model system	Characteristics	Coupling	Web pages/references
EcoDynamo	Same mesh as HD model, ecological modules	Online/ offline	(Duarte et al. 2008; Pereira et al. 2006)
CAEDYM	Same mesh as HD model, ecological modules	Online/ offline	http://ecobas.org/www-server/rem/mdb/caedym.html (Hipsey et al. 2008)
FVCOM	Same mesh as HD model, ecological modules	Online/ offline	http://fvcom.smast.umassd.edu/fvcom/ (Tian et al. 2015)
Simile	Same mesh as HD model, Visual Modelling Environment with ecological sub-models	Offline	http://www.simulistics.com/index.htm (Filgueira et al. 2012)
EcoWin2000	Same mesh as HD model, an object oriented programming tool to implement ecological modules	Offline	http://www.ecasatoolbox.org.uk/the-toolbox/eia-species/models/ecowin (Ferreira et al. 2014)
DELFT3D-GEM	Same grid as HD model, ecological modules	Online/ offline	http://oss.deltares.nl/web/delft3d/delwaq (Blauw et al. 2009)
MIKE Eco-lab	Same mesh as HD model, complete numerical laboratory for ecological modelling	Online/ offline	https://www.mikepoweredbydhi.com/products/eco-lab (Edelvang et al. 2005)
Atlantis	Polygon mesh, aggregated physics from HD models, end-2-end food web model	Offline	http://atlantis.cmar.csiro.au/ (Fulton et al. 2011)
LTRANS	Same mesh as HD model, Lagrangian particle tracking model	Offline	http://northweb.hpl.umces.edu/LTRANS.htm (Schlag, 2012)
Flexsem	Same or converted mesh (structured to unstructured) from HD model, ecological modules	Offline	http://marweb/flexsem/ Present study

The new offline advection method described in this paper is applied to an open water system, the Kattegat, located in the western Baltic Sea with strong salinity gradients and narrow straits (Maar et al. 2011). The method combines Flexsem, a flexible 3D ecological modelling framework based on an unstructured mesh with hydrodynamics derived from a traditional structured 3D hydrodynamic model (HBM).

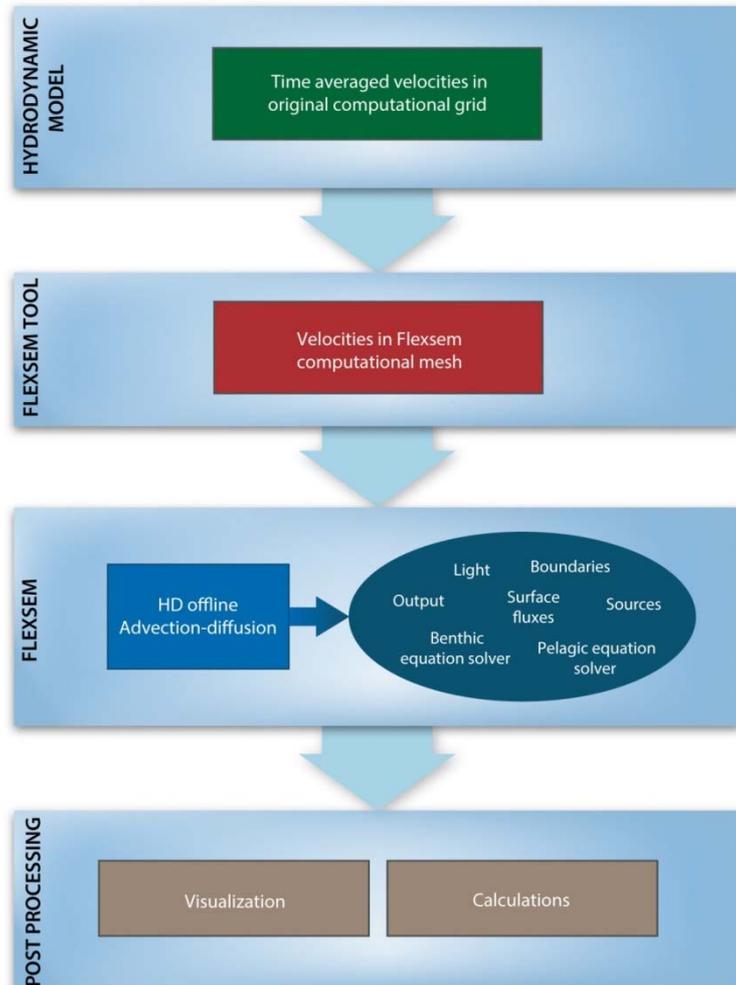
The method is assessed by examining the errors of the transformation of a known analytical solution and tested by releasing passive tracers on different computational mesh types and time-steps, comparing the tracer distributions with output from the original hydrodynamic model providing the forcing data. Computational details are presented in Section 2, the model test cases are described in 3 and the results presented in Section 4. Section 5 is a discussion of the applicability of this offline coupling method in open water systems and Section 6 summarizes the major conclusions and perspectives.

2 Method

2.1 Flexsem framework

The Flexsem framework is designed to construct 3D marine ecological models in a flexible and easy way with respect to hydrodynamic forcing, model domain, mesh type and resolution, and implementation of biogeochemical processes. Ease of use has been prioritized in the system design allowing scientists and students to perform 3D ecological modelling without requiring advanced programming skills. The user can setup the model, including the ecological equation system, by editing a text file and running the model with a precompiled executable. A modular build-up of Flexsem allows the user to run different parts of a model system separately, a feature that is useful e.g. for testing sediment modules separately before the model coupling. The offline hydrodynamic (offline HD) approach presented in this paper requires forcing from an external hydrodynamic model. Before the standard Flexsem modules can be used in combination with the HD offline module, the external velocity fields must be pre-processed to obtain a file with the necessary information to solve the advection-diffusion equation in Flexsem. After using the Flexsem framework to model tracer advection or ecological processes, results can be visualized with Flexsem or post-processed and visualized in a different environment such as R or Matlab. This workflow is illustrated in *Fig. 2.1*.

Figure 2.1. Schematic illustration of the structure and modular construction of Flexsem and the offline system. In Flexsem, all the sub-models shown in the oval can be run in any combination.



The existing modules include a 3D pelagic equation system, two-way coupled benthic equation system, atmospheric exchanges and simplified shallow estuary hydrodynamics (HDLite) (Larsen et al. 2013). In the present study, a fully 3D offline advection method was implemented in the Flexsem framework, as an alternative to the HDLite module.

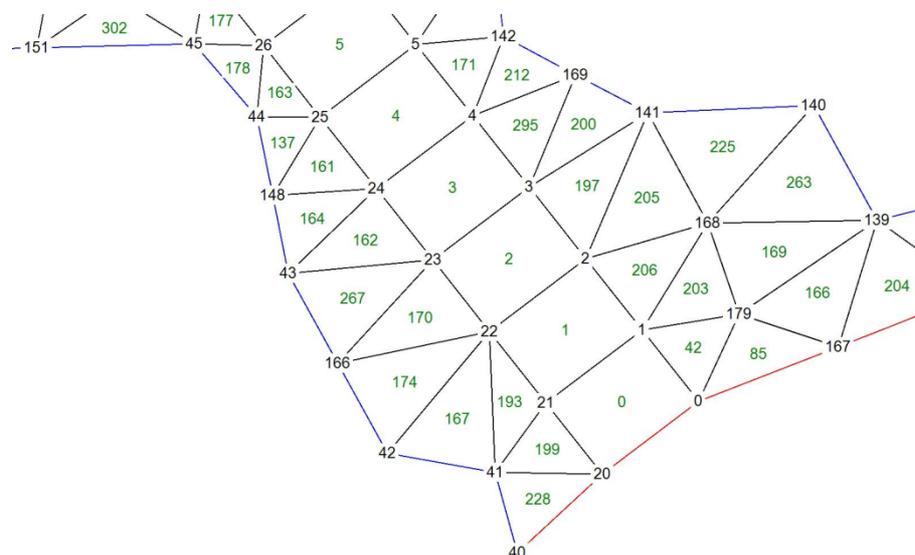
The 3D unstructured marine modelling software Flexsem was developed by Department of Bioscience, Aarhus University, Denmark. Flexsem is licensed under the GNU General Public License (GPL) version 3 and is freely available on the website.

2.2 Flexsem computational mesh

In an offline model system, the downstream (biogeochemical/tracer) model, needs to read in pre-calculated velocity fields and solve the advection-diffusion equation for the state variables/passive tracers.

The offline advection method described here, is implemented on an unstructured computational mesh. The mesh is defined by a number of nodes, faces and elements. Each node consists of a pair of position coordinates (XCoor, YCoor). Nodes are connected by faces and three (or more) faces make up a polygon defining a mesh element (Fig 2.2). In the horizontal plane, there are three types of faces: internal faces, which have an element on each side, land faces, which have an element on one side and land on the other and open boundary faces, which have an element on one side and a boundary condition on the other (Fig. 2.2).

Figure 2.2. Part of an unstructured mesh. Element numbers are given in green and node numbers in black. Blue lines are land faces, red lines are open boundary faces and black lines are internal faces.



The method is implemented in z coordinates, i.e. the separation between computational cells in the vertical are defined at fixed depths. The top layer has a free surface to allow for water level changes and the remaining layer depths can be freely defined by specifying thicknesses for all layers.

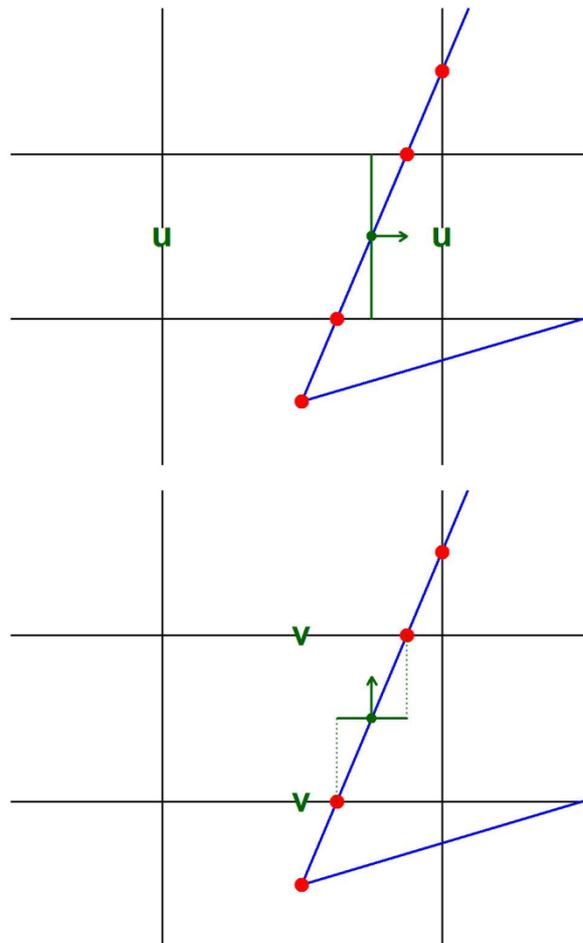
The model bathymetry, i.e. the depth of each element, and the number of layers in each element defines the vertical discretization. Each computational cell will have a number of vertical faces that connects it to the adjacent water filled cells as well as top and bottom horizontal faces. There is no volume transport across the bottom in the deepest layer. The surface layer has a top face that allows for free surface movement.

2.3 Calculating the fluxes

In order to calculate the advection, the flux of water has to be known at all internal faces that have a water-filled computational cell on each side and at all open boundary faces. These fluxes can be obtained by solving the Navier Stokes equations with the shallow water approximation on the unstructured mesh (Casulli & Walters 2000). In the present offline method, these equations have been solved on a structured computational grid and mass conservative average velocities and surface heights were made available by the 3D ocean circulation model Hiromb-BOOS Model (HBM) (She et al. 2007; Berg & Poulsen 2012) (see *Appendix A*).

In order to calculate the fluxes through the faces in the unstructured mesh from the structured velocities, a ‘mapping’ between the model computational meshes was made. Each unstructured face was divided into sections according to the intersections between the meshes - see *Fig. 2.3*. For each of the sections between two intersections, the flux was calculated by linear interpolation of the adjacent u and v velocities to the center point of the section. The interpolated velocities were multiplied by the length of the orthogonal projection of the sections (green lines in *Fig. 2.3*) onto the structured grid and the layer thickness to obtain the section flux. The face flux is then the sum of the u and v fluxes through all sections of the face.

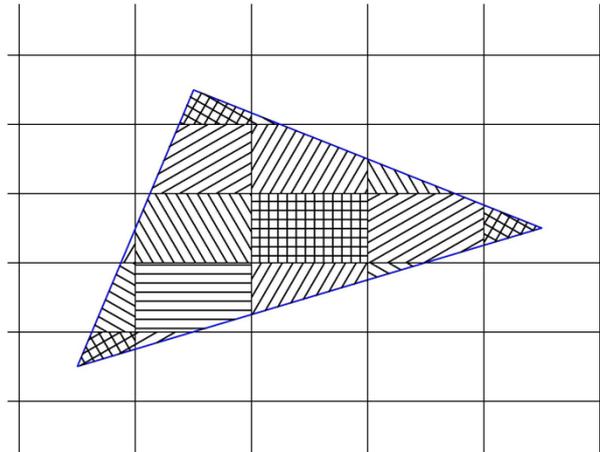
Figure 2.3. The flux through a face in the unstructured mesh is calculated by finding the intersections between the face and the grid cell boundaries in the structured mesh.



The vertical fluxes through the horizontal top of each unstructured computational cell were calculated by an area average of the overlap between the unstructured element and the structured grid (*Fig. 2.4*). The area of the poly-

gons that make up the overlap between the unstructured element and the structured grid was found by polygon clipping (Vatti 1992).

Figure 2.4. The vertical velocity in each unstructured element is calculated by an area average of the overlapping structured grid cells. The overlaps are indicated with different patterns in the figure.



2.4 Adjusting unstructured fluxes to ensure conservation of mass

One approach for ensuring conservation of mass would be to use the horizontal fluxes to calculate the vertical velocities by integrating from the bottom and upward. However, that would cause all errors from the interpolation and numerical issues to be absorbed in the vertical velocities. Since the accuracy of the vertical velocity is of great importance to ecological modeling and considering the fact that in the ocean vertical velocities are much smaller than horizontal velocities, the adjustment to the obtained fluxes to ensure mass conservation is done in the horizontal fluxes.

The adjustment of the advective horizontal fluxes is done in one layer at a time. The residual in all computational elements of fixed height is calculated by adding up all fluxes to the current element:

$$R_e = \left[A_e(w_t - w_b) + \sum_f^n L_f dz_f u_f \right] dt$$

where R_e is the residual in element e , A_e is the element area, w_t and w_b are the vertical velocities at the top and bottom of the cell, L_f is the length of face f , dz_f is the face height, u_f the horizontal velocity, n is the number of faces (polygon sides) in element e and dt the length of the time step.

A system of linear equations with one equation for each element and one unknown for each horizontal flux (corresponding to an internal or boundary face) in the current layer is set up. In each equation, the sum of corrections to the horizontal fluxes relevant for the current element equals the residual. Assuming no corrections to the vertical velocities, the relation between horizontal velocity corrections and the residuals become:

$$dt \sum_f^n L_f dz_f u_{f,c} = R_e$$

where $u_{f,c}$ is the unknown velocity correction to u_f .

The system, which is overdetermined if there are more elements than faces, is solved by the LSQR; an algorithm for Sparse Linear Equations and Sparse Least Squares (Paige & Saunders 1982), to obtain $u_{f,c}$.

2.5 Advection scheme on the structured mesh

Once the mass-conservative fluxes have been obtained, the advection of passive tracers or ecological state variables can be calculated by different numerical methods. Here the semi-implicit finite volume method suggested by Casulli and Zanolli (Casulli & Zanolli 2002) is used. An offline file stores the horizontal flux for each internal and boundary face at all offline time steps. At runtime, the vertical fluxes and the free surface height is calculated by integrating the fluxes from the bottom and up in each element. Any river inflow that originates from the forcing hydrodynamic model contributes to the mass balance in the relevant elements and is thus also included in the offline file.

The temporal interval at which the fluxes are stored in the offline file, i.e. the offline time step, can be set to any multiple of the advection time step in the hydrodynamic model. Depending on the timescale of the processes studied it is practical to optimize offline file size versus temporal resolution. The offline time step may be longer than necessary for ensuring numerical stability of the advection method and a sub-cycling of the advection method was therefore implemented as suggested by Casulli and Zanolli (Casulli & Zanolli 2002). The length of the time-step that ensures numerical stability can be estimated from the Courant-Friedrichs-Lewy (CFL) stability criterion, which states that time-step must be smaller than the time taken to travel the distance of the spatial step (Courant et al. 1928). Since the velocities and distances are known, the maximum time-step length can readily be calculated and if longer than the offline time step, the advection solved using a sub-cycling necessary to ensure numerical stability.

An offline model will typically require access to state variables from the hydrodynamic model, e.g. a biogeochemical model that requires information about salinity and temperature. In Flexsem, such variables can optionally be treated as offline state variables, thus be advected by the offline model or accessed by outputting them from the hydrodynamic model and adding them to the offline model as 3D time varying forcing.

The advection of independent state variables is very suitable for parallelization with OpenMP on a shared memory computer. This has been implemented in the Flexsem code, and it scales very well; on an eight core computer, eight tracers are advected in the same time as one tracer. However, output of results to a file is not parallelized, so in practice there is some overhead of multiple tracers when outputting the results.

3 Computational experiments

The above method of reconstructing fluxes from a structured grid model to fluxes on an unstructured mesh was implemented in c++. The program reads time averaged velocity field outputs from the HBM model (see *Appendix A*) in netCDF format, calculates the fluxes on the faces of the unstructured mesh, adjusts them to obtain exact conservation of volume and outputs the information to an offline file. A semi-implicit advection-diffusion scheme following Casulli and Zanolli (Casulli & Zanolli 2002) were implemented as a module in Flexsem. In each time step, the HD module reads the fluxes and calculates the advection and diffusion of any state variable defined in the pelagic equation solver. In order to test the method described above, a number of tests were conducted. No explicit diffusion was used in HBM nor in Flexsem in these offline test cases, thus any diffusion originate from the computational diffusion of the advection schemes.

3.1 Test cases

In order to assess the accuracy of the method and compare the general distribution patterns of a passive tracer on different computational meshes versus the HBM tracer advection (Case 1a), three meshes were created; one identical to that of the HBM model (Case 1b), one coarse triangulated mesh (Case 1c) and one with very high resolution around an open water point source and the rest of the domain triangulated in a coarse resolution (Case 1d).

To evaluate the accuracy of the transport and mass conservation adjustment, a mass conservative artificial velocity field on the structured HBM mesh was created. The method described in section 2 was used to calculate the fluxes on the different test meshes and mass balance adjustment carried out. Finally the resulting velocities were compared to the analytical solution that created the artificial velocities. The function used was:

$$v(x, y) = u(x, y) = 0.25(\cos(6x) + \sin(6y))$$

Where x and y are the coordinates of the velocity locations. Because the HBM grid is staggered, u and v are not at the same locations and therefore not identical.

Furthermore, a case study (Case 2) was conducted for different time-steps (3, 15 and 60 min) using the HBM identical mesh (Case 1b). The HBM computational grid and the three Flexsem meshes cover the Kattegat Sea between Denmark and Sweden and there is one point source for the passive tracer release (*Fig. 3.1*). A statistical summary of the meshes is given in *Table 3.1*.

Table 3.1. Total number of computational cells and element size range for the test cases on different computational meshes. The HBM model setup (Case 1a) covers a larger area, but here only cells within the relevant area are counted. The CPU times from HBM were not comparable with the offline set-ups due to the different area and that HBM was run on a 48 core micro supercomputer.

Case	Description	Coupling	No. cells	Smallest element [m ²]	Largest element [m ²]	CPU time [s]
1a	HBM	Online	108970	3.1E6	3.2E6	-
1b and 2	HBM identical	Offline	108970	3.1E6	3.2E6	213
1c	Coarse unstructured	Offline	12079	1.6E6	7.6E7	6.4
1d	Sub HBM resolution	Offline	22501	2E5	7.6E7	13.4

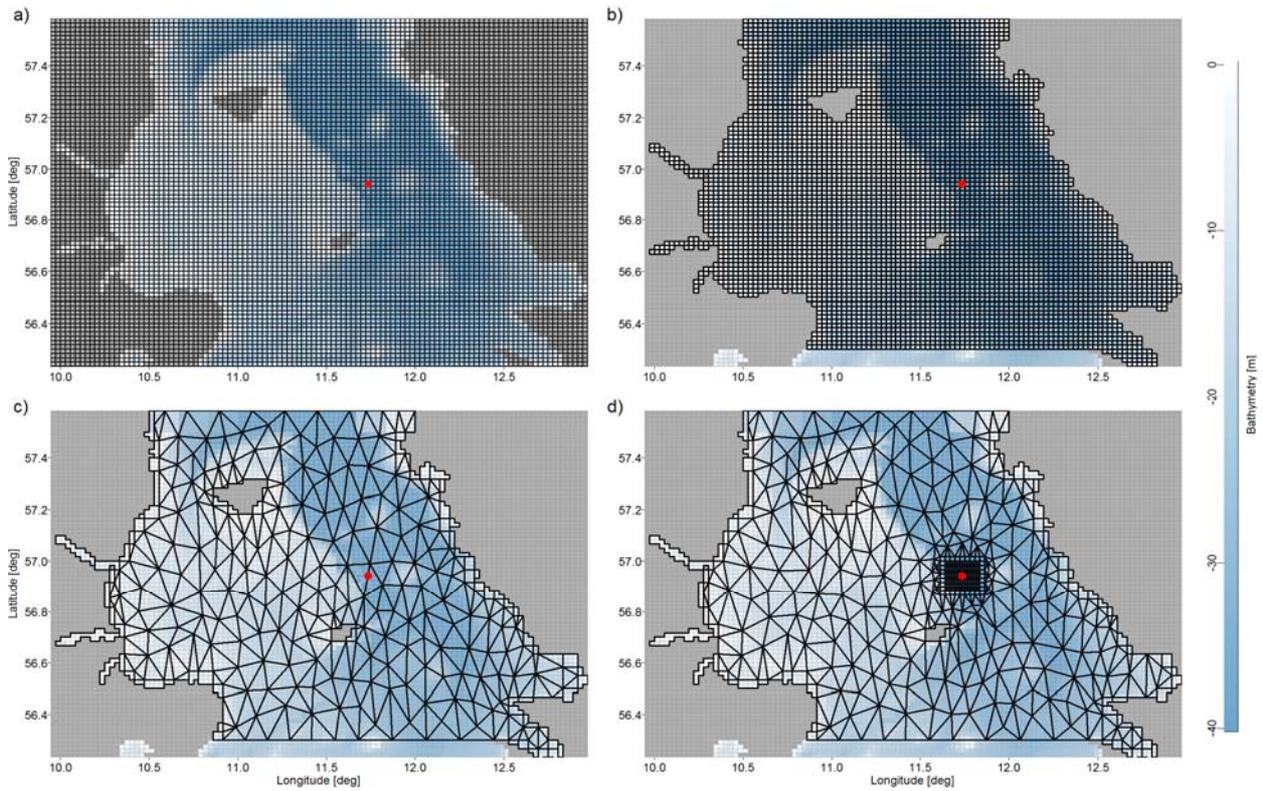


Figure 3.1. The computational mesh of a) the HBM hydrodynamic model (case 1a), b) the Flexsem computational mesh identical to that of the HBM model in the area (case 1b), c) the coarse triangulated computational mesh (case 1c) and d) the mesh with high resolution in the vicinity of the point source (case 1d).

In the triangulated meshes (*Fig. 3.1c* and *3.1d*), the coastal areas are of less interest for the present study and are therefore only very coarsely resolved using large polygons, hence saving computational time. The initial tracer value was set to zero, and the tracer value at the open boundaries was also set to zero. The point source added a tracer corresponding to an inflow of $1 \text{ m}^3/\text{s}$ and with a tracer concentration of 1. The models simulated January 2001 and 3D tracer concentrations were obtained from both models for comparison.

4 Results

4.1 Mesh types

All test cases (1a-d) showed the same general distribution pattern of the passive tracer after 3.5 days, although with some deviations (*Fig. 4.1*). When comparing the HBM results with the Flexsem results on the same spatial resolution (Cases 1a-b), it can be seen that the different advections schemes and the offline temporal interpolation gave a higher diffusion of the tracer in Flexsem (*Fig. 4.1a, b*). The coarse mesh did not show spatial details (Case 1c), but still retained the general pattern (*Fig. 4.1c*). The high-resolution offline run (Case 1d) with linear interpolation of the velocity field to HBM sub-resolution, showed details of the tracer plume, which was not included in the original HBM model run.

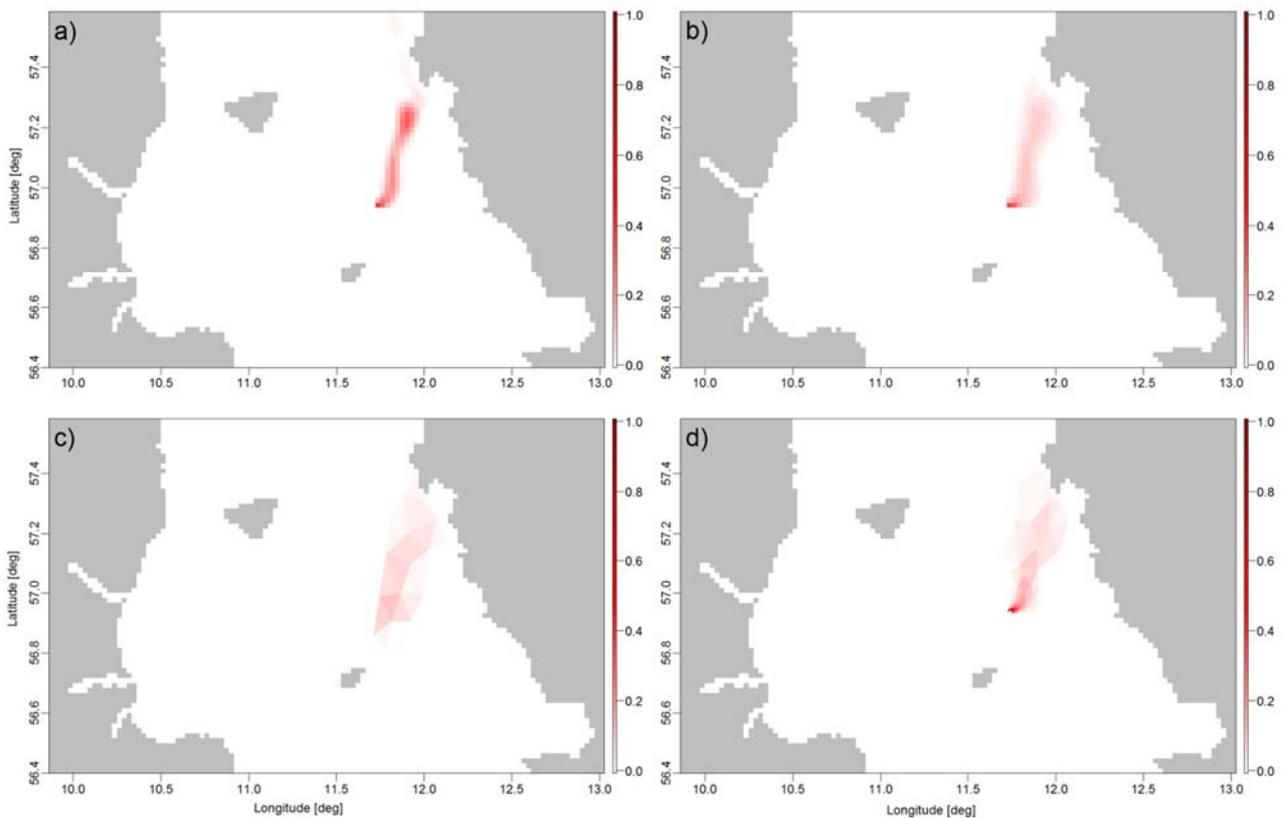


Figure 4.1. Surface tracer concentrations in test case 1 (a, b, c, d) model setups. Top left is HBM (a); top right Flexsem with computational mesh identical to that of HBM (b); bottom left, coarse Flexsem computational mesh (c) and bottom right, coarse Flexsem computational mesh, with high resolution in the vicinity of the open water source (d).

Furthermore, the CPU time was tested for three different Flexsem computational meshes (*Table 3.1*). The offline Flexsem code advected one tracer for one month in 213 seconds, on a 3.4 GHz Intel i7 processor when using the mesh identical to that of HBMs computational grid (Case 1b). In comparison, this took 6.4 seconds with the coarse Flexsem mesh (Case 1c), whereas the mesh with the high spatial resolution around the open water point source (Case 1d) took 13.4 seconds.

4.2 Accuracy of the method

The accuracy of the method was evaluated by creating an artificial 3D velocity field on the structured grid from an analytical solution, calculating the fluxes on the unstructured mesh and enforcing conservation of mass by the methods described above. The solution was evaluated in a 0.5×0.5 deg. area around the location of the open water source. *Table 4.1* summarizes the errors, i.e. the difference between velocities given by analytical solution and the velocities calculated by the described method on the unstructured meshes. The more the mesh deviates from the structured grid, the larger the error. The temporal interpolation implemented as a sub-cycling of the offline time-step in solution of the advection-diffusion equation is linear and hence first order accurate.

Table 4.1. Errors of the velocities on the different unstructured meshes when compared to an analytical solution.

Case	Mean error	Error RMS
1b	1.8×10^{-4}	9.8×10^{-4}
1c	3.6×10^{-3}	4.8×10^{-2}
1d	3.2×10^{-2}	1.2×10^{-1}

4.3 Conservation of mass

Based on the HBM output, the method described in the previous sections was used to calculate the transport fluxes in the different flexible meshes. Due to loss of precision in the output format of HBM and the interpolation in time and space of the fluxes, the resulting velocity fields were very close to, but not exactly mass conservative. To enforce mass conservation, the method described in section 2 was used to adjust the velocity fields thereby obtaining exact mass conservation. Typical maximum residuals were in the order of 10 to 30 m³, in element sizes of 10-100 e⁶ m³, corresponding to less than 1e⁻⁴ percent. When adjusting the velocity field to obtain mass conservation within floating point precision, this resulted in adjustments to the horizontal velocities in the order of 1e⁻⁵ to 1e⁻⁶ ms⁻¹. In meshes that were identical to that of the original HBM, spatial interpolation was avoided and the residuals were smaller, typically 5-15 m³.

Surface tracer concentrations in the HBM and Flexsem model simulations at 3, 8 and 14 days after model start for cases 1a and 1b are shown in *Fig. 4.2*. It can be seen that the general advection distribution patterns were the same for the two models, however, the numerical diffusion was larger in the Flexsem advection than in HBM. In order to verify mass conservation and quantify the concentration differences, the total tracer mass was calculated over time (*Fig. 4.3*). The tracer stayed inside the domain for approximately 2.5 days, after which it started to flow out of the model domain through the open boundaries. This is illustrated in *Fig. 4.3* where the circles (model tracer mass) deviate from the line (cumulative tracer mass). After the tracer flows out of the domain, the total mass differed in the two models due to the slightly different distribution patterns. E.g. after 4.5 days the total tracer mass differed by 2.5 %.

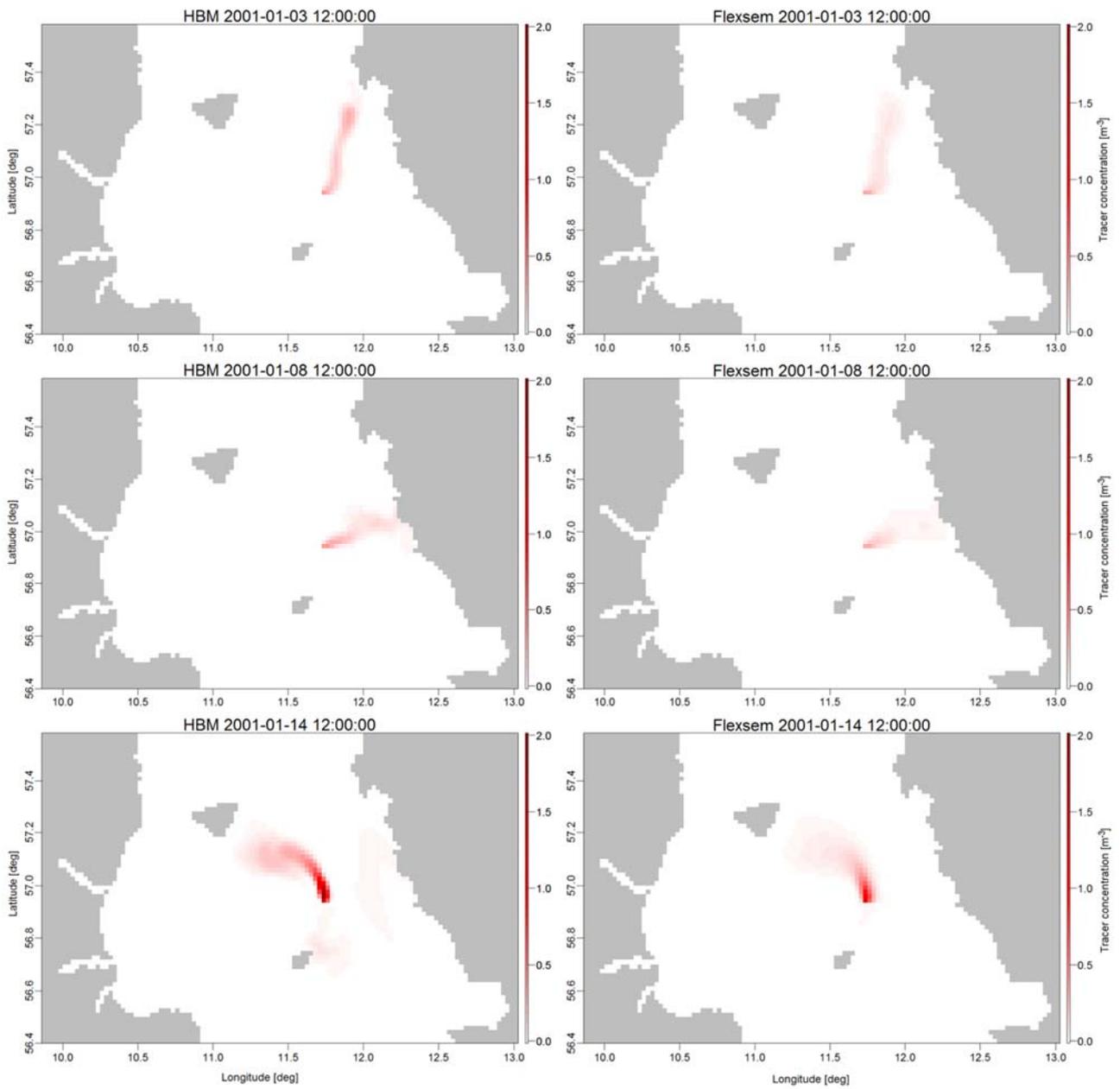
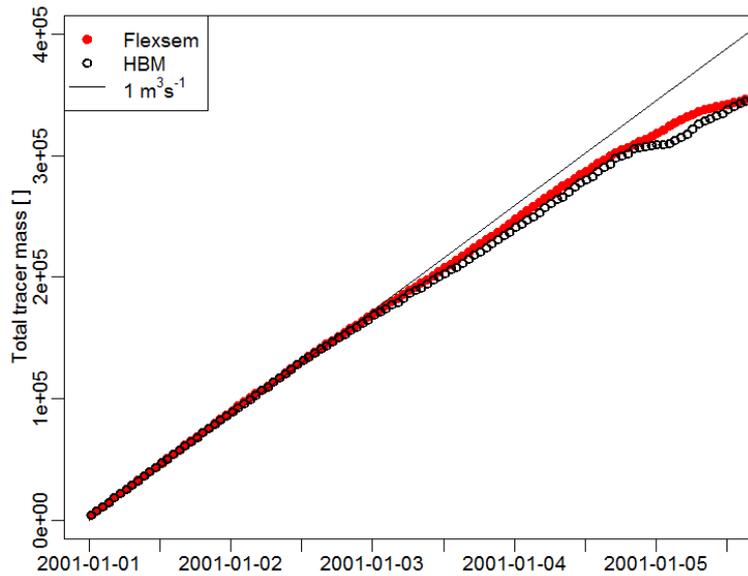


Figure 4.2. Colour coded maps of surface tracer concentrations at three different times for identical computational meshes. Left column is HBM (case 1a) and right column is Flexsem (case 1b).

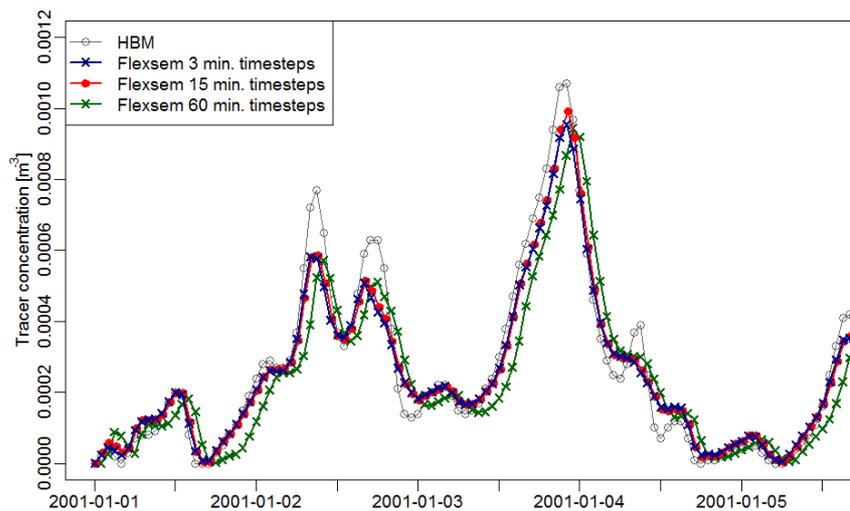
Figure 4.3. The total tracer mass in the domain (case 1b) has been calculated, by multiplying the tracer concentration in each computational cell with the volume of the cell and summing it up. The inflow rate of $1 \text{ [m}^3\text{s}^{-1}\text{]}$ and concentration of $1 \text{ [m}^{-3}\text{]}$ are constant in time. Until tracer mass starts to flow across the open boundaries approximately 2.5 days after model start, the total tracer mass in the models (circles) equals the inflow flux times the tracer concentration of the inflow (line).



4.4 Time-steps

Test case 2 was used to evaluate the effect of different lengths of the offline time-step. The averaged HBM velocities were stored at 3, 15 and 60 minutes intervals. In the 60 minutes case, a factor 4 was used in the sub-cycling, so that the 60 minutes averaged HBM velocities were linearly interpolated to 15 minutes in the solution of the advection equation. Time-series of tracer concentration in the surface cell east of the source cell for HBM and the 3 Flexsem simulations were compared (Fig. 4.4). The coefficient of determination R^2 between the HBM concentrations and the 3 minute Flexsem concentrations was 0.9222. The R^2 value measuring the difference between the 3 minute Flexsem simulation and the 15 and 60 minute Flexsem simulations were 0.9988 and 0.8903, respectively.

Figure 4.4. Test case tracer concentration in the cell to the east of the source cell in HBM and in Flexsem for three different lengths of the offline time-step.



5 Discussion

The concept of offline tracer advection, and thereby potentially an ecological model, from the hydrodynamic computations by storing the fluxes in a file, thus saving the computational effort of solving the hydrodynamic equations when rerunning the tracer advection/ecological model is well known and widely used (Filgueira et al. 2012; Ferreira et al. 2014; Blauw et al. 2009). However, this is typically done on the same computational mesh and in the same model system. Here, the concept has been taken further by developing and implementing a method to solve the tracer advection on a different computational mesh in a separate model system. This has the advantage of being much more flexible when defining resolution and spatial coverage of the ecological model, without having to calibrate and validate a new hydrodynamic model. It also enables coupling of one ecological model system to several different hydrodynamic models.

The combined velocity field interpolation and mass conservation was validated by accessing the accuracy of the method. On coinciding meshes, the errors were in the order of 10^{-3} to 10^{-4} and between 10^{-1} and 10^{-2} using a fully unstructured mesh on a structured grid (*Table 4.1*). These errors are in the same order of magnitude as unstructured mesh interpolation methods (Wang et al. 2011).

Tracer advection in the offline system was also validated by comparing it to a tracer advected by the original HBM model and it was found that the passive tracer concentrations in Flexsem is close, but not identical to that of the HBM model. The difference between the tracer distributions in HBM and Flexsem is mainly due to the difference in advection schemes; the semi-implicit upwind scheme of Flexsem is more diffusive than the flux-corrected transport scheme of HBM, thus leading to lower Flexsem surface tracer concentrations after 14 days (see *Fig. 4.2*). Time averaging in the HBM output and the optional linear temporal interpolation in the sub-cycling of the advection-diffusion calculation may also lead to differences.

Exact mass conservation is obtained by calculating adjustments to the interpolated velocity fields. These adjustments compensate for the inaccuracies arising from the interpolations and loss of precision in the output formats. The velocity adjustments are in the order of $1e^{-5}$ to $1e^{-6}$ ms^{-1} which is considerably smaller than the characteristic velocities in open water of 0.1-1 ms^{-1} (Nielsen 2005). Thus, this adjustment of the velocity field does not alter the general flow pattern.

As expected too long offline time-steps results in reduced accuracy (*Fig. 4.4*). The difference between 3 minute and 15 minute offline time-steps is very small ($R^2 = 0.9988$), but in the case of a 60 minute offline time-step the tracer concentration differs relative to the 3 minute offline time-step during some periods ($R^2 = 0.8903$). This is expected as 60 minutes is too long to resolve the higher frequency spectrum of the water movement in the study area. The appropriate length of the offline time-step will be dependent on the characteristic timescales of the physical processes in the modelled area.

In test case 1d, a computational mesh with elements smaller than that of HBM was constructed for Flexsem (*Fig. 3.1d*). The velocities in these cells are

calculated as linear interpolations of the HBM field. Although the subscale resolution does not contribute to additional information about the flow field itself, it still allows to study phenomena in open water associated with offshore structures that not alter the general flow field itself, e.g. offshore aquaculture facilities or wind farms. The high resolution can be used in an ecological model to simulate small-scale distribution of nutrients- and chlorophyll concentrations and Secchi depths around a point source. In addition, computational effort is optimized by using a high vertical resolution in the upper part of the water column and a coarser in the deeper. The higher resolution of the computational mesh in the area of interest is compensated by the coarse resolution in the rest of the domain and in the vertical, thus resulting in a much faster advection model. This setup (mesh in *Fig. 3.1d*) is 15 times faster than the mesh identical to that of HBM and simulates advection of a tracer for one month in only 13.4 seconds (*Table 3.1*).

Because the offline method implies a one-way coupling, it leaves out the possibility that processes in the offline model can affect the hydrodynamic model. In the case of biogeochemical models, such feedback is low and rarely taken into account. However, in water columns with high particle concentrations, self shading (i.e. modulation of light intensity in the presence of algae) can affect the water temperature (Burchard et al. 2006).

6 Conclusions

Scientific and management challenges of complex biogeochemical processes in open oceanic and coastal zone ecosystems often stimulate the use of equally complex and resource intensive modelling tools. The emphasis of Flexsem is on a flexible and easy adaptation to different areas of interest, as well as on low computational effort. The scope of possible applications includes ecological modelling, tracer studies and particle tracking. However, the implementation of a fully unstructured 3D offline tracer and ecological state variable advection-diffusion formulation allows multi-scale offline coupling with data from independent model output, without traditional requirements of using the same computational mesh in the offline model as in the hydrodynamic model.

We have demonstrated that the method presented here is accurate and yields general distribution patterns of passive tracers in an offline unstructured model is comparable to the original structured grid tracer distribution. Choice of spatial resolution in the unstructured model affects the advection significantly, as do temporal resolution in the offline output and choice of the advection-diffusion scheme.

Further, we have shown that the flow field provided by the external hydrodynamic model can be interpolated to create a higher spatial resolution in the offline unstructured model. Although this will not add additional information to the flow pattern, it will enable high resolution modelling of e.g. nutrients and pollutants leaking from open water aquacultures or particle tracking. Hence, the method has a high potential for future implementation of offline models in various areas including fjords, estuaries, coastal and open marine waters with any available hydrodynamic forcing.

7 References

<http://www.matlab.com/>

<http://www.r-project.org/>

<http://marweb.dmu.dk/Flexsem/>

Baretta JW, Ebenhoh W, Ruardij P. 1995. The European-Regional-Seas-Ecosystem-Model, a Complex Marine Ecosystem Model. *Netherlands Journal of Sea Research* 33:233-246.

Berg P, Poulsen JW. 2012. Implementation details for HBM. Report no.

Blauw AN, Los HFJ, Bokhorst M, Erfteimeijer PLA. 2009. GEM: a generic ecological model for estuaries and coastal waters. *Hydrobiologia* 618:175-198.

Brüning T, Janssen F, Kleine E, Komo H, Maßmann S, Menzenhauer-Schumacher I, Jandt S, Dick S. 2014. Operational Ocean Forecasting for German Coastal Waters. *Die Küste* 81:273-290.

Burchard H, Bolding K, Kuhn W, Meister A, Neumann T, Umlauf L. 2006. Description of a flexible and extendable physical-biogeochemical model system for the water column. *Journal of Marine Systems* 61:180-211.

Cailleau S, Fedorenko V, Barnier B, Blayo E, Debreu L. 2008. Comparison of different numerical methods used to handle the open boundary of a regional ocean circulation model of the Bay of Biscay. *Ocean Modelling* 25:1-16.

Casulli V, Walters RA. 2000. An unstructured grid, three-dimensional model based on the shallow water equations. *International Journal for Numerical Methods in Fluids* 32:331-348.

Casulli V, Zanolli P. 2002. Semi-implicit numerical modeling of nonhydrostatic free-surface flows for environmental problems. *Mathematical and Computer Modelling* 36:1131-1149.

Courant R, Friedrichs K, Lewy H. 1928. Partial differential equations of mathematical physics. *Mathematische Annalen* 100:32-74.

Daewel U, Schrum C. 2013. Simulating long-term dynamics of the coupled North Sea and Baltic Sea ecosystem with ECOSMO II: Model description and validation. *Journal of Marine Systems* 119:30-49.

Dick S, Kleine E, Müller-Navarra SH, Klein H, Komo H. 2001. The operational circulation model of BSH (BSH cmod). Model description and validation. *Berichte des Bundesamtes für Seeschifffahrt und Hydrographie* 29/2001.

Duarte P, Azevedo B, Guerreiro M, Ribeiro C, Bandeira R, Pereira A, Falcao M, Serpa D, Reia J. 2008. Biogeochemical modelling of Ria Formosa (South Portugal). *Hydrobiologia* 611:115-132.

Edelvang K, Kaas H, Erichsen AC, Alvarez-Berastegui D, Bundgaard K, Jorgensen PV. 2005. Numerical modelling of phytoplankton biomass in coastal waters. *Journal of Marine Systems* 57:13-29.

EU 2008. Directive 2008/56/EC of the European Parliament and of the Council of 17 June 2008 establishing a framework for community action in the field of marine environmental policy (Marine Strategy Framework Directive). Pages 22: Official Journal of the European Union.

Ferreira JG, Saurel C, Silva JDLE, Nunes JP, Vazquez F. 2014. Modelling of interactions between inshore and offshore aquaculture. *Aquaculture* 426: 154-164.

Filgueira R, Grant J, Bacher C, Carreau M. 2012. A physical-biogeochemical coupling scheme for modeling marine coastal ecosystems. *Ecological Informatics* 7:71-80.

Fulton EA. 2010. Approaches to end-to-end ecosystem models. *Journal of Marine Systems* 81:171-183.

Fulton EA et al. 2011. Lessons in modelling and management of marine ecosystems: the Atlantis experience. *Fish and Fisheries* 12:171-188.

Fulton EA, Smith ADM, Johnson CR. 2004. Effects of spatial resolution on the performance and interpretation of marine ecosystem models. *Ecological Modelling* 176:27-42.

Grant J, Curran KJ, Guyondet TL, Tita G, Bacher C, Koutitonsky V, Dowd M. 2007. A box model of carrying capacity for suspended mussel aquaculture in Lagune de la Grande-Entree, Iles-de-la-Madeleine, Quebec. *Ecological Modelling* 200:193-206.

Hipsey MR, Antenucci JP, Brookes JD. 2008. A generic, process-based model of microbial pollution in aquatic systems. *Water Resources Research* 44.

Janssen F, Schrum C, Backhaus JO. 1999. A climatological data set of temperature and salinity for the Baltic Sea and North Sea. *German Journal of Hydrography (Suppl. (9))*:1-245.

Larsen J, Mohn C, Timmermann K. 2013. A novel model approach to bridge the gap between box models and classic 3D models in estuarine systems. *Ecological Modelling* 266:19-29.

Mason E, Molemaker J, Shchepetkin AF, Colas F, McWilliams JC, Sangra P. 2010. Procedures for offline grid nesting in regional ocean models. *Ocean Modelling* 35:1-15.

Maar M, Moller EF, Larsen J, Madsen KS, Wan ZW, She J, Jonasson L, Neumann T. 2011. Ecosystem modelling across a salinity gradient from the North Sea to the Baltic Sea. *Ecological Modelling* 222:1696-1711.

Neumann T. 2000. Towards a 3D-ecosystem model of the Baltic Sea. *Journal of Marine Systems* 25:405-419.

- Nielsen MH. 2005. The baroclinic surface currents in the Kattegat. *Journal of Marine Systems* 55:97-121.
- North EW, Schlag Z, Hood RR, Li M, Zhong L, Gross T, Kennedy VS. 2008. Vertical swimming behavior influences the dispersal of simulated oyster larvae in a coupled particle-tracking and hydrodynamic model of Chesapeake Bay. *Marine Ecology Progress Series* 359:99-115.
- OSPAR. 2012. Advice document on Good environmental status - Descriptor 7: Hydrographical conditions. OSPAR Commission. Publication number 583/2012.
- Paige CC, Saunders MA. 1982. LSQR: An Algorithm for Sparse Linear-Equations and Sparse Least Squares. *ACM Transactions on Mathematical Software* 8:43-71.
- Paris CB, Helgers J, van Sebille E, Srinivasan A. 2013. Connectivity Modeling System: A probabilistic modeling tool for the multi-scale tracking of biotic and abiotic variability in the ocean. *Environmental Modelling & Software* 42:47-54.
- Pereira A, Duarte P, Norro A. 2006. Different modelling tools of aquatic ecosystems: A proposal for a unified approach. *Ecological Informatics* 1:407-421.
- Piroddi C, Teixeira H, Lynam CP, Smith C, Alvarez MC, Mazik K, Andonegi E, Churilova T, Tedesco L, Chifflet M, Chust G, Galparsoro I, et al. 2015. Using ecological models to assess ecosystem status in support of the European Marine Strategy Framework Directive. *Ecological Indicators* 58:175-191. <https://doi.org/10.1016/j.ecolind.2015.05.037>.
- (<http://www.sciencedirect.com/science/article/pii/S1470160X1500285X>)
- Raillard O, Menesguen A. 1994. An Ecosystem Box Model for Estimating the Carrying-Capacity of a Macrotidal Shellfish System. *Marine Ecology Progress Series* 115:117-130.
- Savchuk OP, Wulff F. 2009. Long-term modeling of large-scale nutrient cycles in the entire Baltic Sea. *Hydrobiologia* 629:209-224.
- Schlag ZR, North E.W. 2012. Lagrangian TRANSport model (LTRANS v.2) User's Guide. University of Maryland Center for Environmental Science, Horn Point Laboratory. Cambridge, MD. 183 pp.
- She J, Hoyer JL, Larsen J. 2007. Assessment of sea surface temperature observational networks in the Baltic Sea and North Sea. *Journal of Marine Systems* 65:314-335.
- Shin YJ, Travers M, Maury O. 2010. Coupling low and high trophic levels models: Towards a pathways-orientated approach for end-to-end models. *Progress in Oceanography* 84:105-112.
- Skogen MD, Soiland H, Svendsen E. 2004. Effects of changing nutrient loads to the North Sea. *Journal of Marine Systems* 46:23-38.

Smith ADM et al. 2011. Impacts of Fishing Low-Trophic Level Species on Marine Ecosystems. *Science* 333:1147-1150.

Tian RC, Chen CS, Qi JH, Ji RB, Beardsley RC, Davis C. 2015. Model study of nutrient and phytoplankton dynamics in the Gulf of Maine: patterns and drivers for seasonal and interannual variability. *Ices Journal of Marine Science* 72:388-402.

Umgiesser G, Canu DM, Solidoro C, Ambrose R. 2003. A finite element ecological model: a first application to the Venice Lagoon. *Environmental Modelling & Software* 18:131-145.

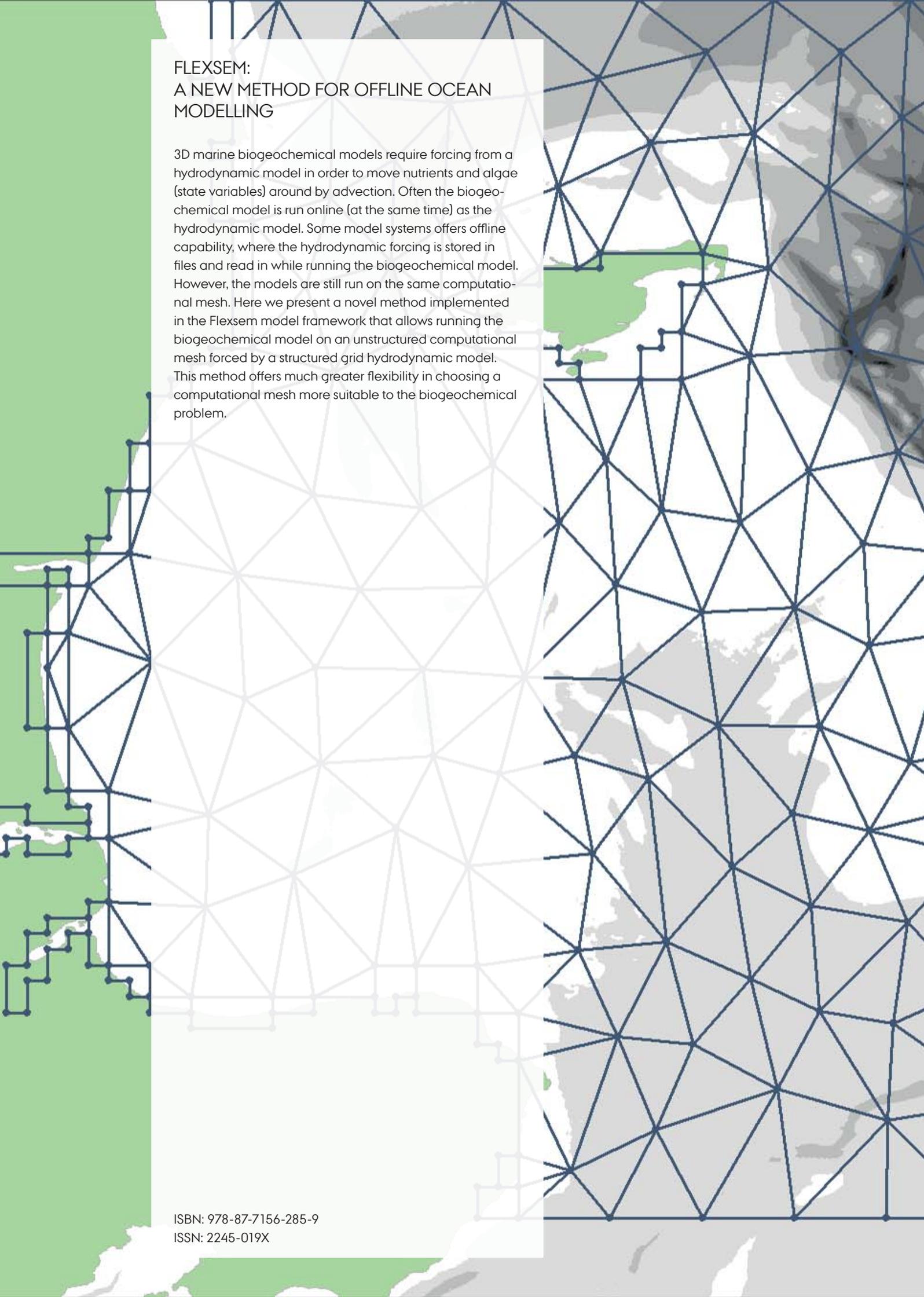
Vatti BR. 1992. A Generic Solution to Polygon Clipping. *Communications of the ACM* 35:56-63.

Wang B, Zhao G, Fringer OB. 2011. Reconstruction of vector fields for semi-Lagrangian advection on unstructured, staggered grids. *Ocean Modelling* 40:52-71.

Appendix A

The velocity fields used as input to the method were generated by the 3D ocean circulation model HBM. The HBM is a further development of the BSHcmod model (Dick et al. 2001) that has been running operationally at DMI since 2009 (Berg & Poulsen 2012) and at BSH since 2013 (Brüning et al. 2014). The model is based on Navier-Stokes primitive equations which are spatially discretized with an explicit finite difference method. The discrete equations are closed with a Smagorinsky formulation for the horizontal diffusivity and a two-equation $k-\omega$ scheme for the vertical turbulence. Advection and diffusion of heat, salt and passive tracers are based on budget equations and are realized by a conservative and fully explicit flux-corrected transport scheme. The model domain in this study covers the North Sea and the Baltic Sea with a coarse rectangular grid of 6 nm (nautical mile) horizontal resolution and 50 vertical z-layers with a thickness of 8 m at the surface, 2 m from 8 metres to 82 metres, 8 m from 82 metres to 98 metres, 25 m between 98 metres and 148 metres and 50 m below 148 metres. In addition a two-way nested fine rectangular grid of 1 nm horizontal resolution and 52 vertical z-layers covering the Baltic Sea transition zone (from Kattegat to Arkona Basin) is used to resolve the narrow Danish Straits and related Baltic-North Sea water and mass exchange. The vertical layers of this finer grid have a thickness of 2 m at the surface, 1 m from 2 metres to 30 metres water depth and 2 m below 30 metres water depth. The model has open lateral boundaries in the English Channel (4° W) and the northern North Sea (59.25° N). To secure stability of the explicit schemes an advection time step of 180 s and a hydrodynamic time step of 90 s in the coarse grid and 45 s in the fine grid is used. HBM is forced by hourly meteorological forcing (wind, air temperature, mean sea level pressure, surface humidity and cloud cover) from January 2001 based on DMI's operational version of the weather model HIRLAM (High Resolution Limited Area Model). Lateral temperature and salinity boundary conditions for the open North Sea boundaries are based on monthly climatologic fields from Janssen et al. (Janssen et al. 1999).

[Blank page]



FLEXSEM: A NEW METHOD FOR OFFLINE OCEAN MODELLING

3D marine biogeochemical models require forcing from a hydrodynamic model in order to move nutrients and algae (state variables) around by advection. Often the biogeochemical model is run online (at the same time) as the hydrodynamic model. Some model systems offers offline capability, where the hydrodynamic forcing is stored in files and read in while running the biogeochemical model. However, the models are still run on the same computational mesh. Here we present a novel method implemented in the Flexsem model framework that allows running the biogeochemical model on an unstructured computational mesh forced by a structured grid hydrodynamic model. This method offers much greater flexibility in choosing a computational mesh more suitable to the biogeochemical problem.