The Scottish Government
Riaghaltas na h-Alba

The Scottish Shelf Model. Part 6: Wider Domain and Sub-Domains Integration

Scottish Marine and Freshwater Science Vol 7 No 8

J Wolf, C Stuiver, D Price, H Johnson, A Gallego and R O'Hara Murray

marinescotland

© Crown copyright 2016

Scottish Marine and Freshwater Science Vol 7 No 8

The Scottish Shelf Model. Part 6: Wider Domain and Sub-Domains Integration

J Wolf, C Stuiver, D Price, H Johnson, A Gallego and R O'Hara Murray

Published by Marine Scotland Science

ISSN: 2043-7722

Marine Scotland is the directorate of the Scottish Government responsible for the integrated management of Scotland's seas. Marine Scotland Science (formerly Fisheries Research Services) provides expert scientific and technical advice on marine and fisheries issues. Scottish Marine and Freshwater Science is a series of reports that publishes results of research and monitoring carried out by Marine Scotland Science. It also publishes the results of marine and freshwater scientific work that has been carried out for Marine Scotland under external commission. These reports are not subject to formal external peer-review.

The Scottish Shelf Model. Part 6: Wider domain and sub-domains integration.

Marine Scotland

14 December 2015

Halcrow Group Limited
City Park, 368 Alexandra Parade, G31 3AU
tel 0141 552 2000
fax 0141 552 2525
halcrow.com

Halcrow Group Limited is a CH2M HILL company
Halcrow Group Limited has prepared this report in accordance with the instructions of client Marine Scotland for the client's sole and specific use. Any other persons who use any information contained herein do so at their own risk.

© Halcrow Group Limited 2016

ch2m.

Document history

The Scottish Shelf Model. Part 6: Wider domain and sub-domains integration

Marine Scotland

This document has been issued and amended as follows:

Version	Date	Description	Created by	Verified by	Approved by
1.0	09-Dec-2014	First draft including methodology	Caroline Stuiver / Hakeem Johnson	Darren Price / Judith Wolf	
2.0	7-Apr-2015	Inclusion of Shelf Model setup and Particle Tracking Methodology. Section 3 has been updated	Judith Wolf /Caroline Stuiver	Hakeem Johnson/Darren Price	
3.0	21-Nov-2015	Final version of Particle Tracking Methodology	Judith Wolf	Hakeem Johnson Caroline Stuiver	John Debenham
4.0	14-Dec-2015	Updated based on comments from Marine Scotland	Judith Wolf/Caroline Stuiver	Hakeem Johnson Caroline Stuiver	John Debenham

The Scottish Shelf Model. Part 6: wider domain and sub-domains integration.

Authors: Judith Wolf, Caroline Stuiver, Darren Price, Hakeem Johnson, Alejandro Gallego, Rory O'Hara Murray.

Acknowledgements:

The Scottish Shelf Model (SSM) contract was funded by the Scottish Government.

The FVCOM model has been developed by the Marine Ecosystem Dynamics Modeling Laboratory at the School for Marine Science and Technology, University of Massachusetts, Dartmouth, led by Dr Changsheng Chen. We would like to acknowledge Dr Chen for authorising the project team to use FVCOM for the development of the Scottish Shelf Model.

We would like to thank the SSM Steering Group for their contribution. In particular, Tracy McCollin (Marine Scotland) as the Project Manager, John Debenham (CH2M HILL) and Alan Hills (Scottish Environment Protection Agency). Daniel Pendrey and Kate Smith (Marine Scotland) and Andrew Berkeley (SEPA) also participated in the Steering Group. We would also like to acknowledge Christina Sommerville (University of Stirling) and Nabeil Salama (MSS) for their input into fish farm connectivity indices.

The Grid2Grid freshwater runoff data were supplied under contract by the Centre for Ecology and Hydrography. We would like to thanks Robert Moore and his colleagues at CEH for those data.

Many individuals and organisations, too numerous to list individually, made data and data products used in the development of this model available free of charge. All relevant data sources are acknowledged through the text of these reports and we refer the readers to that information.

Contents

Abbreviations 4

1. Introduction 6
1.1 Background 6
1.2 Study areas 6
1.3 Aims and scope of numerical modelling works 7
1.4 Project Team 9
1.5 This Report 9
1.6 Datums 9
1.7 Acknowledgments 9

2. Methodology for developing integrated models 11
2.1 Introduction 11
2.2 Options for integrated modelling 11
2.2.1 Method 1 - One way coupling 11
2.2.2 Method 2 - Two way coupling 11
2.2.3 Method 3 - New model including S1 and S2 models 11
2.2.4 Method 4 - Method 1 + Combination of S1 and S2 model results in integrated file. 12
2.2.5 Method 5 - FVCOM one-way nesting module for S2 + Combined S1 and S2 result files 13
2.3 Selected option for integrated modelling 14

3. Integration of model results from shelf and local models 15
3.1 Introduction 15
3.2 Integrated model mesh 15
3.3 Interpolation of results onto particle tracking mesh 21
3.4 Issues and solution 30

4. Model Setup 32
4.1 Introduction 32
4.2 Shelf model 32
4.3 Local models 33
4.3.1 One-way coupling (nesting) approach in FVCOM 34
4.3.2 Integrated model results for stage 3 35

5. Particle tracking model 37
5.1 Introduction 46
5.2 Particle Tracking in FVCOM 48
5.2.1 Theory 48
5.2.2 Offline particle tracking code 56
5.3 Particle Tracking in SSM 58
5.4 Results 62

6. Connectivity Indices 64
6.1 Methodology 64
6.2 Sea Lice Connectivity 64
6.3 ISAV Connectivity 71
6.4 IPNV Connectivity 80

7. Summary and Conclusions 89

8. Recommendations for future work 90

9. References 91

Particle Tracking and Connectivity Methodology 93

Abbreviations

Abbreviation	meaning
ADCP	Acoustic Doppler Current Profiler
AMM	Atlantic Margin Model
BODC	British Oceanographic Data Centre
CEFAS	Centre for Environment, Fisheries and Aquaculture Science
CEH	Centre for Ecology and Hydrology
CTD	Conductivity, Temperature and Depth instrument
DHI	Danish Hydraulic Institute
DTM	Digital Terrain Model
ECLH	East Coast of Lewis and Harris
ECMWF	European Centre for Medium range Weather Forecasting
EMODNet	European Marine Observation and Data Network
G2G	Grid-to-Grid
GEBCO	General Bathymetric Chart of the Oceans
GSHHS	Global Self-consistent, Hierarchical, High-resolution Shoreline
ICES	International Council for the Exploration of the Sea

Abbreviation	meaning
MHW	Mean High Water
MHWS	Mean High Water Spring
MS	Marine Scotland
MSL	Mean sea level
NGDC	National Geophysical Data Centre
NOAA	US National Oceanic and Atmospheric Administration
NOC-L	National Oceanography Centre - Liverpool
NODB	National Oceanographic Database
NTSLF	National Tide and Sea Level Facility
ODYSSEA	Ocean Data analYsis System for SEA
OS	Ordnance Survey
PFOW	Pentland Firth and Orkney Waters
SEPA	Scottish Environment Protection Agency
SMB	St Magnus Bay
UKHO	United Kingdom Hydrographic Office
WLLS	Wider Loch Linnhe System
WVS	World Vector Shoreline

1. Introduction

1.1 Background

CH2M (formerly Halcrow Group Ltd.) was commissioned by Scottish Ministers to develop a 'Hydrodynamic model of Scottish Shelf waters'. The contract was commissioned under the Scottish Government Framework Contract for the Provision of Strategic Environmental Assessment, Appropriate Assessment and Marine Planning Services and Advice to Support Sustainable Economic Development in Scottish Marine Waters (REF: 177895) – Call Off Number 11 - Provision of a Hydrodynamic Model of Scottish Shelf waters – 16 May 2012. The project is managed on behalf of the Scottish Ministers by Marine Scotland.

The Scottish Government is committed to the development of a successful marine renewable energy industry in Scotland, which is currently also the largest producer of farmed Atlantic salmon in the EU and third largest globally. To achieve the sustainable development of both the offshore renewable energy industry and the aquaculture sector, Marine Scotland has adopted a planning approach to identify potential developmental areas.

Both of these factors are drivers for the development of a regional hydrodynamic model of the Scottish Shelf Waters and four more localised models which will be used to inform their planning approach. Marine Scotland will take ownership of the hydrodynamic models at the end of the study enabling them and other community organisations they work with, to undertake simulations and further development to meet their planning and research needs.

One of the key aims of the integrated model is to use it in the development of connectivity indices between various fish farms. This will ensure a seamless flow of hydrodynamic modelling data from the high resolution local area models into the larger Scottish shelf model, thereby ensuring that the model covers the entire region of influence of each fish farm. The integrated model will therefore contribute to improved understanding of potential sea lice dispersal, to help inform management and mitigation measures.

1.2 Study areas

The overall study area includes all of the Scottish shelf waters out to the 200m depth contour at the edge of the continental shelf. This model simulates the hydrodynamic conditions in three-dimensions, including

meteorological and tidal forcing. The shelf model resolution varies from 10km offshore to 1km at the coast.

Within this region-wide shelf waters model, four local three-dimensional models have been setup providing higher resolution to resolve key bathymetry, coastline and physical processes over smaller more local areas. These four model areas have been defined as case studies and cover the following regions:-

Case Study 1: Pentland Firth and Orkney Waters (PFOW)
Case Study 2: Wider Loch Linnhe System (WLLS)
Case Study 3: East Coast of Lewis and Harris (ECLH)
Case Study 4: Northwest Shetland mainland – St Magnus Bay area (SMB)

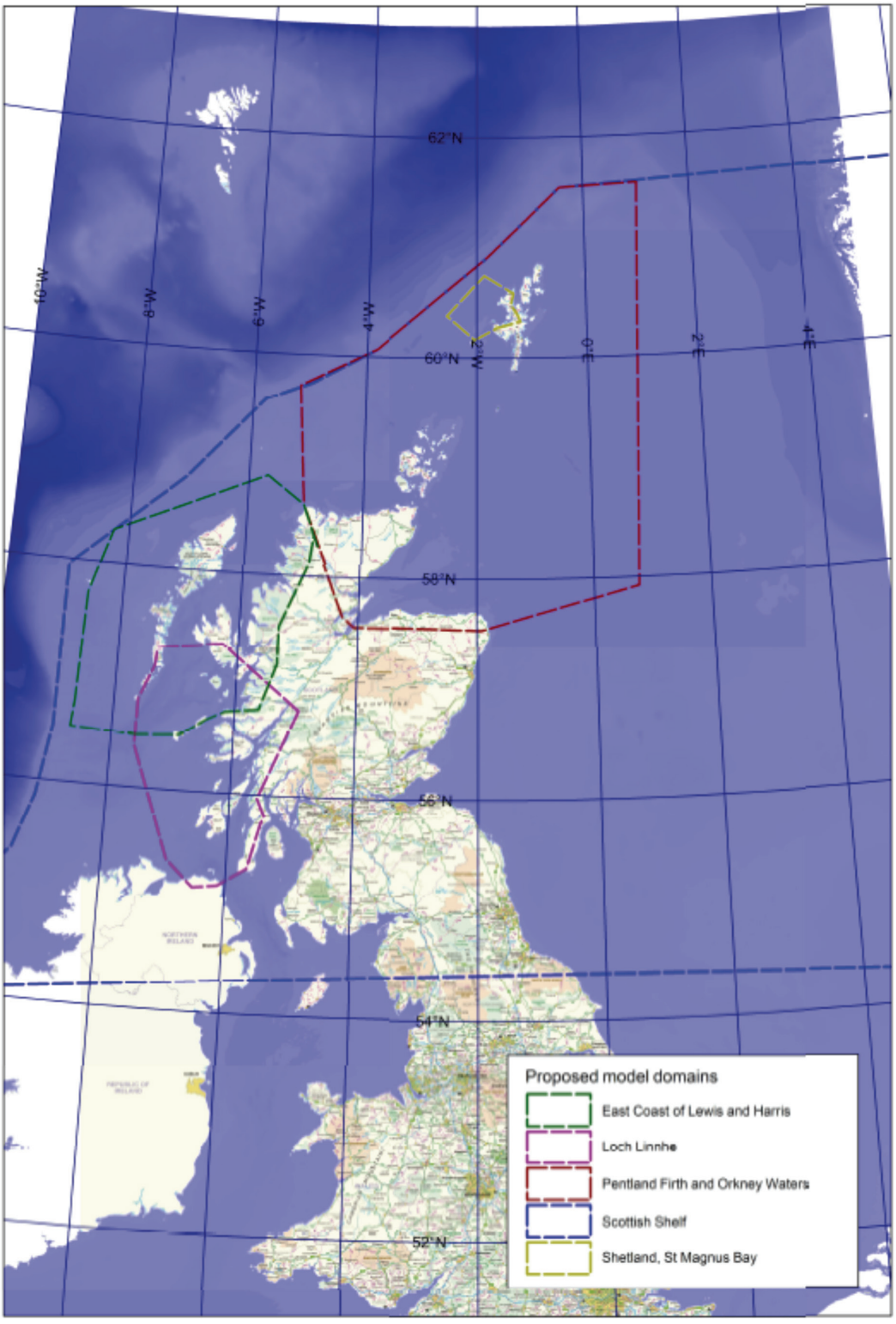
The locations and approximate areas of these models are shown in Figure 1-1.

1.3 Aims and scope of numerical modelling works

The main aims of the project are to: 1) develop a validated three dimensional hydrodynamic model for the Scottish shelf waters; 2) develop a validated three dimensional hydrodynamic model for each of the four identified case studies, plus a validated wave model for the Pentland Firth and Orkney Waters (Case Study 1); and 3) integrate the case study sub-models into the wider domain shelf model.

The modelling is aimed at providing a quantitative description of marine currents and water properties for the whole of Scottish waters on a range of spatial scales. The outputs of this study will be a validated hydrodynamic model capable of predicting tidal and non-tidal currents for the whole of the Scottish shelf and inshore waters and include a more accurate assessment of the connectivity of different regions, and the available energy resources in those regions. It will also include description of methods for assessing the impact of extracting some of that energy upon the physical environment.

The modelling has been undertaken using an open-source three-dimensional (3D) hydrodynamic model called FVCOM. One of the reasons behind the choice of this modelling software is that the models developed in this project will be freely available to others at the end of the Project. Marine Scotland have a vision that the models will be used and developed further by Marine Scotland staff and the marine modelling community as more data becomes available and/or other needs are identified.



Contains Ordnance Survey data © Crown copyright and database right 2011

Client	Consulting Engineer	Project:	**Figure 1-1**
Marine Scotland	ch2m	Scottish Shelf Waters Model	Location of the Shelf and individual case study model domains

1.4 Project Team

The project team delivering this study consists of:

- CH2M (formerly Halcrow Group Ltd) as the main contractor, responsible for co-ordination of team and development of the hydrodynamic models for the four case studies.
- National Oceanography Centre, Liverpool (NOC-L) as subcontractor, responsible for development of the Scottish shelf model.
- Centre for Ecology and Hydrology (CEH) responsible for delivering river outflow discharge data covering the entire Scottish waters and Northern Ireland using the Grid to Grid model.
- Prof. Chen of University of Massachusetts, USA, responsible for providing technical support on the application of the FVCOM software.
- Prof Christina Sommerville of University of Stirling, UK, responsible for providing technical support on sea lice and development of connectivity indices.

1.5 This Report

This report documents the work carried out in Stage 3 - developing the integrated model and its application for particle tracking modelling and development of connectivity indices.

1.6 Datums

Unless explicitly stated otherwise the following reference datums are used in this study:

- All horizontal co-ordinates are referenced to latitude and longitude.
- All vertical levels are relative to MSL.

1.7 Acknowledgments

We gratefully acknowledge with thanks the contributions of the following organisations and individuals to this project.

- Marine Scotland (Alejandro Gallego, Rory O'Hara Murray, Berit Rabe and George Slesser) for providing, requesting and collecting available data.
- UKHO for the bathymetry datasets we have received.
- BODC/NOC-L for the wide range of oceanographic data and metadata; this is a great source of data. Thanks to Polly Hadziabdic at BODC for helping us with our enquiries.
- SEPA for providing tide gauge and fish farm data, which were very useful for this study.
- CEH (Robert Moore and team) for their work towards providing river discharges data using the Grid-to-Grid model for this study.
- CEFAS for the provision of wave data from their WAVENET website. Thanks to David Pearce at CEFAS for his help with clarifying the terms of use of these data.
- Dr Susana Baston Meira and Dr David Woolf at Heriot-Watt University for their help with obtaining ADCP data in the Pentland Firth.
- Professor Chen at the University of Massachusetts (Dartmouth) and his team for making the FVCOM software available for this project.

We also acknowledge with thanks the owners of the internet websites mentioned below for the valuable data downloaded from them for this study.

- Tide gauge data (class 'A') from the National Tide and Sea Level Facility (NTSLF – available from www.pol.ac.uk/ntslf) will be downloaded and used for calibration purposes.
- ICES database (http://ocean.ices.dk/) which proved to be a good source of data.
- Bathymetric metadata and Digital Terrain Model data products have been derived from the EMODNet Hydrography portal - http://www.emodnet-hydrography.eu. This portal was initiated by the European Commission as part of developing the **European Marine Observation and Data Network** (EMODNet).

2. Methodology for developing integrated models

2.1 Introduction

A number of methods were considered for the integration of the shelf (Wolf et al. 2015) and local models (Price et al. 2015 a-d). These methods are presented and discussed in Section 2.2, and the selected method is presented in Section 2.3.

2.2 Options for integrated modelling

2.2.1 Method 1 - One way coupling

In this method, the shelf model is used to provide initial and boundary data (water level, temperature and salinity) for driving the local area models. The tools delivered will comprise Matlab scripts required for extracting initial and boundary data for any local area in the shelf model (hereafter S1 model).

The advantages of this method are: a) information flow from S1 (Stage 1 shelf model) to S2 (Stage 2 local models); b) reduced computational resources (effort and cpu times) as each model is run separately, and c) reduced data handling effort and storage space requirements.

The disadvantages are: a) no feedback from S2 to S1 model; and b) flow output data will be in separate files, and therefore inconvenient for use as an integrated set for particle model simulations.

2.2.2 Method 2 - Two way coupling

In this method, the S2 models would be incorporated into the S1 model, such that dynamic coupling occurs across the interface of the S1 and S2 models. The S1 and S2 model grids need to be designed so that the embedding occurs at logical boundaries (common nodes, elements and cross-sectional areas). This method of dynamic nesting is used in some structured grid models (e.g. MIKE 21 Nested HD). However, this feature is not available in FVCOM. Thus, this is not considered further.

2.2.3 Method 3 - New model including S1 and S2 models

In this method, the S1 model mesh would be designed to incorporate the high resolution mesh in the areas covered by S2 models. This approach would deliver a new model, which is outside the scope of the present project.

The advantages of this method are: a) full dynamic coupling between S1 and S2 model areas; b) model results in one integrated file that can be used for particle model simulations.

The disadvantages are: a) it is practically not possible to develop such a new mesh, and at the same time preserve the properties of the already developed S1 and S2 meshes. This is because it is necessary that the S1 and S2 meshes have common cells (with identical properties) at the interface in order to preserve the properties of the S1 and S2 meshes in the combined S3 mesh. This is however practically impossible to achieve as the S1 and S2 models were developed in parallel; b) the computational time step will be constrained by smallest mesh size, hence such a model will be very expensive to run (in terms of computational times). The CPU time required is expected to be at least 1 order of magnitude more than that required for the S1 model; c) this method does not take advantage of work already done in S1 and S2. There would be a need for model re-calibration and validation and d) such a model would be difficult (impossible) to extend to other S2 areas. Each new S2 area would require complete redevelopment of integrated model.

2.2.4 Method 4 - Method 1 + Combination of S1 and S2 model results in integrated file.

This method consists of the following steps:

a) The method described in Section 2.2.1 (hereafter referred to as Method 1) is used to develop the S2 model results.

b) Next, an integrated mesh (S3 mesh) is developed including the mesh used in S1 and the mesh used in S2 in the appropriate model areas.

c) Finally, a Matlab script is used to generate the S3 model results by interpolation in the S1 and S2 results.

The tools delivered: As in method 1 + Matlab script for interpolating model results onto S3 mesh.

The advantages of this method are: a) the method makes use of development work in S1 and S2; b) it is expected to be significantly faster than the method in Section 2.2.3 (developing a new model), since S1 and S2 models can be developed separately; c) the output file will be one integrated result file; and d) the method can be adapted to incorporate more or fewer S2 areas.

The disadvantages are: a) it is practically not possible to develop such a new S3 mesh, and at the same time preserve the properties of the S1 mesh and S2 meshes as the S1 and S2 models were developed separately. In order to preserve the properties of the S1 and S2 meshes in the S3 mesh, it is necessary that the S1 and S2 meshes have common cells at the interface. However, it is expected that this will not be a problem, since the model results are to be obtained from the calibrated S1 and S2 models, rather than a new numerical solution; b) the interpolation may yield unphysical results at some locations. This will need to be checked especially at the interface of the S1 and S2 meshes; c) the integrated result file may be very large. It is expected to be slightly smaller than the sum of the file sizes for the S1 and S2 files. The large result file can be minimised by saving the results in smaller chunks (e.g. daily).

2.2.5 Method 5 - FVCOM one-way nesting module for S2 + Combined S1 and S2 result files

This method is similar to the method described in Section 2.2.4 (Method 4). The only difference (an important difference) is that the S2 model results are obtained using boundary data obtained with the one-way nesting feature in FVCOM. Thus, for each S2 model, a nested file required as boundary data is obtained as output from the S1 model simulation using the NCNEST feature in FVCOM.

In order to use the NCNEST feature, the cells at the interface of the two models (S1 and S2) should be common. According to the FVCOM manual for v3.1.6 (see p91), two types of nesting are available for unstructured models – direct nesting and indirect nesting.

QUOTE:

For "direct nesting", the small domain FVCOM is driven directly with the nested boundary output from the large domain FVCOM. In this case, only the variables at boundary nodes and cells are required.

For "indirect nesting", the small domain FVCOM will retain its own tidal forcing at the nesting boundary and nest with the large domain FVCOM using the subtidal values of variables at boundary nodes and cells.

END QUOTE

This method requires that the cells at the interface between the S1 and S2 models are common to allow for the possibility to prepare the nesting file directly from S1 run using the NCNEST feature. However, this type of compatibility is not feasible in general. A workaround is to create the nesting file by interpolation from the S1 results file.

A key advantage of this method is in the use of native nesting module in FVCOM. This ensures compatibility of hydrodynamic conditions at the interface, and improved stability of the nested models since the combined elevation and current forcing from the S1 model are applied at the boundary of the S2 models.

The disadvantages are: a) it is practically not possible to develop such a new S3 mesh, and at the same time preserve the properties of the S1 mesh and S2 meshes at the interfaces. Special measures are required at the interface between S1 and S2; b) the integrated result file may be very large. It is expected to be slightly smaller than the sum of the file sizes for the S1 and S2 files. The large result file can be minimised by saving the results in smaller chunks (e.g. daily).

2.3 Selected option for integrated modelling

Due to practical difficulties in combining the shelf and local model meshes while maintaining the node positions of all models and the large computational demand to run a fully integrated model, the method described in Section 2.2.5 (Method 5) was chosen. The results from the shelf and local models are combined using a Matlab script and output onto a new mesh which retains the best resolution of nodes from each of the individual model. Further details on how the results are combined are presented in Section 3. The integrated result file is used as input to the particle tracking model.

The adopted method involves one way coupling between the S1 model and the S2 models using the FVCOM nested boundary data files. Since the cells at the boundary of the S2 models and the S1 model are not common, the nested boundary files were obtained by interpolation in the S1 results file. Further details on the adopted approach for creating the nesting boundary data are presented in Section 4.

3. Integration of model results from shelf and local models

3.1 Introduction

As outlined in Section 2, a number of methods were considered for the integration of the shelf and local models. The selected method is described in Section 2.2.5 (Method 5). A new mesh is created incorporating the shelf and local model meshes and the results from the shelf and local models are interpolated onto the new mesh to create the integrated results file. This integrated file is required as an input file for the particle tracking model. Daily hydrodynamic model result files are required for the particle tracking model, therefore the process was repeated for each day of the year. Results for the PFOW and WLLS models are available for the full year. However the results for ECLH and SMB models are only available May through to October. Therefore it was necessary to create two different integrated meshes, one including all the local model meshes (Figure 3-1 to 3-2) and one including only the PFOW and WLLS model meshes (Figure 3-3 to 3-4). A full description of this method is outlined here.

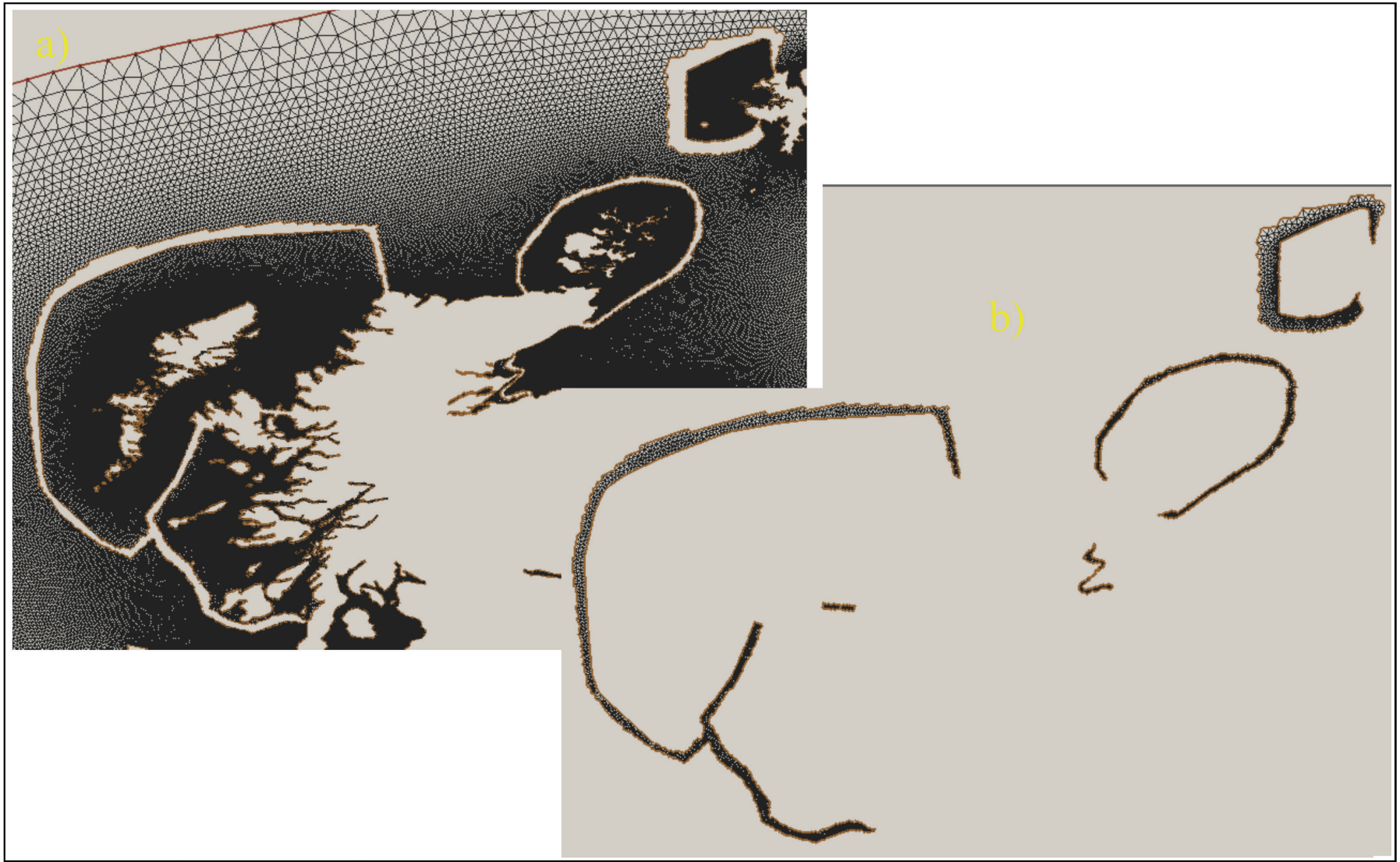
3.2 Integrated model mesh

The local model meshes were inserted into the shelf model mesh in SMS using the following method:

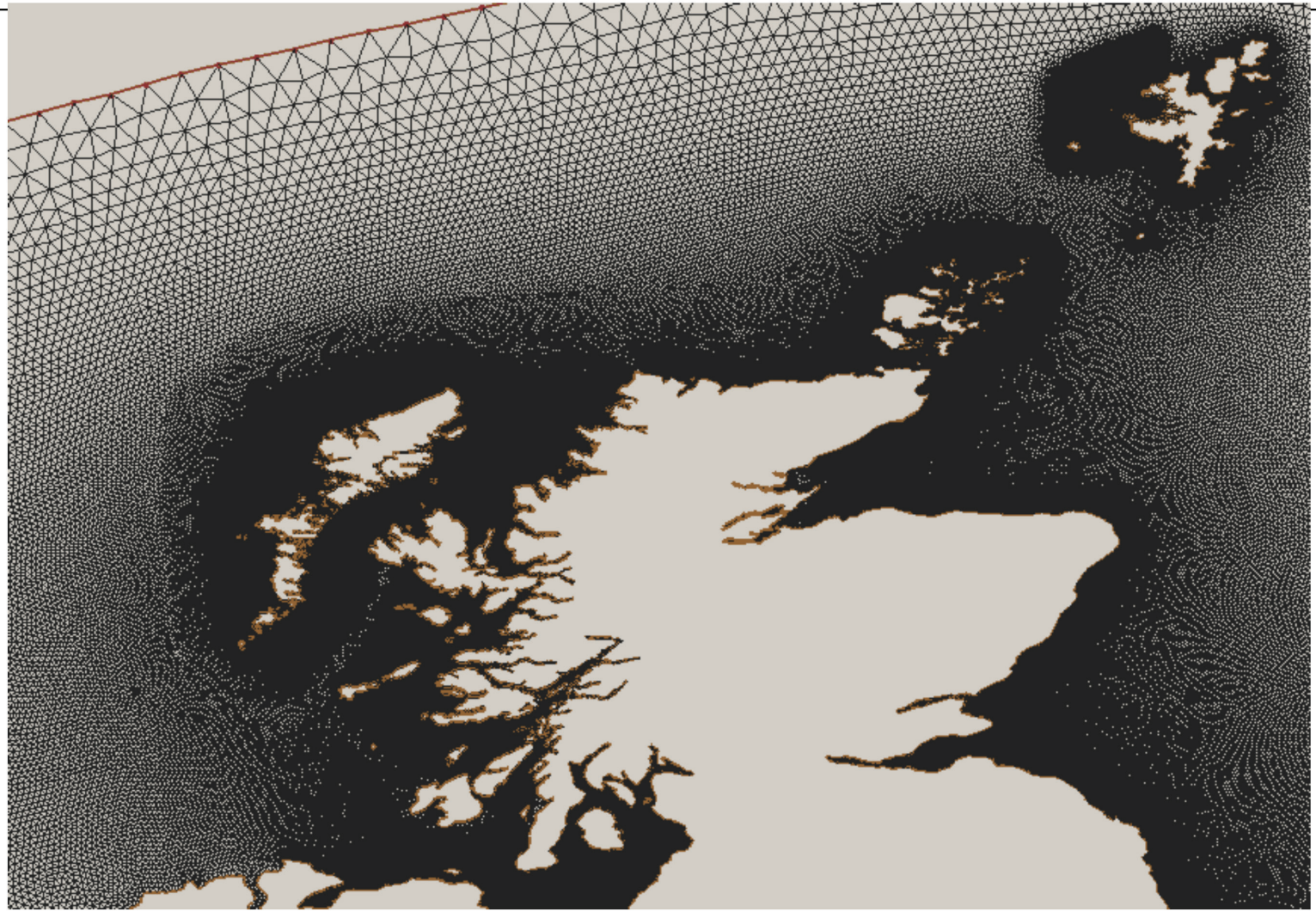
1) Nodes in the shelf model mesh in areas that are covered by the local model meshes, where the resolution in the local model meshes is better than the shelf model, were deleted. This creates an area where the higher resolution mesh of each local model mesh can be slotted in without any overlapping elements. In cases where the local model domains overlapped, it was necessary to delete the overlapping nodes from the local model mesh with the lower resolution.

2) All the cropped meshes where imported into SMS, care was taken to ensure no overlapping nodes remained, the highest resolution mesh available was used, and a buffer between the various meshes existed (Figure 3-1a and Figure 3-3a). The buffer was created manually, its width varied based on the surrounding mesh resolution and varies between 1 and 6 elements across. The gaps between the meshes were converted into polygons and the mesh generation function was used to produce a mesh in these areas (Figure 3-1b and Figure 3-3b). In the newly combined mesh (Figure 3-2 and Figure 3-4), the mesh quality was maintained where possible,

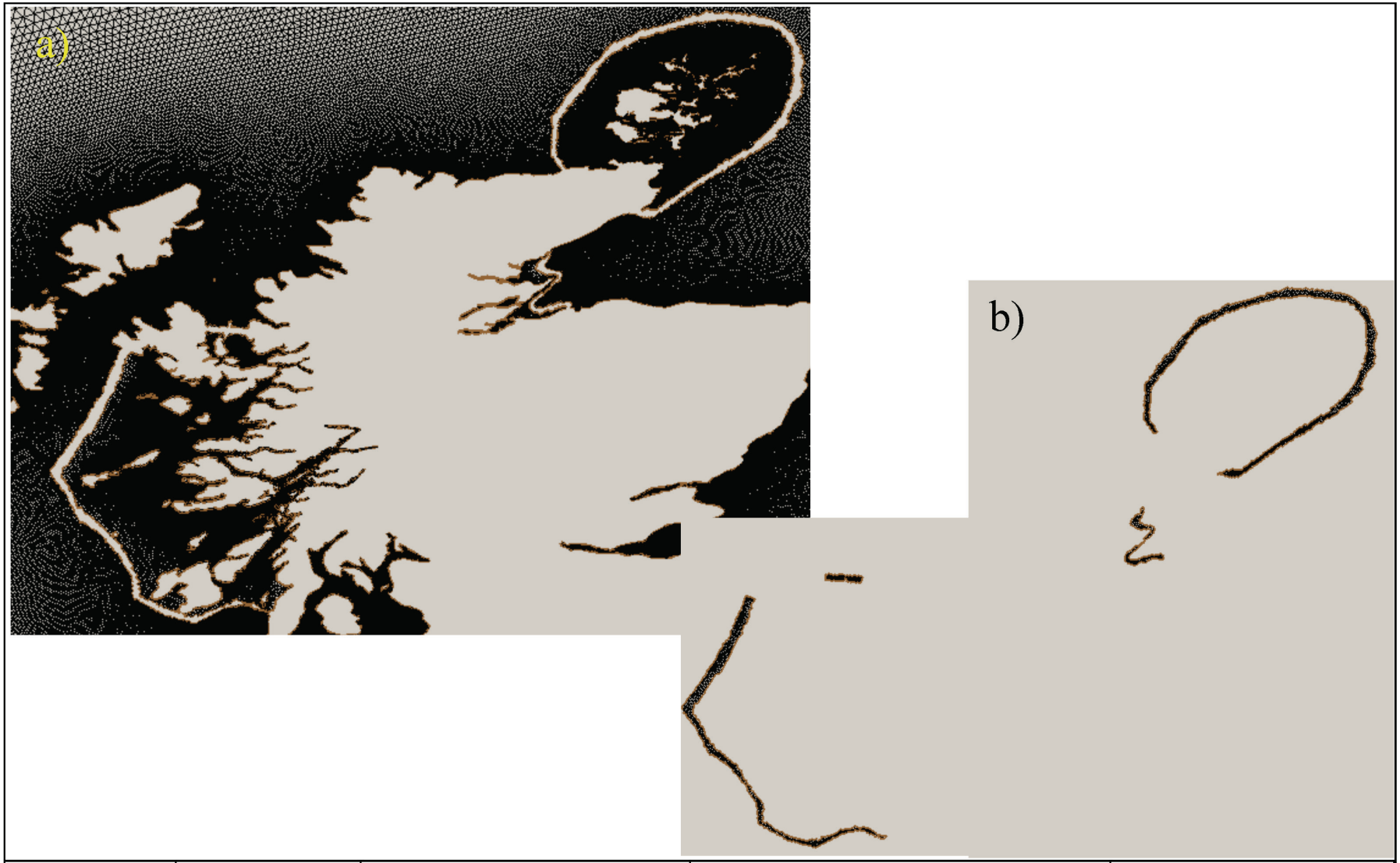
ensuring that adjacent element areas do not differ by more than a factor of 0.5, the minimum interior angle was 30 degrees, maximum interior angle was 130 degrees and that the maximum number of connecting elements was 8, as specified in the FVCOM manual. For the SMB model, which was run on OSGB and not longitude/latitude, it was not possible to satisfy the minimum interior angle without remeshing.



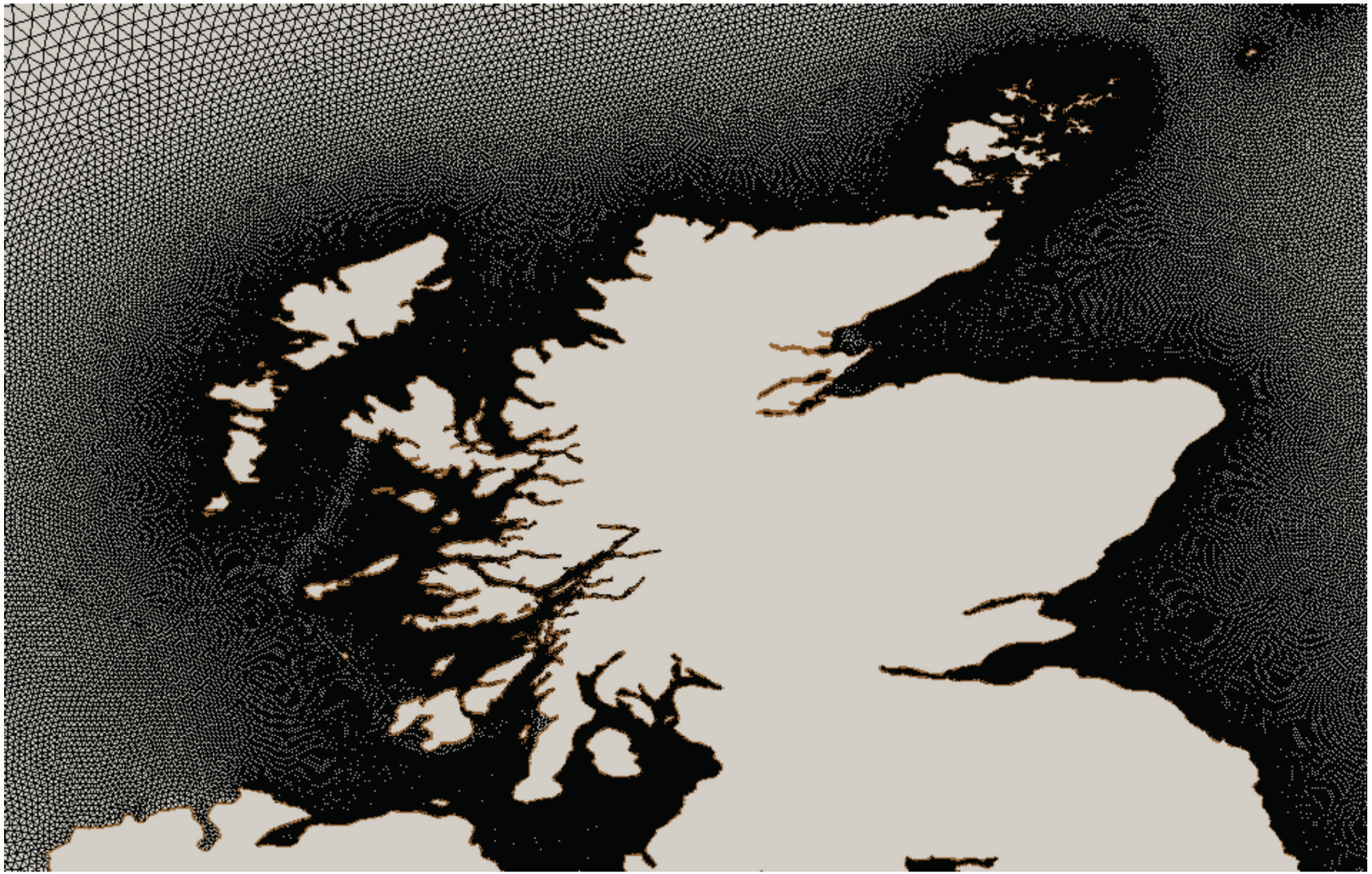
Client	Consulting Engineer	Project:	Figure Title:	Figure 3-1		
Marine Scotland	ch2m.	Scottish shelf waters model	Shelf and all local model meshes slotted together with gaps (a) and mesh created to fill the gap (b)	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-2		
Marine Scotland	ch2m.	Scottish shelf waters model	Combined model mesh for particle tracking using all local model s	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-3		
Marine Scotland	ch2m.	Scottish shelf waters model	Shelf, PFOW and WLLS model meshes slotted together with gaps (a) and mesh created to fill the gap (b)	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-4		
Marine Scotland	ch2m.	Scottish shelf waters model	Combined model mesh for particle tracking using the PFOW and WLLS models only	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014

3) A number of mesh metrics are required by the FVCOM particle tracking model, including Momentum Stencil Interpolation Coefficients (a1u and a2u) and Element Based Interpolation Coefficients (aw0, awx and awy). Node connectivity (nv) and the coordinates in the centre of elements (lonc and latc) were also required. To obtain these metrics for the new mesh (Stage 3 mesh or S3 mesh), the mesh was used in an FVCOM run with no boundary conditions for one time step. Siglay and Siglev, parameters that describe the relative thickness of the model layers are specified as 10 equally spaced layers and 11 equally spaced levels.

3.3 Interpolation of results onto particle tracking mesh

The interpolation of the shelf and local models onto a new integrated mesh (for the particle tracking model) is carried out in Matlab. The process has been schematised in Figure 3-5 and described below:

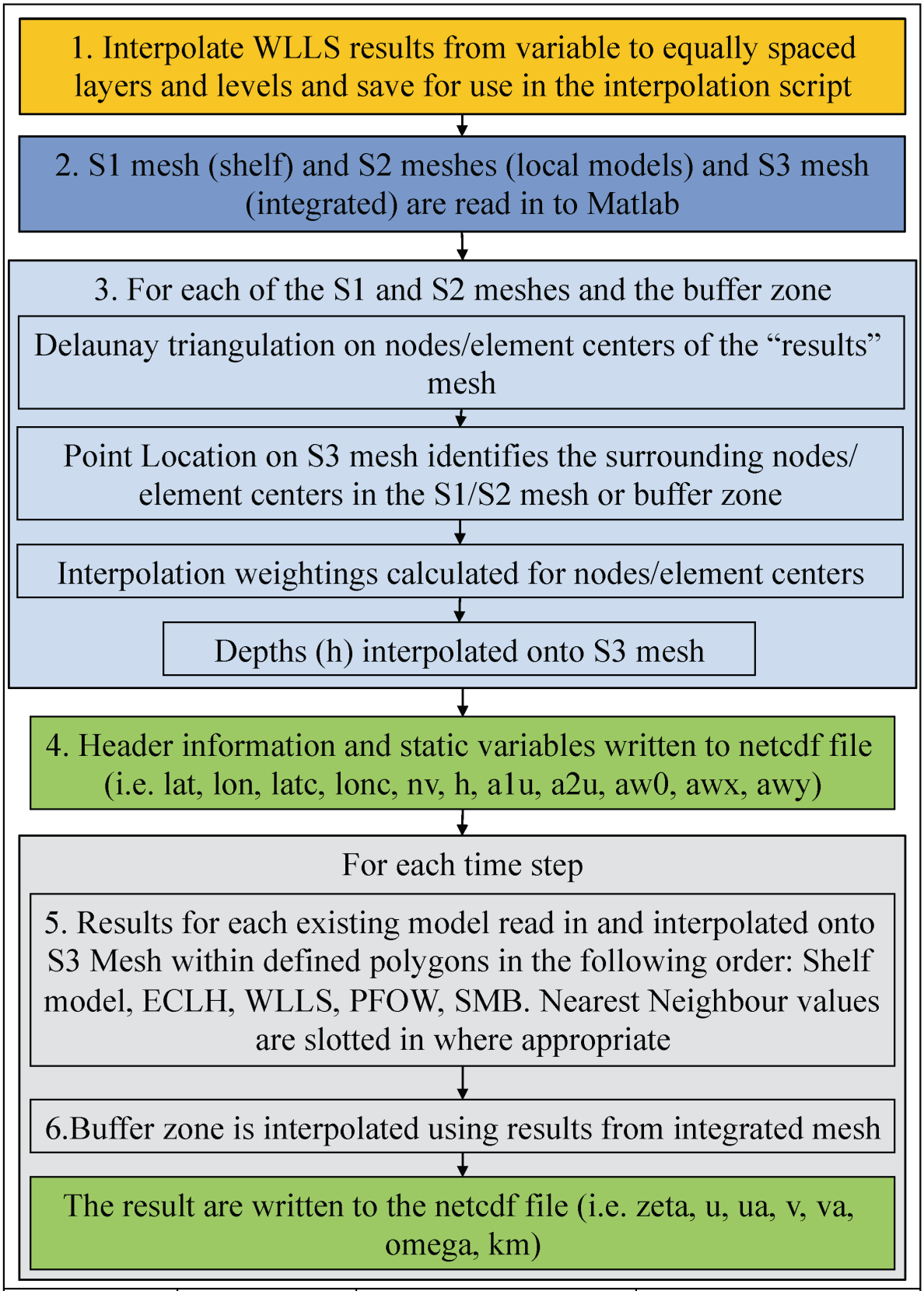
1) The WLLS model has 10 layers of variable thickness, therefore prior to running the interpolation script the results need to be interpolated on to 10 equally spaced layers. N.b. This process is completed outside of the main script to reduce computational times, see section 3.4 for more details

2) First the interpolation weightings are calculated for each mesh and stored for use later in the process. The interpolation weightings are calculated based on the triangulation of the nodes and element centres of the “results” mesh, i.e. the mesh containing the results to be interpolated. The point location function is used to determine where within the triangulation of the “results” mesh the nodes and element centres of the “integrated” mesh (the mesh the results will be interpolated onto) lie. The nearest neighbour is also calculated in case any of the nodes or element centres fall outside the valid triangulation zone (Figure 3-6).

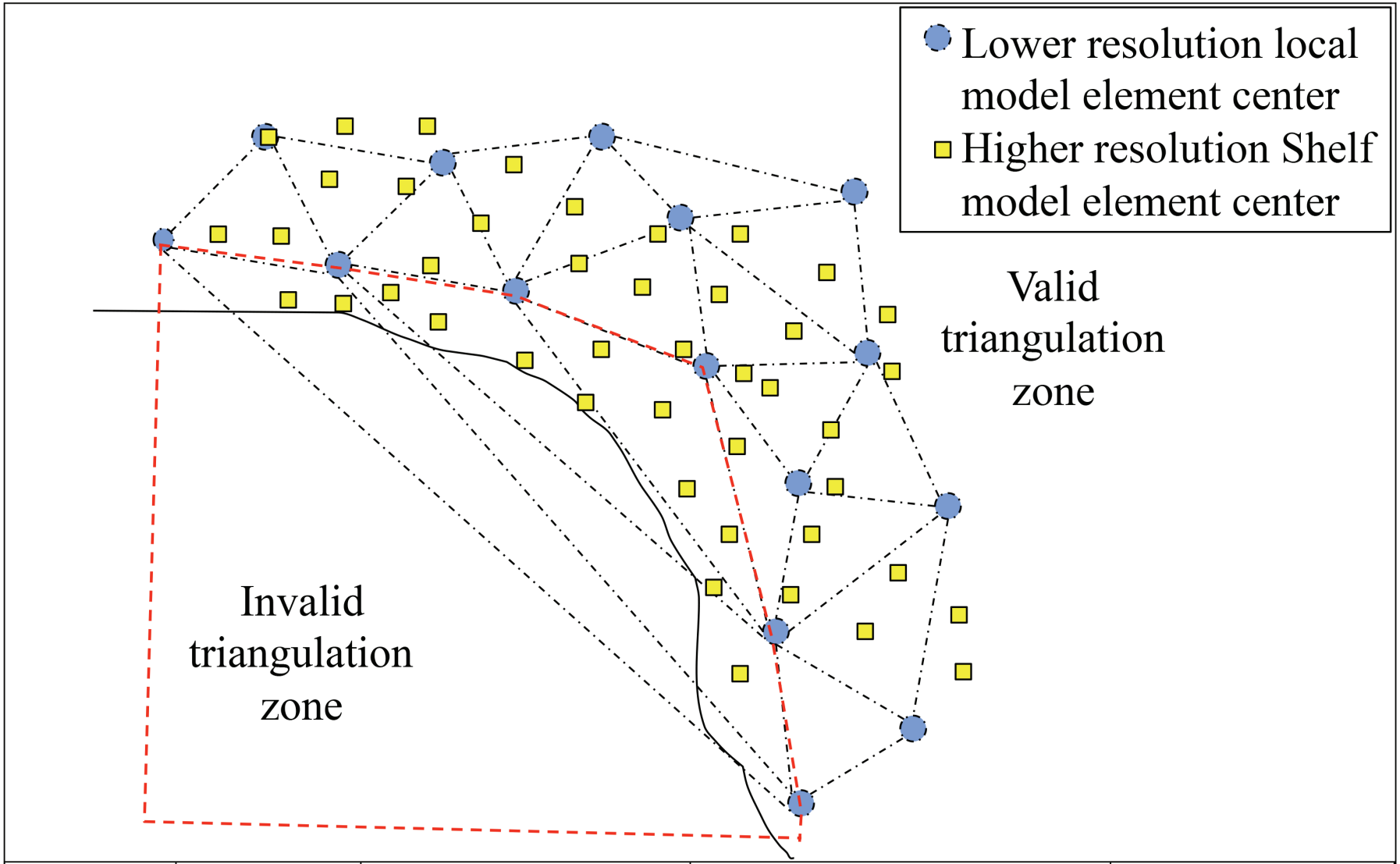
3) Interpolation weightings are also calculated for an interpolation buffer used later to smooth the transition between the various model results as shown in Figure 3-7a and b. The triangulation is carried out on the points within the inner and outer buffer polygons and the point location is carried out on the buffer polygon. Again, the nearest neighbour is also calculated in case any of the nodes or element centres fall outside the valid triangulation zone (Figure 3-6a and b).

4) The header information and static variables are written to the NetCDF file.

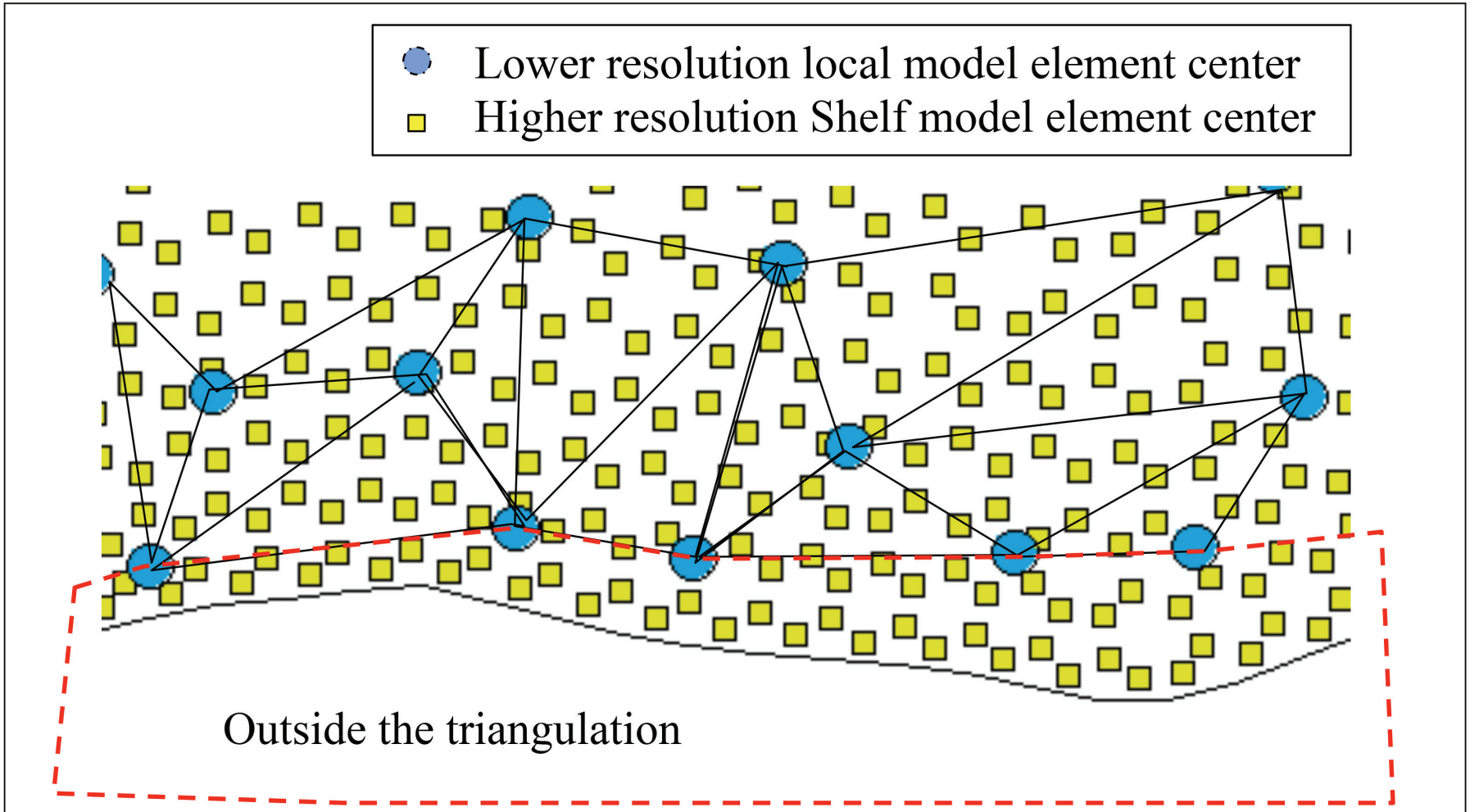
5) For each time step the time dependent variables were interpolated from the shelf and local models into the new integrated mesh one model at a time, using the *inpolygon* function in Matlab to determine which nodes/elements to interpolate onto. The polygons are defined as shown in Figure 3-8. Note that the polygons for interpolation of the local model results follow the same line as the inside line of the buffer polygon and lie within the local model domain boundary. This is to avoid any issues at the boundaries being transferred to the particle tracking model and to ensure the buffering from the local models to the shelf model is successful.



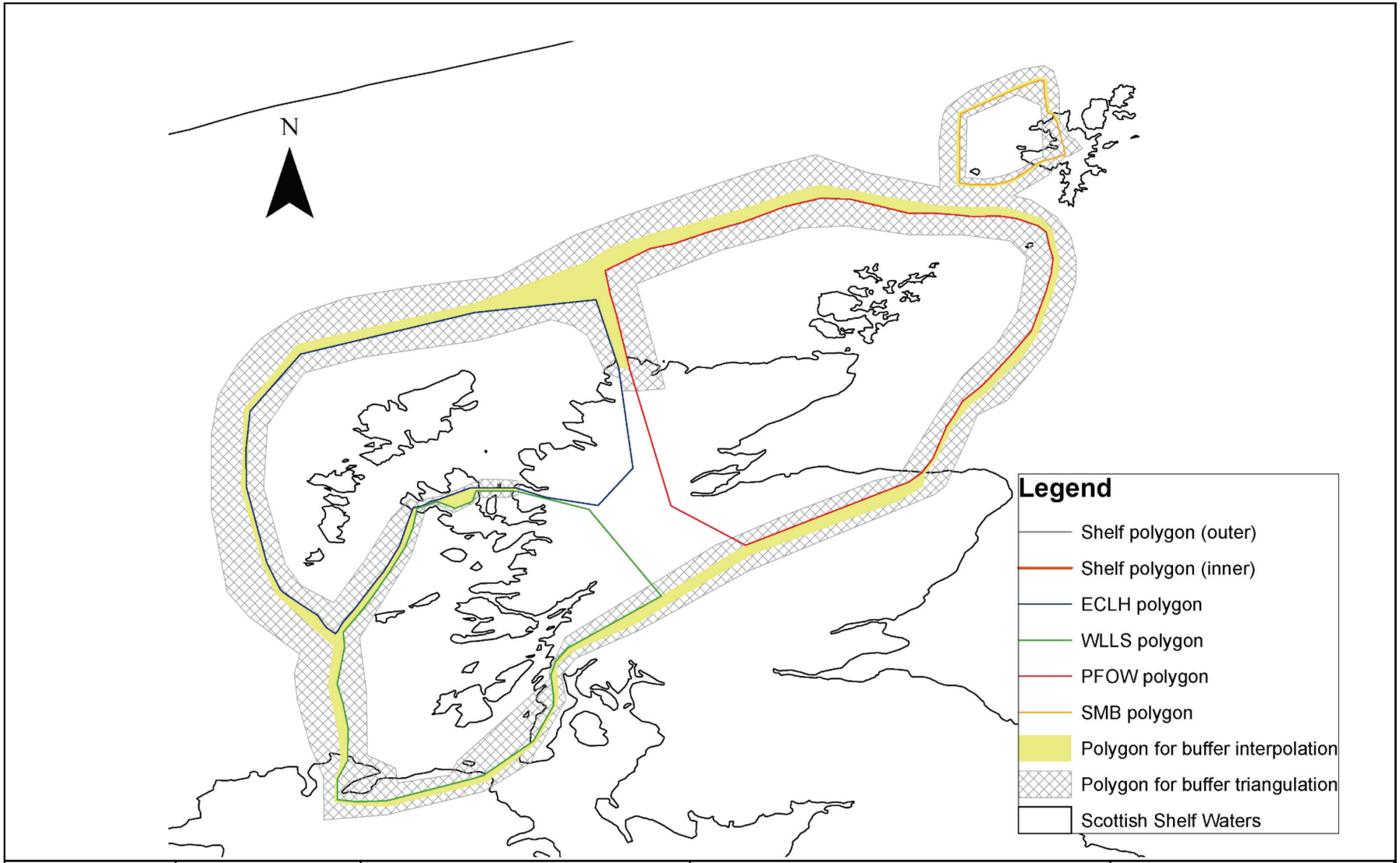
Client	Consulting Engineer	Project:	**Figure 3-5**
Marine Scotland	ch2m	Scottish Shelf Waters Model	Matlab script work flow for creation of combined results file for particle tracking model input



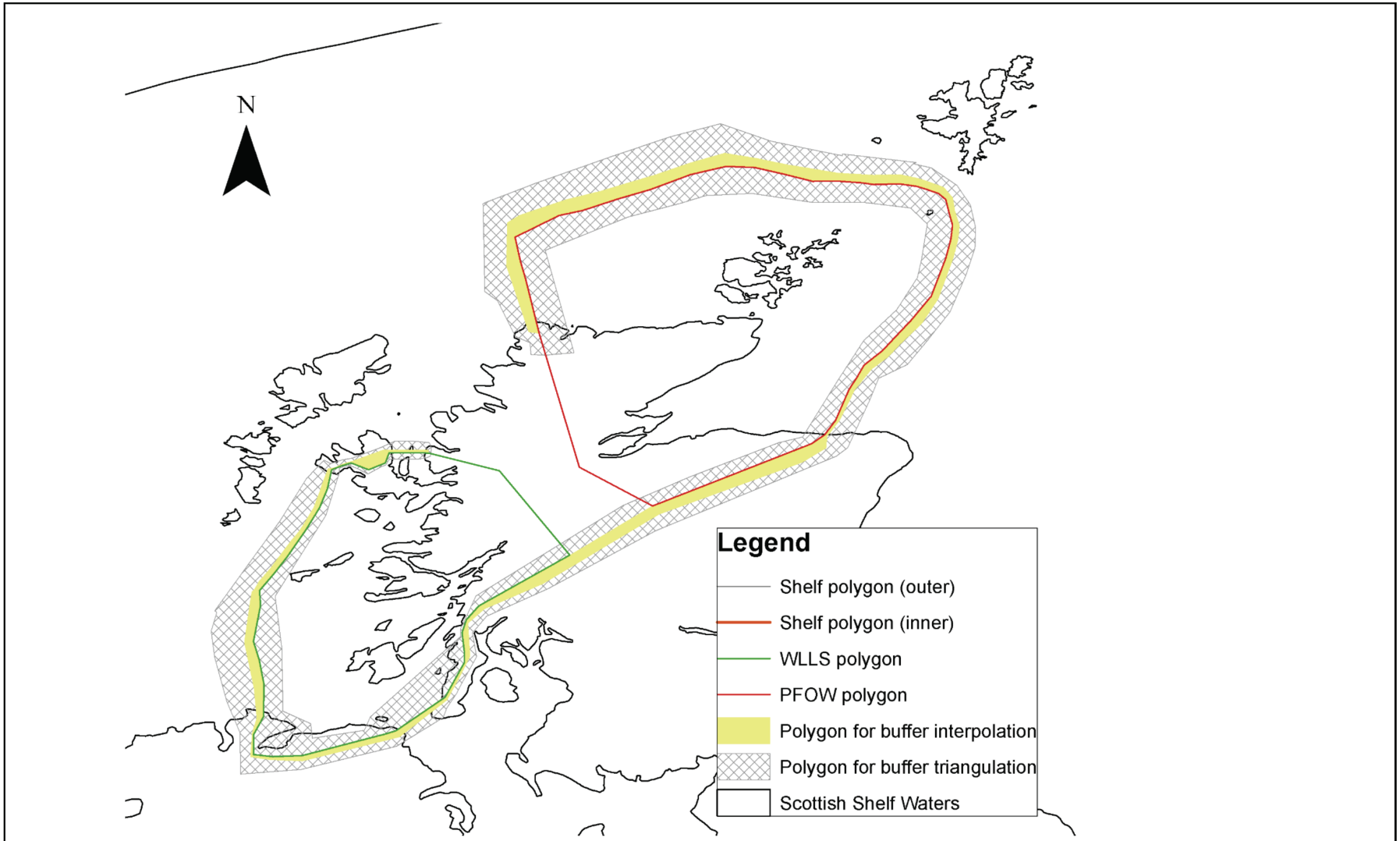
Client	Consulting Engineer	Project:	Figure Title:	Figure 3-6a		
Marine Scotland	ch2m.	Scottish shelf waters model	Schematic showing the potential for elements in the higher resolution mesh to fall in the invalid triangulation zone. In these areas the nearest neighbour should be used	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



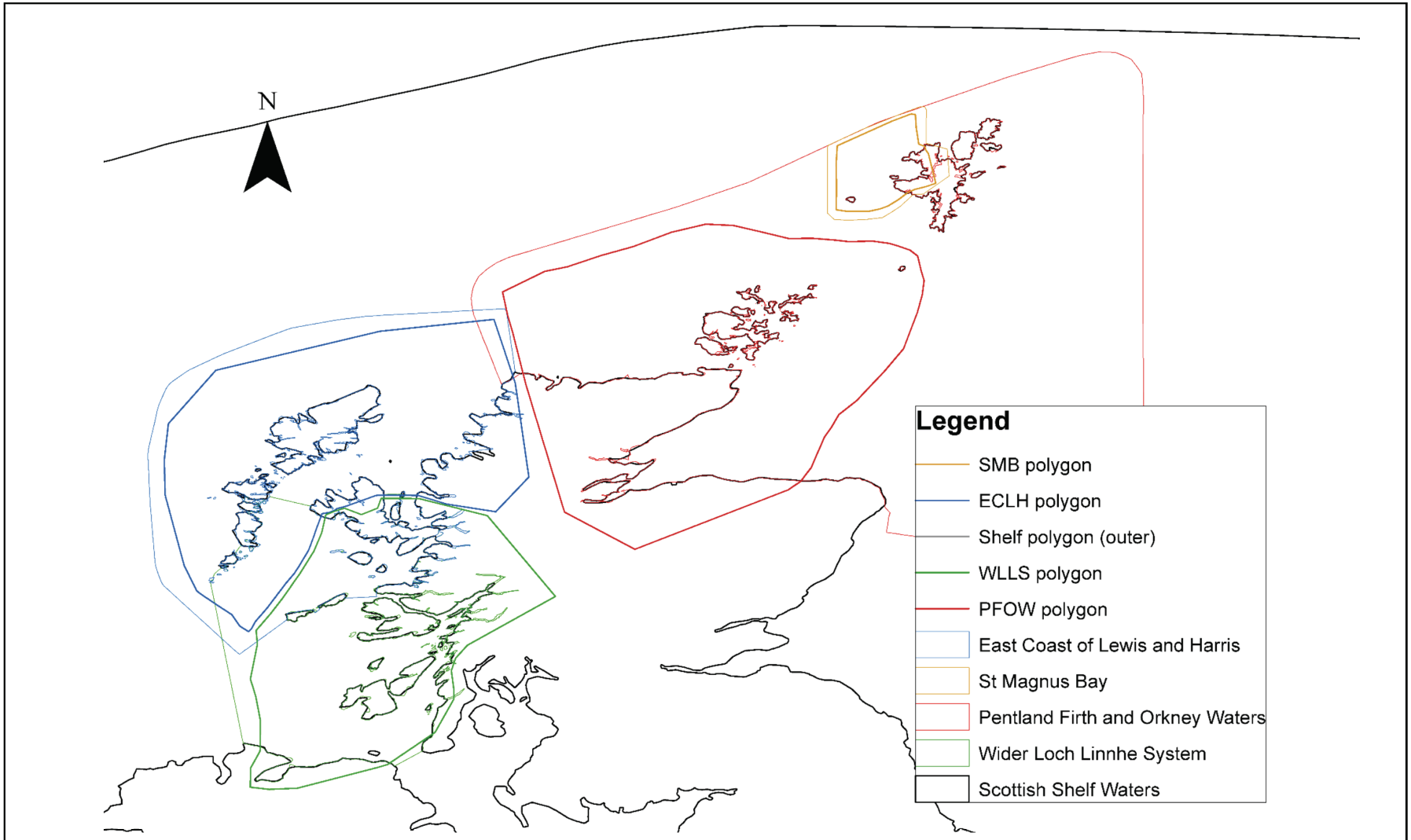
Client	Consulting Engineer	Project:	Figure Title:	Figure 3-6b		
Marine Scotland	ch2m:	Scottish shelf waters model	Schematic showing the potential for elements in the higher resolution mesh to fall outside of the triangulation zone. In these areas the nearest neighbour should be used	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



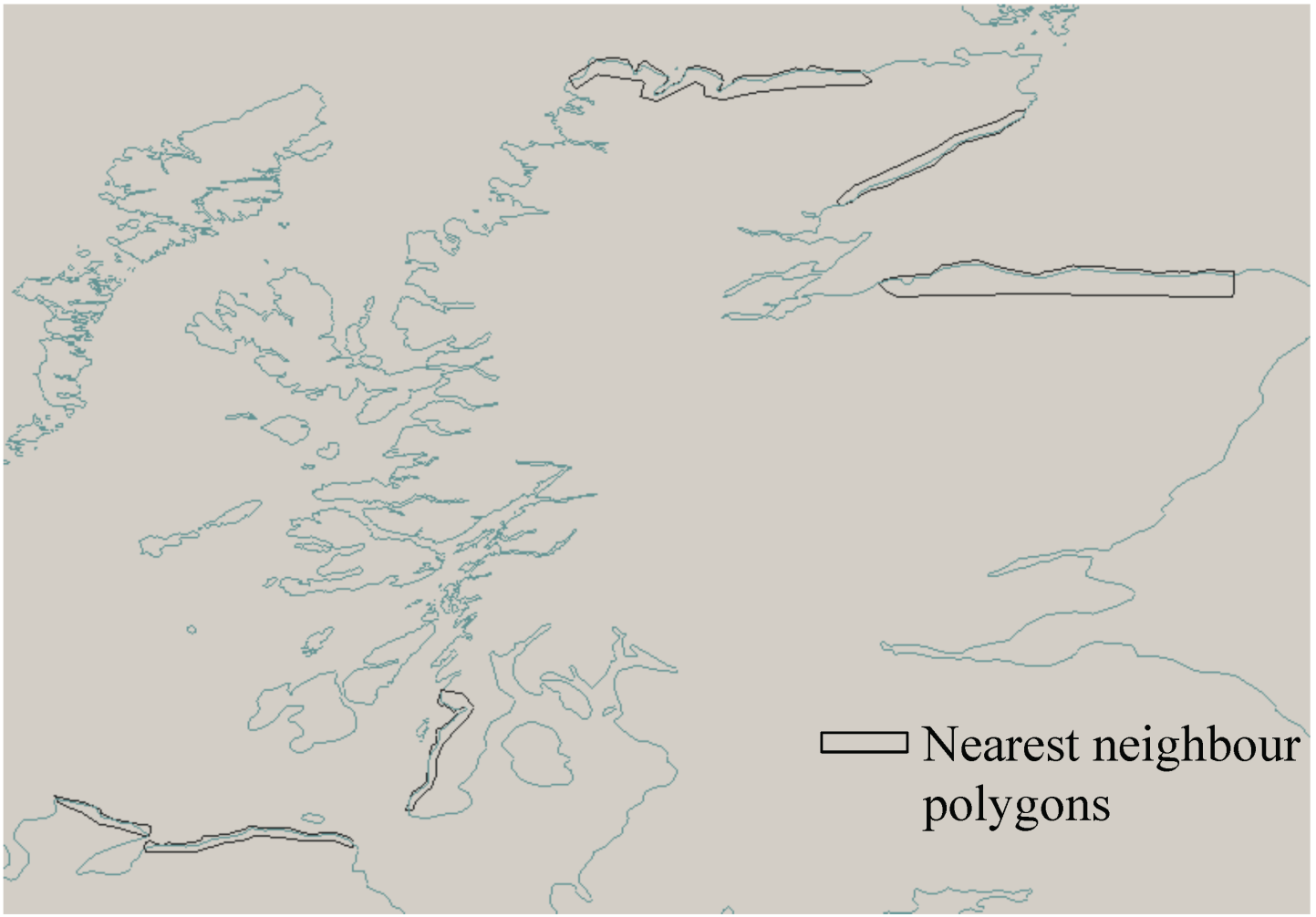
Client	Consulting Engineer	Project:	Figure Title:	Figure 3-7a		
Marine Scotland	ch2m.	Scottish shelf waters model	Extent of polygons used to extract the combined results for triangulation and the polygon defining the buffer area for interpolation of those results, for all local models.	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-7b		
Marine Scotland	ch2m.	Scottish shelf waters model	Extent of polygons used to extract the combined results for triangulation and the polygon defining the buffer area for interpolation of those results, for PFOW and WLLS only.	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-8		
Marine Scotland	ch2m.	Scottish shelf waters model	Model extents (outlines) and polygons within which results are interpolated on to the new particle tracking mesh	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 3-9		
Marine Scotland	ch2m.	Scottish shelf waters model	Polygons defining the areas where nearest neighbour must be used	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014

6) In areas close to land where the “integrated” model mesh had a higher resolution than the local (“results”) model mesh, the element centres of the “integrated” mesh will fall outside the valid triangulation of the local model element centres (Figure 3-6a). In these areas the nearest neighbour function was used to avoid unrealistic results being passed into the particle tracking model. The areas where this was necessary were defined as a polygon and shown in Figure 3-9.

7) When all the model results have been combined the boundary between the different models is smoothed using the method described below:

    a. Results either side of the interpolation buffer are extracted from the combined mesh (Figure 3-7a and b).

    b. The results on the nodes and element centres within the buffer are interpolated from the integrated results either side of the buffer and slotted back into the integrated mesh. Close to land where necessary the nearest neighbour value was used.

8) The interpolated results on the integrated model mesh are written to the NetCDF file at each time step. Daily input files are required for the particle tracking model, therefor the process was repeated for each day of the year.

3.4 Issues and solution

An initial attempt to develop the Matlab script for combining the results presented issues with unrealistic computational times and insufficient memory. The interpolation weightings calculations were performed as matrix calculations, meaning the interpolation weights for all nodes or elements could be calculated in one step, instead of looping through the nodes/elements one at a time, thus increasing the computational speed. Since the interpolation weights are calculated based on the geometry of the mesh, which is static, the interpolation weights were calculated prior to the interpolation of the results. This means the interpolation weightings for the nodes and elements only had to be calculated once and could then be used for all time steps and relevant parameters. Using the *inpolygon* function allowed the interpolation to be carried out only in the relevant areas of the mesh.

The polygon for the shelf model has an inner and outer boundary. This prevents results from the shelf model being interpolated to the S3 mesh in the areas covered by the local models only to be over written (when

the results of each local model is interpolated to the S3 mesh), thus improving efficiency. The polygon for the PFOW model does not include the area of the SMB model, again preventing data being written to the same area twice.

The shelf model has 20 layers while the local models have 10 layers. To reduce computational times and memory requirements it was decided to reduce the number of layers in the shelf model to 10 instead of increasing the number of layers in the local models, due to the higher horizontal resolution in the local models. For parameters calculated on the layers the results were averaged using Equation 3-1 and for parameter calculated on the levels every second value was used.

$$Integrated\ Mesh\ layer_n = \frac{Shelf\ Mesh\ layer_{(n\times 2)-1} + Shelf\ Mesh\ layer_{n\times 2}}{2} \quad (3\text{-}1)$$

The WLLS model has 10 variable thickness layers and 11 variable thickness levels, therefore to incorporate these results into the combined mesh it was necessary to interpolate the results on to 10 equally spaced layer and 11 equally spaced levels. This was carried out prior to running the script to save time. Since it is necessary to loop through all the nodes with the selected interpolation method it was quicker to do this for all time steps within a results file at once instead of looping through all the nodes and elements one time step at a time in the main script.

The issue of insufficient memory was tackled by reading in the model results, performing the interpolation and writing out the results to the NetCDF file one time step at a time.

Another issue was the realisation that around land the triangulation may not be valid and would produce unrealistic results. This would only be an issue when the results from a local model were being interpolated onto a higher resolution mesh. The issue was solved by defining polygons in which the results of the nearest neighbour is used (Figure 3-9).

4. Model Setup

4.1 Introduction

In this section, a brief description of the setup of the Shelf and Local hydrodynamic models used for the climatology runs is presented. The results from these models are combined together in an integrated grid (as described in Section 3) for the overlapping periods. The combined results are used for the particle model simulations (described in Section 5), and the development of connectivity indices.

4.2 Shelf model

The Stage 1 report (Scottish Shelf Waters Model) describes the process of setting up the Scottish Shelf Waters FVCOM model from the assembling of data sets, through development of a stable grid, implementation of forcing (tidal, meteorological and river discharge), calibration and validation. The calibration period was March-June 2009 inclusive, while the validation has been carried out over the period May 2008- March 2009.

The model grid has been set up to provide at least 1km resolution around the Scottish coast. The model extends over the whole NW European continental shelf and into the North Atlantic in order to properly represent the tidal regime.

It was found necessary to use the HEATING_CALCULATED option rather than HEATING_ON, within the FVCOM model, in order to get a reasonable evolution of the sea surface temperature (SST). The sources of met forcing data have been explored, including which variables to download from the Met Office Unified Model output and ERA40/ERA-Interim reanalysis datasets.

During the model calibration phase the bottom friction drag coefficient was varied (although kept constant spatially) and the optimum settings were found to be a roughness length (z_0) of 0.01m and a minimum drag coefficient of 0.005. The best turbulence closure scheme was GOTM and better results were obtained with 20 vertical levels rather than 10.

The model has then been used to assess the tidal energy resource and, using climatological forcing, the monthly mean circulation pattern. These results have been assessed qualitatively against previously published work and found to be in good agreement.

The most difficult part of the model implementation was to develop a stable grid. In the end, by trial and error and also advice from various sources, including Prof Chen, via CH2M, it was found that the model was sensitive to the connectivity of the mesh (no more than 8 elements must be connected to a single node), steep gradients in bathymetry and issues related to the river forcing. Some smoothing of bathymetry was necessary, near the shelf edge and the Norwegian Trench. At river nodes it was necessary to ensure that the depth was at least 5m in order to ensure that the river inflow could be accepted and propagated into the main body of the model grid.

The model was calibrated by adjusting the number of vertical layers, the bottom friction and the turbulent closure scheme. Validation was carried out by comparison with water surface elevation data, from coastal and offshore tide gauges, current meter data and CTD profiles.

The detailed instructions for running the Shelf Model are provided in a separate document (Model Documentation Report, February 2015) prepared for Marine Scotland training. This includes sections on model installation, data sources, data preparation (pre-processing), running the model and post-processing of the output. It also includes Appendices on using SMS to Prepare Grids (Appendix A), Documentation of MatLab Scripts (Appendix B) and Frequently Asked Questions (FAQ's, Appendix C).

4.3 Local models

Four local models (PFOW, ECLH, WLLS and SMB) were developed in Stage 2 (S2) of this project. Each of the four local models have been described in a corresponding technical report. As in the Stage 1 (S1) report, each report describes the process of setting up the model from the assembling of data sets, through development of a stable model, implementation of forcing (tidal, meteorological and river discharge), calibration and validation.

In addition to the challenges with developing a stable model mesh (described in Section 4.2), it was also found necessary to use a nested boundary approach in order to eliminate stability problems in the SMB model. This instigated this approach with all of the local models.

The models were calibrated and validated against available measured water levels, current velocities at current meter locations and transects, and CTD measurements. The calibration was carried out by adjusting the bottom friction and the parameters for the turbulent closure scheme (horizontal and vertical mixing). It was also found necessary to adjust the structure of the vertical layers for the WLLS. The validation was

carried out by running the model for a different time interval without any further change to the model parameters.

Each of the local models has been used to determine the mean circulation pattern for the period May to October (Jan – Dec in the case of PFOW and WLLS) using climatological forcing. The derivation of the climatological forcing data is described in detail in the Stage 1 report.

As discussed in Section 2.3, the adopted method for integrating the S1 and S2 models involves one way coupling between the S1 model and the S2 models using the FVCOM nested boundary approach. Further details on the approach used to create the nesting boundary data are presented in Section 4.3.1.

4.3.1 One-way coupling (nesting) approach in FVCOM

There are a number of ways to provide boundaries conditions to an FVCOM model, however for stage 3 the nested relaxation boundary approach has been used. This allows water levels, velocity components, temperature and salinity to be prescribed along the local model boundaries using results from the Shelf model. The relaxation boundary approach was originally developed for use with a regular structured grid model that was coarser than the model that was being nested within it.

This approach has been used for the nesting of the four local models within the Shelf model, it is not always the case that the Shelf model is coarser than the local model at the boundaries but this does not affect the approach.

As the variables from the Shelf model are required to be interpolated onto the local model boundary nodes/elements, the values from the Shelf model cannot ensure mass and volume conservation, in addition the model output from the Shelf model may vary from the local model results in the region of the local model boundary. Therefore a relaxation zone is defined within which a weighting factor is used to proportion the values from the Shelf model and those within the local model to enable a smooth transition between the two models.

Figure 4-1 shows a schematisation of how the relaxation nested boundary works. The blue triangles represent the local model mesh, with the open boundary shown by the light green line, and the boundary elements indicated by the yellow dots. The nodes attached to the boundary elements are indicated by the green dots and are all used for the relaxation boundary. The shelf model mesh is represented by the black-edged triangles, which are slightly finer than the local model

(as is the case for the WLLS model western boundary). Water levels, temperature and salinity values are interpolated (triangulation) from the Shelf mesh onto the green dots/ local model nodes along the open boundary and through each of the vertical layers. Likewise the velocity components from the Shelf model are interpolated onto the yellow dots/local model elements adjoining the open boundary.

Whilst the relaxation boundary can be more than one element deep, we have found that one element wide has been sufficient. The boundary nodes/elements each have a weighting factor associated with them, these can be seen in Figure 4-1 Adjacent to each of the nodes/elements on the model boundary.

The weighting factor relates to the proportion of the Shelf model variable to be used compared with the variable already calculated within the local model. For example on the model boundary nodes the factor is 0.75. This means that the elevation at this point is made up of 75% of the values contained within the boundary file (derived from the Shelf model values interpolated onto the boundary nodes) and 25% of the values already calculated within the local model. For the boundary nodes within the model domain, 25% is made up from the values in the boundary file and 75% is taken from the values already calculated within the local model.

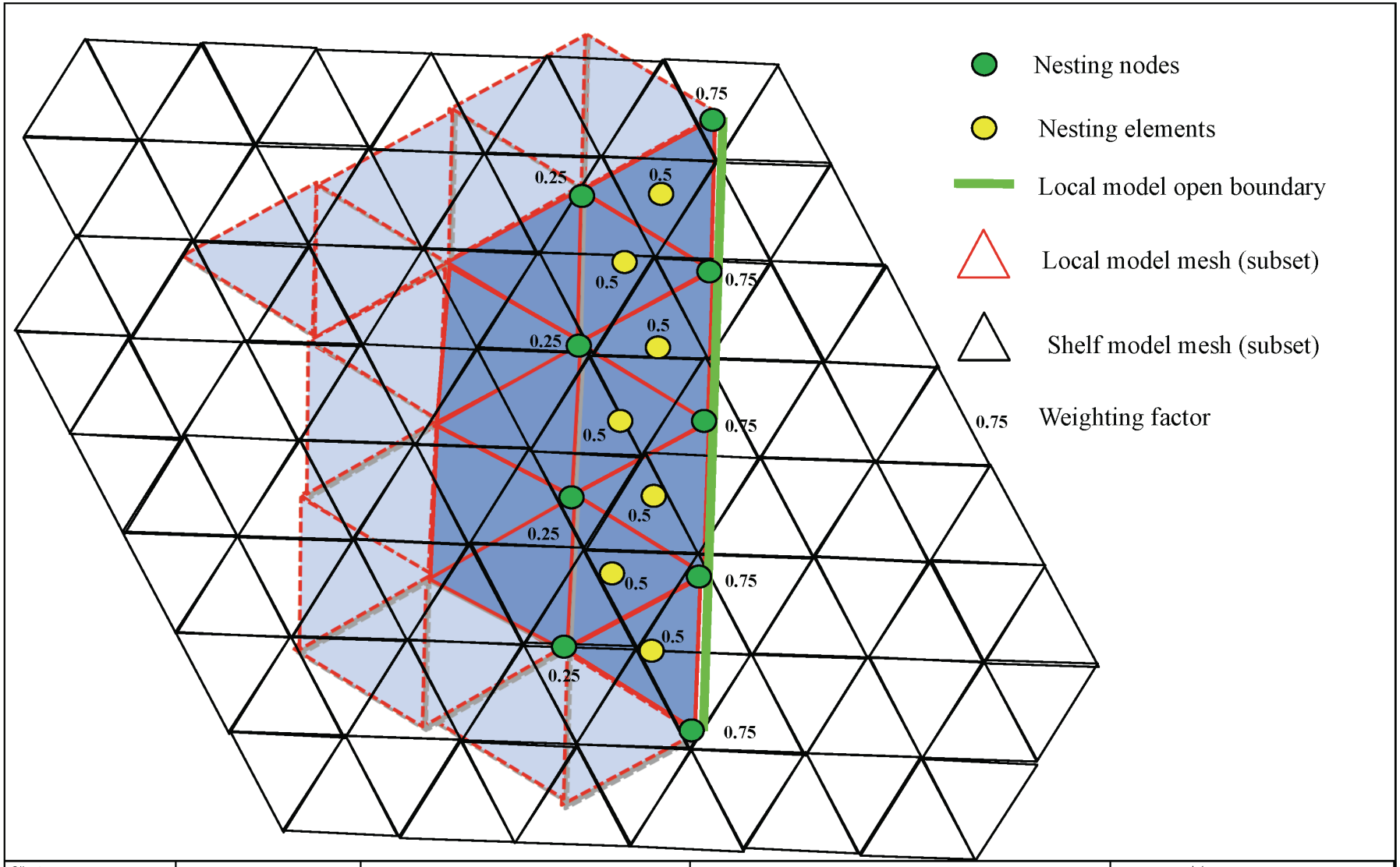
For the current speed components, as the relaxation zone is only one element wide then there is only one layer of weights. In this case a weighting factor of 0.5 (or 50%) was used, meaning current components imposed on the model were derived equally between the values contained within the boundary file (derived from the Shelf model values interpolated onto the boundary nodes) and the current speed components already calculated within the local model. This approach smooth's out any discontinuities that may exist between the two models avoiding instabilities that may otherwise occur.

The resulting nesting file is a netcdf file which is produced by the scripts created as part of this project. It contains the data for each of the variables used as well as the weights for the nodes and elements (variables within the netcdf nesting boundary file are called *weight_node* and *weight_elem*).

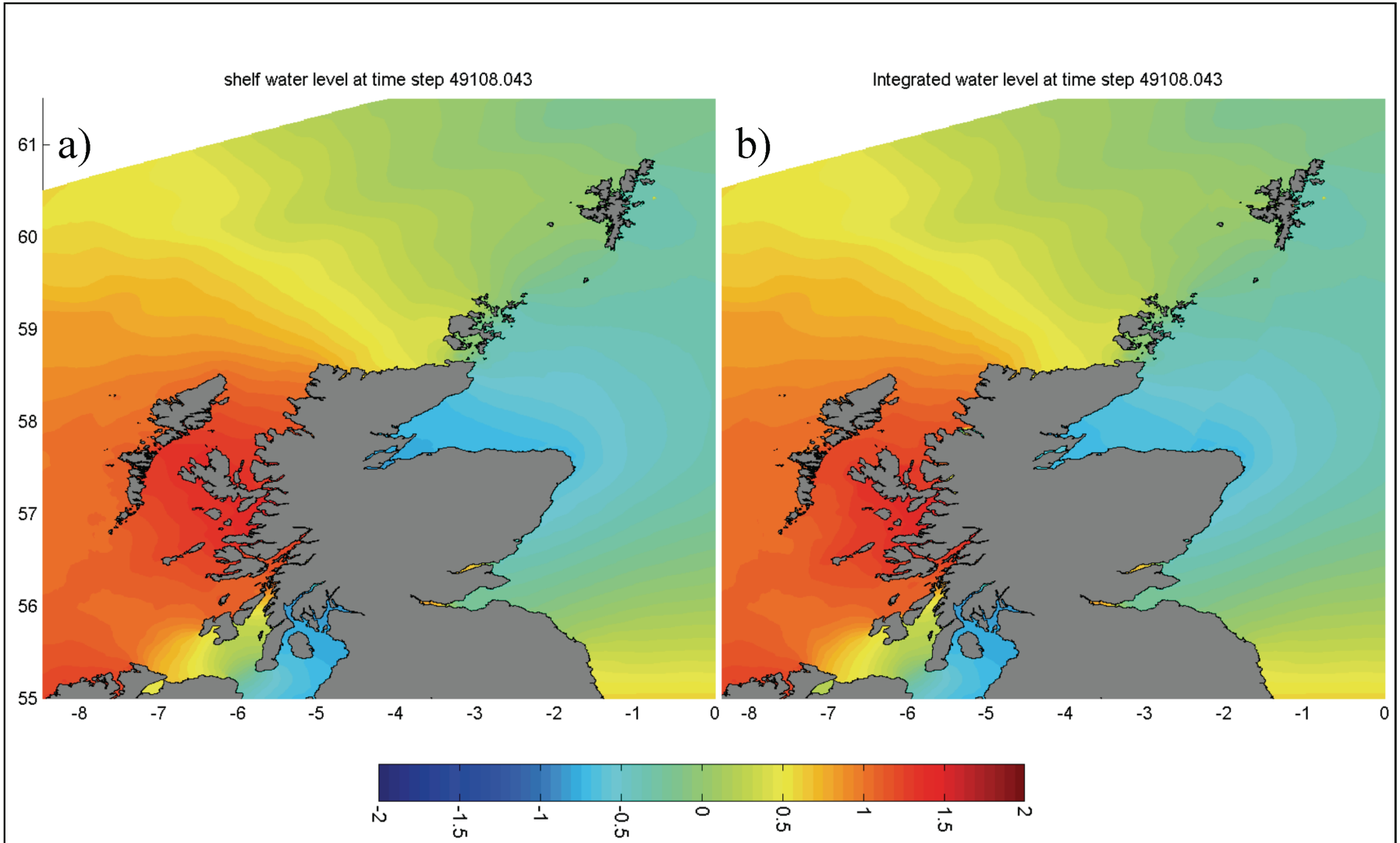
4.3.2 Integrated model results for stage 3

Figure 4-2 shows the combined mesh water levels including the shelf, ECLH, PFOW, WLLS and SMB models, compared with the shelf model only for the same time step in May. Comparison of the shelf and combined mesh for surface, mid-depth and bottom currents are

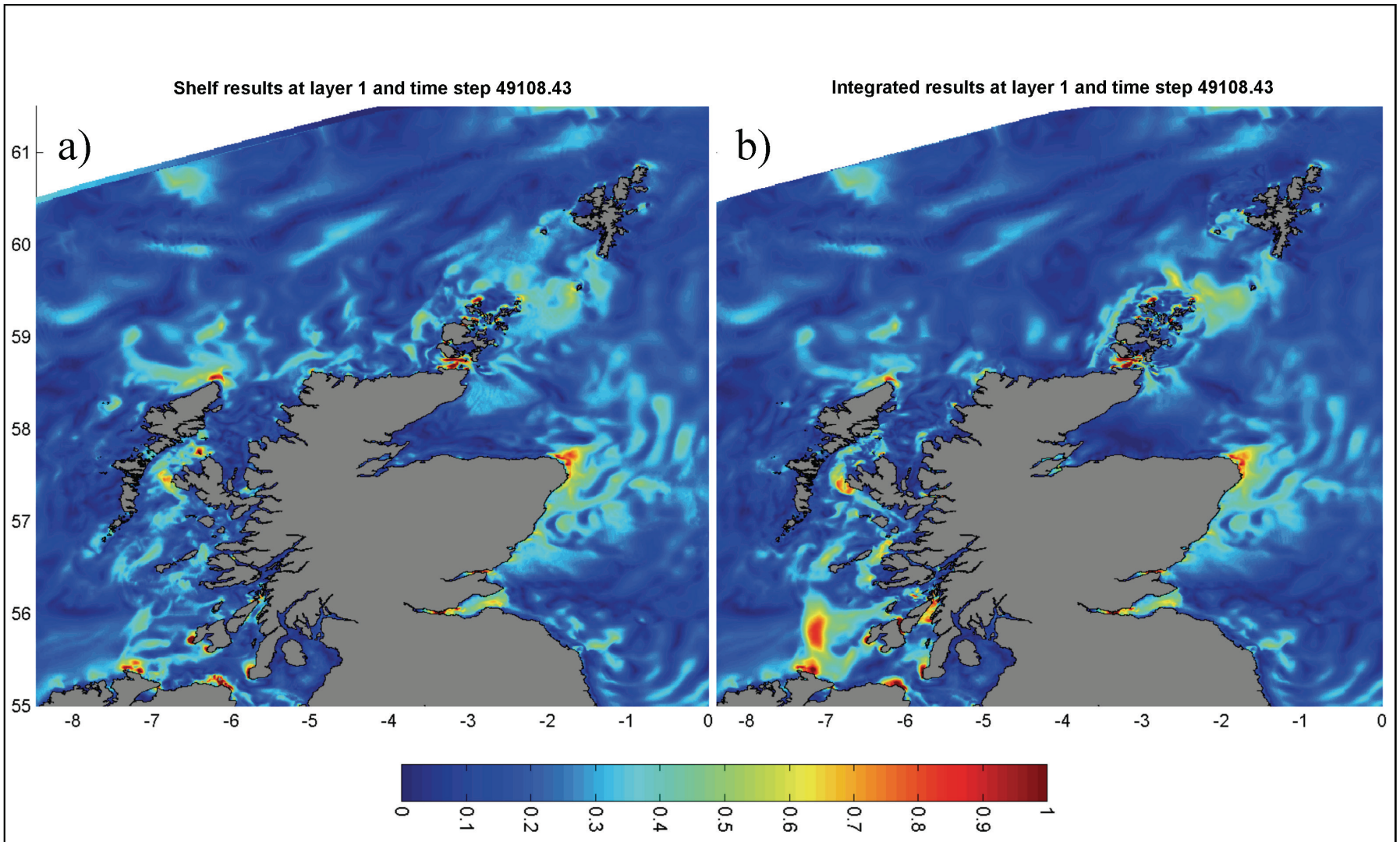
presented in Figure 4-3a to c. Water levels show a seamless transition between the shelf and local models. For the current speeds the transition between the shelf and local models is visible in places, particularly for the bottom currents, however the current speeds in these areas are low <0.2m/s. Figure 4-4 show a comparison of the shelf water levels and the integrated water levels with the shelf and PFOW results only for one time step in January. Figure 4-5a to c show the surface, mid-depth and bottom current speed comparison for the same time step. These results indicate that the method used to combine the model results has been successful.



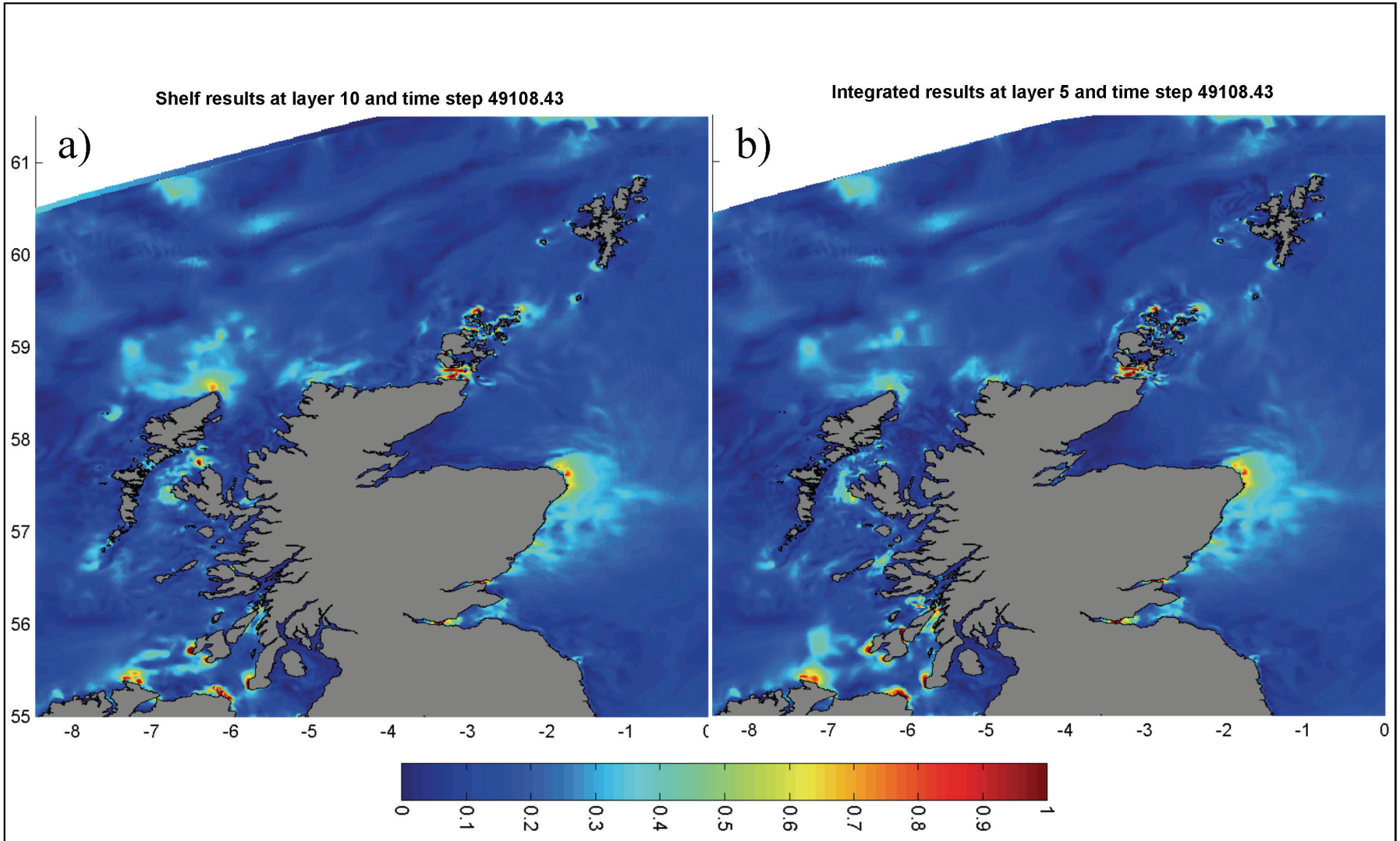
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-1		
Marine Scotland	ch2m:	Scottish shelf waters model	Shelf and local model meshes with nesting boundary nodes/ elements	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



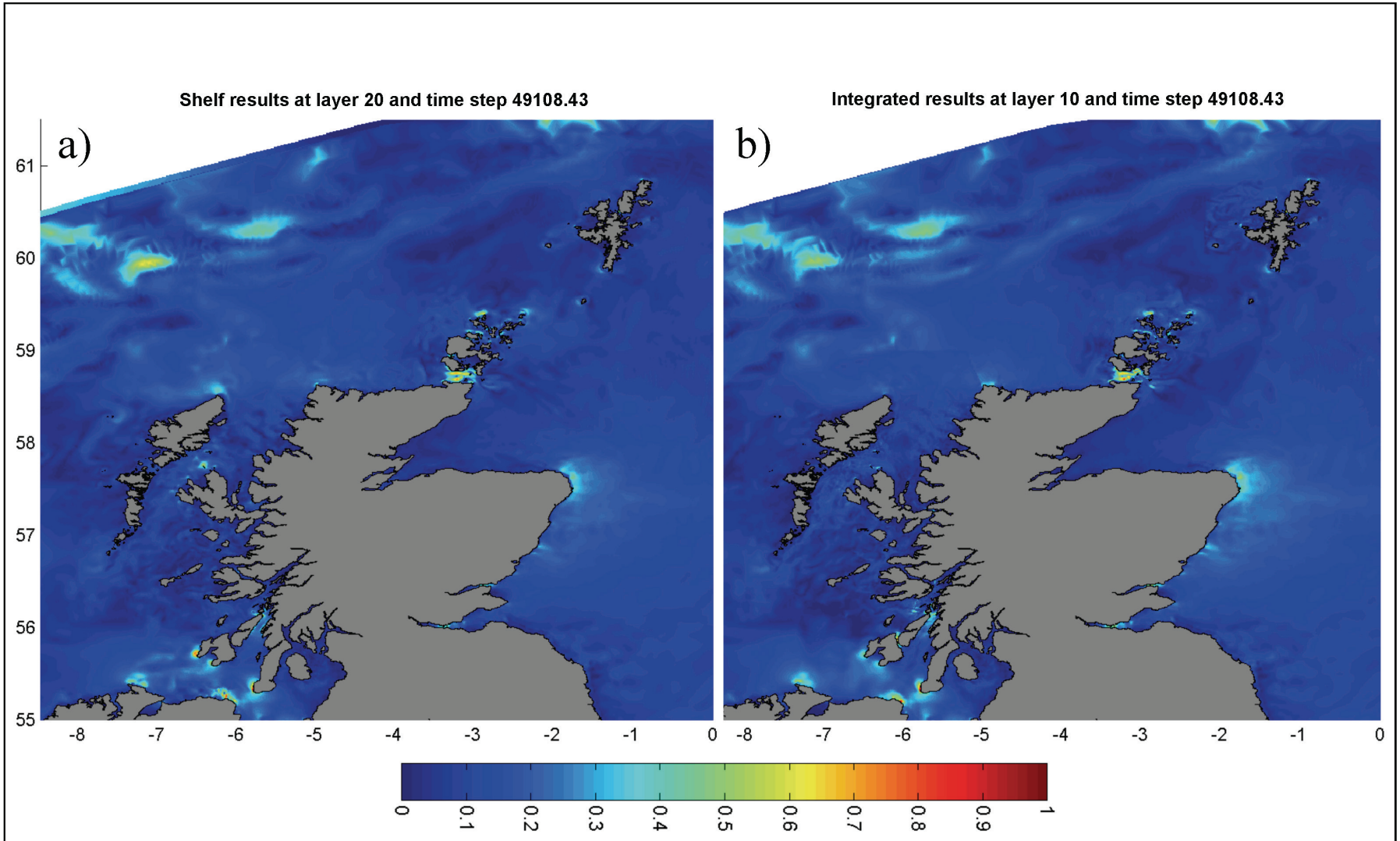
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-2		
Marine Scotland	ch2m.	Scottish shelf waters model	Water level from a) the shelf model and b) the integrated mesh including the shelf, ECLH, PFOW, WLLS and SMB results	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



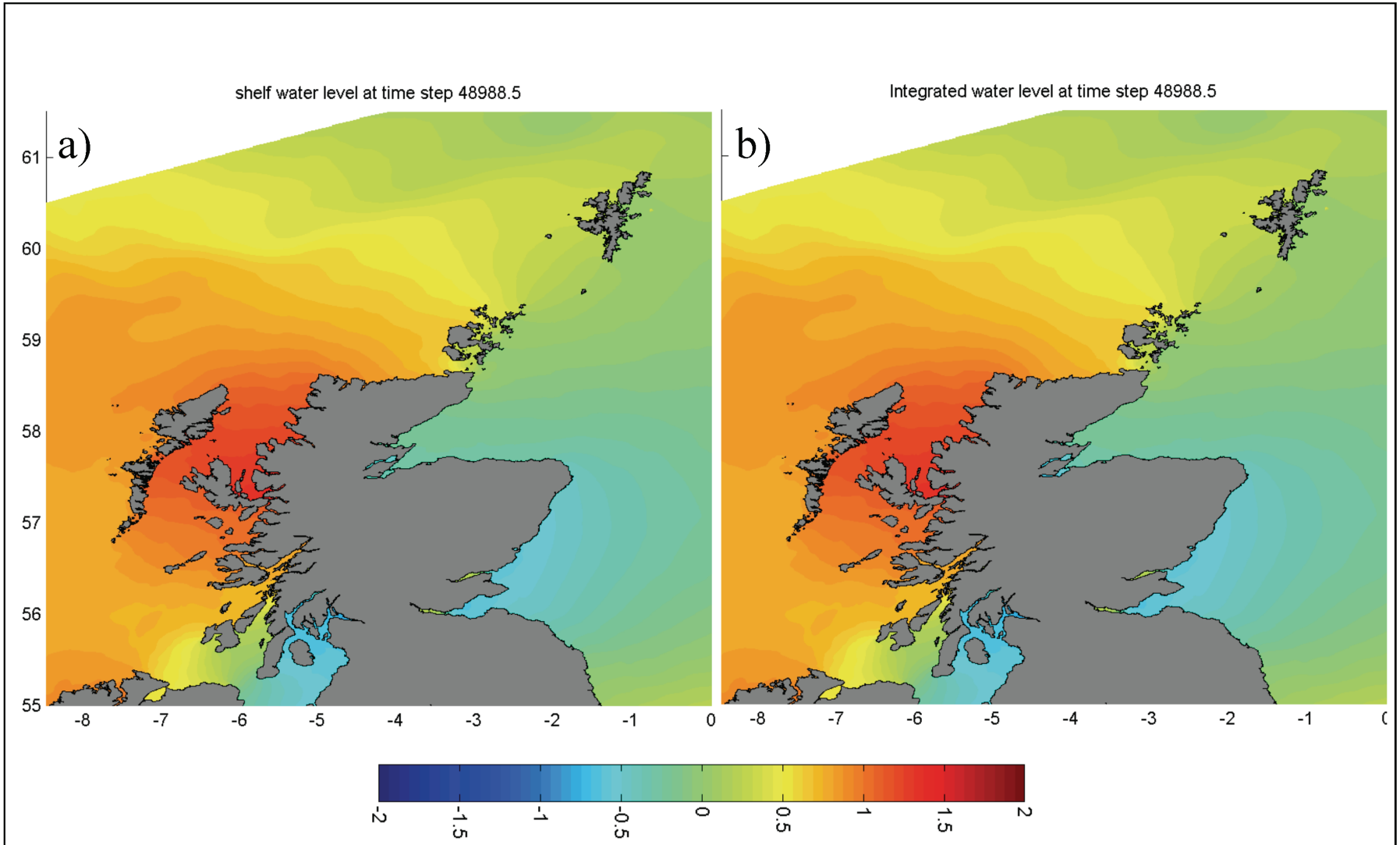
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-3a		
Marine Scotland	ch2m.	Scottish shelf waters model	Surface currents from a) the shelf model and b) the integrated mesh including the shelf, ECLH, PFOW, WLLS and SMB results	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



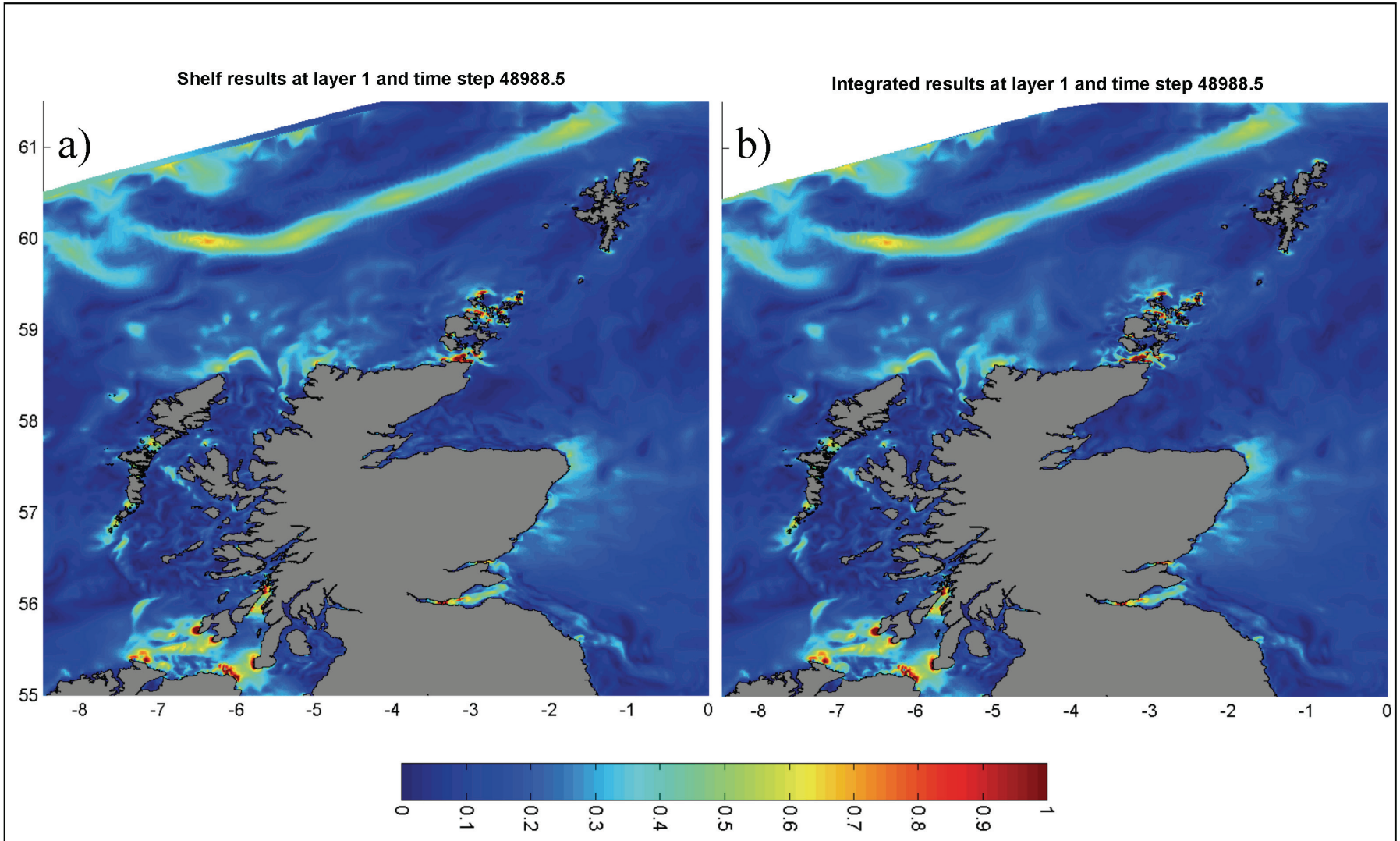
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-3b		
Marine Scotland	ch2m.	Scottish shelf waters model	Mid-depth currents from a) the shelf model and b) the integrated mesh including the shelf, ECLH, PFOW, WLLS and SMB results	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



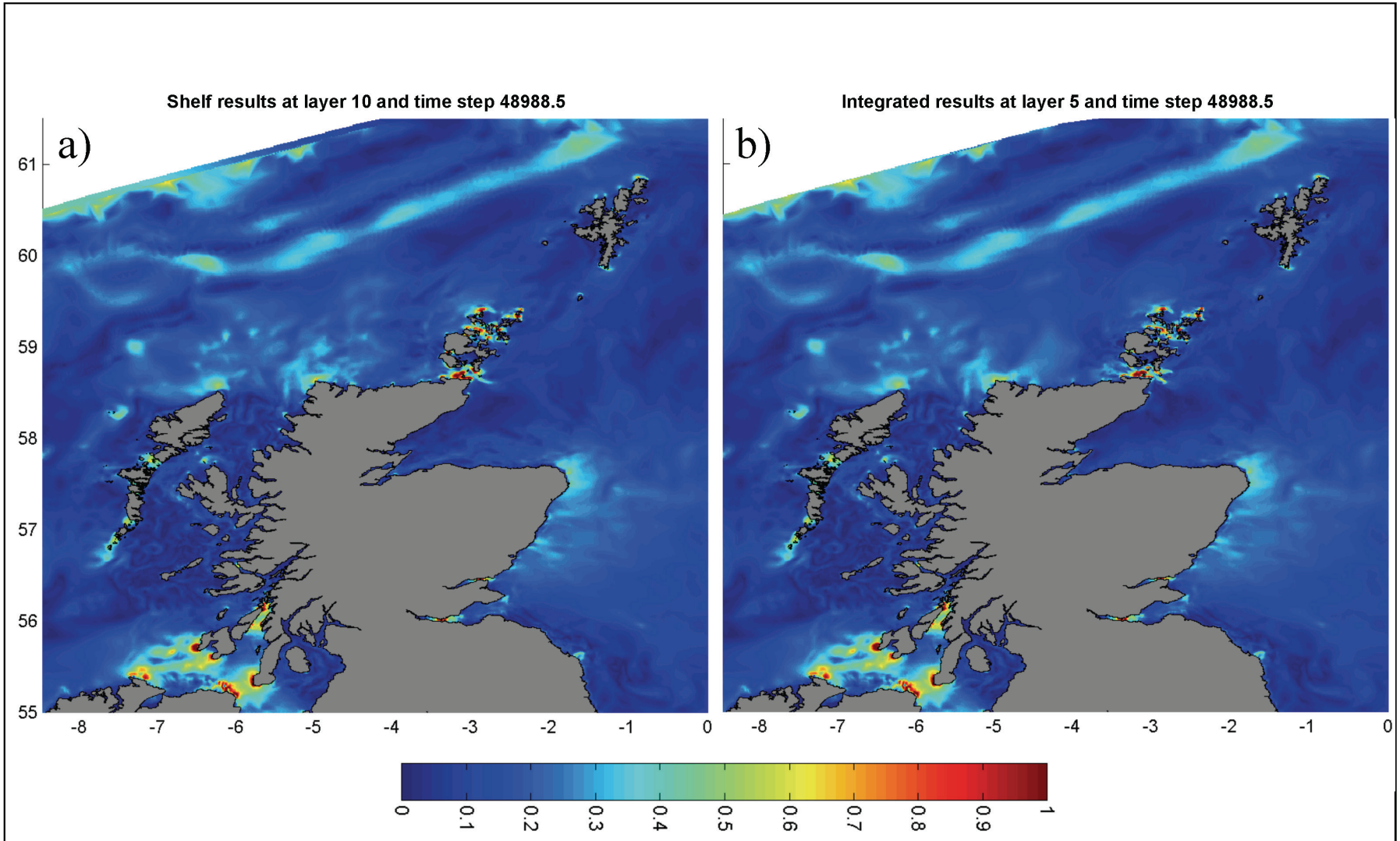
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-3c		
Marine Scotland	ch2m.	Scottish shelf waters model	Bottom currents from a) the shelf model and b) the integrated mesh including the shelf, ECLH, PFOW, WLLS and SMB results	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



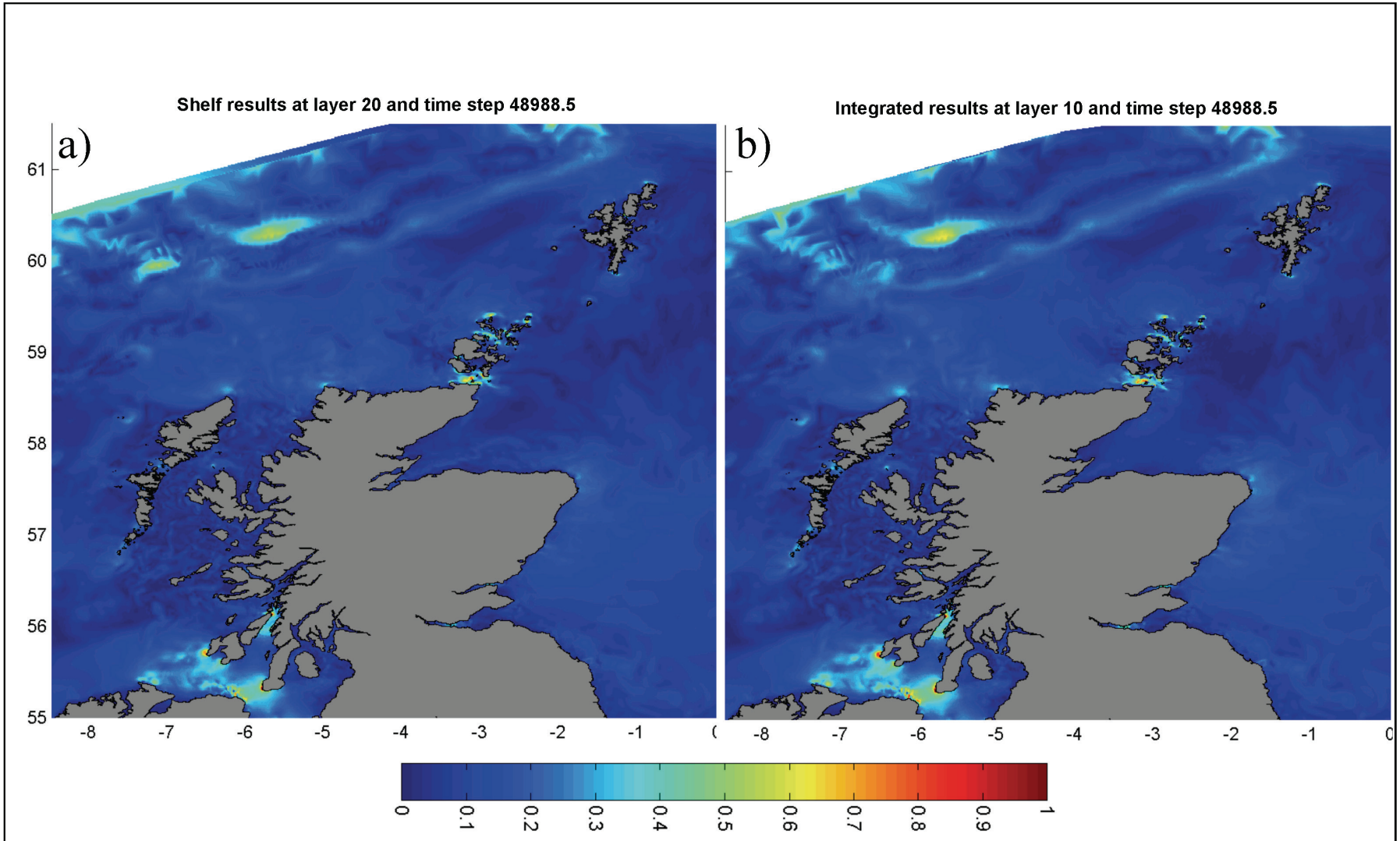
Client	Consulting Engineer	Project:	Figure Title:	Figure 4-4		
Marine Scotland	ch2m.	Scottish shelf waters model	Water level from a) the shelf model and b) the integrated mesh including the shelf and PFOW results only	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 4-5a		
Marine Scotland	ch2m.	Scottish shelf waters model	Surface currents from a) the shelf model and b) the integrated mesh including the shelf and PFOW results only	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 4-5b		
Marine Scotland	ch2m.	Scottish shelf waters model	Mid-depth currents from a) the shelf model and b) the integrated mesh including the shelf and PFOW results only	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014



Client	Consulting Engineer	Project:	Figure Title:	Figure 4-5c		
Marine Scotland	ch2m.	Scottish shelf waters model	Bottom currents from a) the shelf model and b) the integrated mesh including the shelf and PFOW results only	Checked	Scale: Not to scale	Rev.: 0
				Designed	Drawn	Date: 29/10/2014

5. Particle tracking model

5.1 Introduction

A particle tracking and connectivity methodology report (Wolf, 2015) has been prepared and reviewed by Alejandro Gallego (Marine Scotland Science) and Prof Christina Sommerville (Emeritus Professor of Aquatic Parasitology, Institute of Aquaculture, University of Stirling). This full report is attached as Appendix A while some extracts are included here. The initial statement of the problem is to deliver "Connectivity indices (which may be defined as the degree of dynamic interactions between geographically separated populations via the movement of individuals), such as transition probability matrices between (finfish aquaculture) Farm Management Areas (FMA)." These FMAs are on the west coast of mainland Scotland, the Western Isles, Orkney and Shetland; 86 FMA polygons are identified, from which particles are released and tracked and their capture by the original or other FMAs is calculated.

The report reviews the background to this study in terms of the dispersal of sea lice, referring to the life cycle of the sea louse *Lepeophtheirus Salmonis* (referred to as *L. Salmonis*, also known as Leps) which is the main species causing concern in the aquaculture industry, as well as the behaviour of 2 other disease vectors: Infectious Salmon Anaemia Virus (ISAV), a representative short-persistence pathogen and Infectious Pancreatic Necrosis Virus (IPNV), a representative long-persistence pathogen. Some previous particle tracking studies are reviewed.

Based on laboratory experiments, the optimum temperature for *L. Salmonis* larvae is 10°C and the optimum salinity is 33-35 psu. The larvae are infectious when they are in the copepodid stage (approximately the last ⅔ of the pelagic larval duration, PLD). At lower salinities copepodids do not thrive (< 25 psu). Copepodids are thought to maintain their position just below the halocline when surface water is less saline than 29 psu. Otherwise they are in the surface waters (they control this by buoyancy and vertical swimming behaviour). Representative particles are therefore released in the surface layer and "target" FMAs reached within the infectious part of the PLD are scored.

ISAV has a pelagic duration of about 3 days and IPNV has a pelagic duration of about 35 days during autumn to spring and 17 days in summer. These disease vectors are assumed to be well-mixed through

the water column and passive, so whole water column releases and passive vertical and horizontal drift (including diffusion) are used. All "target" FMAs reached within the pelagic duration period are scored.

The method adopted is to use the offline particle tracking module available in FVCOM (described in section 5.2). Some code fixes were necessary in order to get the horizontal and vertical diffusion parts of the code to work. The particle tracking is run in post-processing mode, using the Climatology output from the combined Stage 1 Shelf Model and Stage 2 models results (sections 3 and 4), using the methodology described in sections 5.3, which utilises hourly current fields, forced by climatological forcing over a standard tidal year.

The FMAs are shown in Figure 5-1 to 5-4. They are represented by 89 shape files within the model grid (Figure 5-5). The nomenclature used in Figs. 5-2 – 5-4 is used hereafter i.e. S1-S11 (Shetland, including S8a and S8b), O1-O4 (Orkney), M1-M49 (Mainland) and W1-W22 (Western Isles). Of these 89 areas, one represents a tiny extension of M13 and another is a westward extension of W14. Most of the FMAs are well-resolved in the combined shelf model mesh, however there are some that do not include any nodes of the model (M12, inner Loch Broom and M43, inner Loch Striven) and some that are only partially resolved (e.g. S10 and M13). The FMAs numbered M11, M12 and M13 have therefore been combined within a boundary further out into the estuary and called LB (Loch Broom), see Fig. 5-6a. The inner FMA in Loch Striven (M43) has been extended south in order to enclose some model nodes (Fig. 5-6b). The resulting 86 polygons have been used to define the areas of sources and sinks for particle tracking.

A large number of particles are released within the 86 Farm Management Areas (FMAs) in Scottish Waters. The experimental design is described further in section 5.3. Example results of the particle tracking are shown in section 5.4

The Connectivity matrices have been calculated from these results, taking into account the length of time for which sea lice larvae and viruses can survive at various temperatures in the sea. This is presented in section 6.

5.2 Particle Tracking in FVCOM

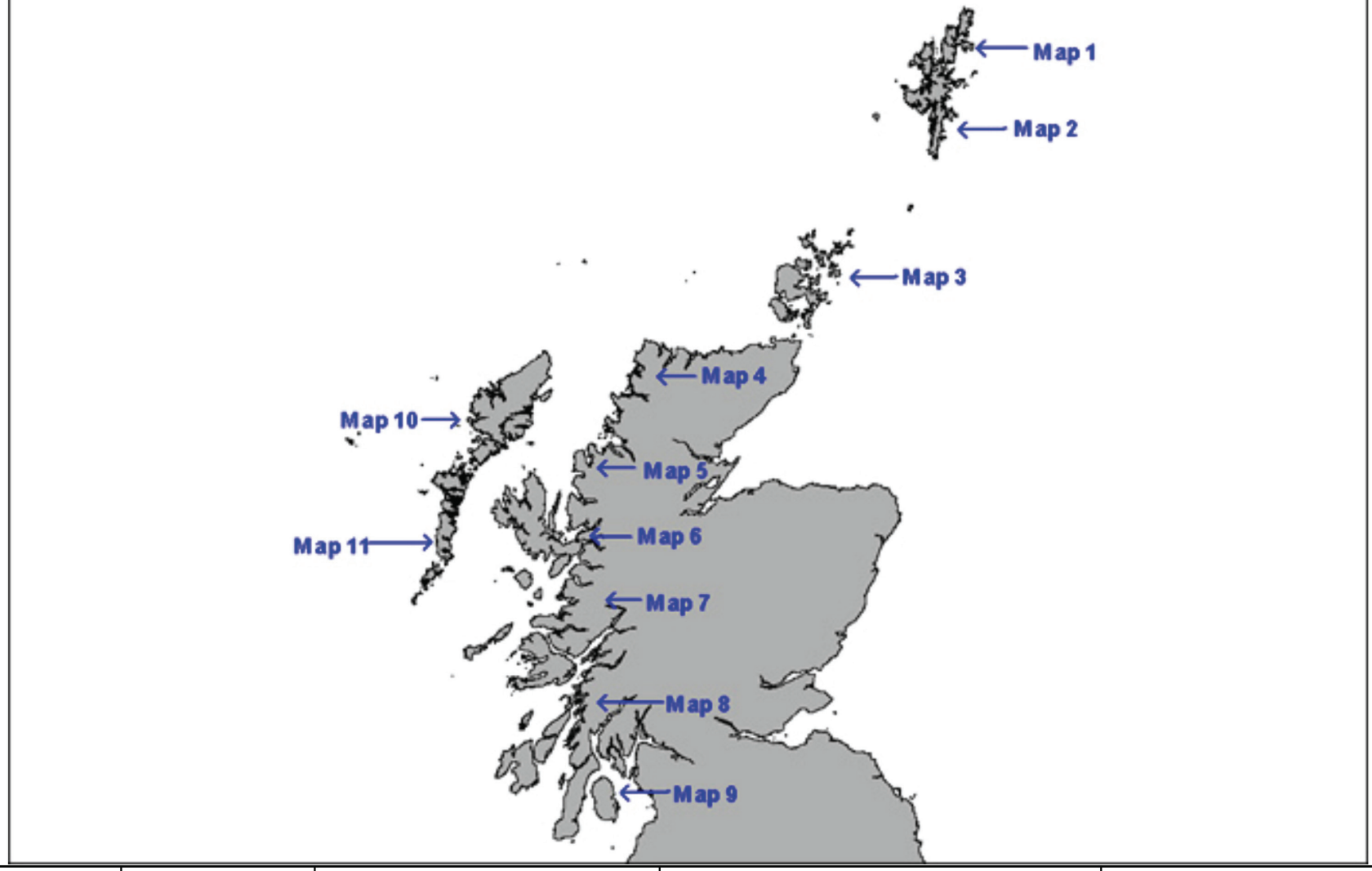
5.2.1 Theory

From the FVCOM manual (Chen et al., 2013) the Lagrangian particle tracking module consists of solving a nonlinear system of ordinary differential equations (ODE) as follows

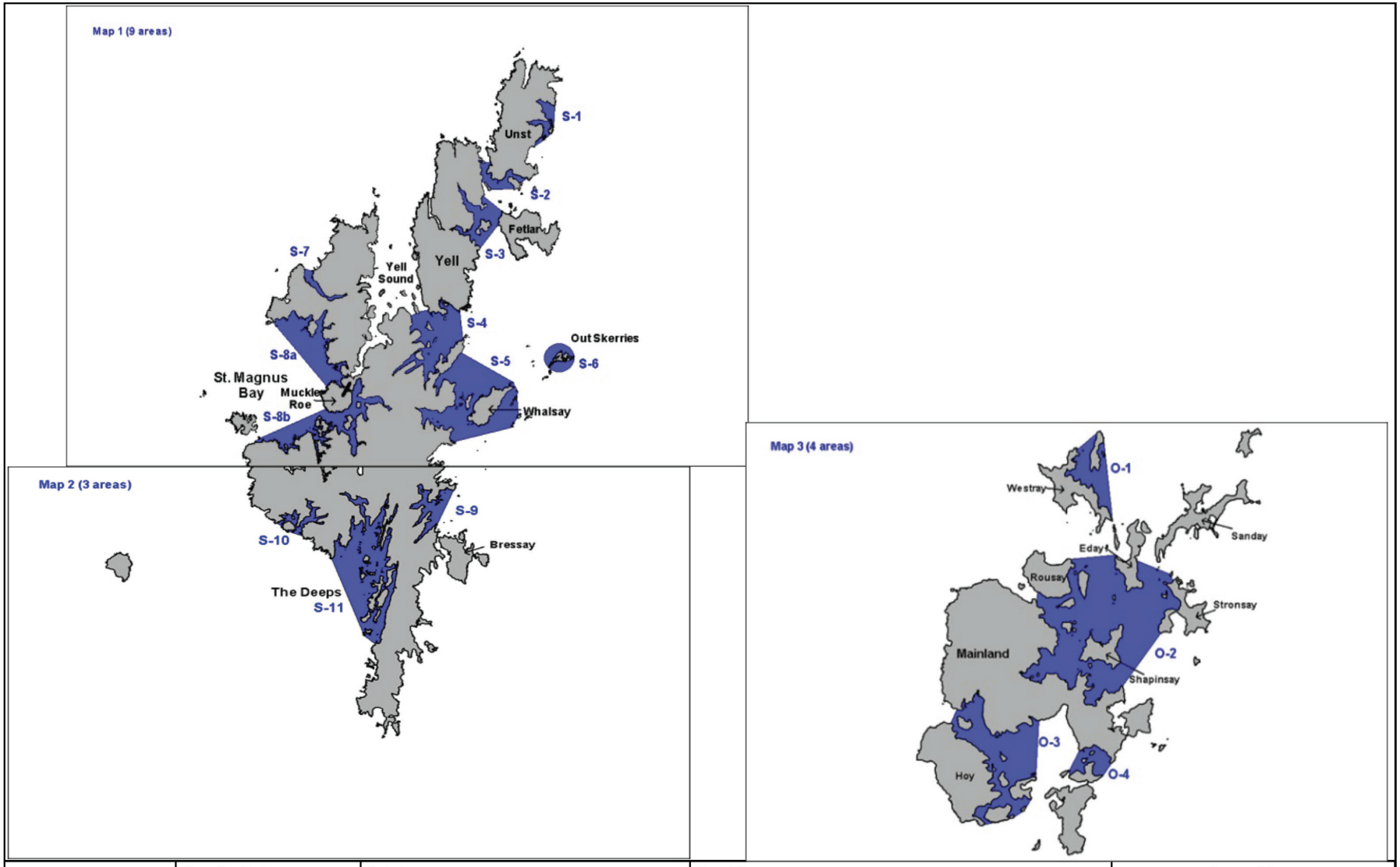
$$\frac{dx}{dt} = \boldsymbol{v}(\boldsymbol{x}(t), t) \tag{5.1}$$

where ***x*** is the particle position at a time *t*, *d***x**/*dt* is the rate of change of the particle position in time and **v**(**x**,*t*) is the 3-dimensional velocity field generated by the model. This equation can be solved using any method suitable for solving coupled sets of nonlinear ODE's such as the explicit Runge-Kutta (ERK) multi-step methods which are derived from solving the discrete integral:

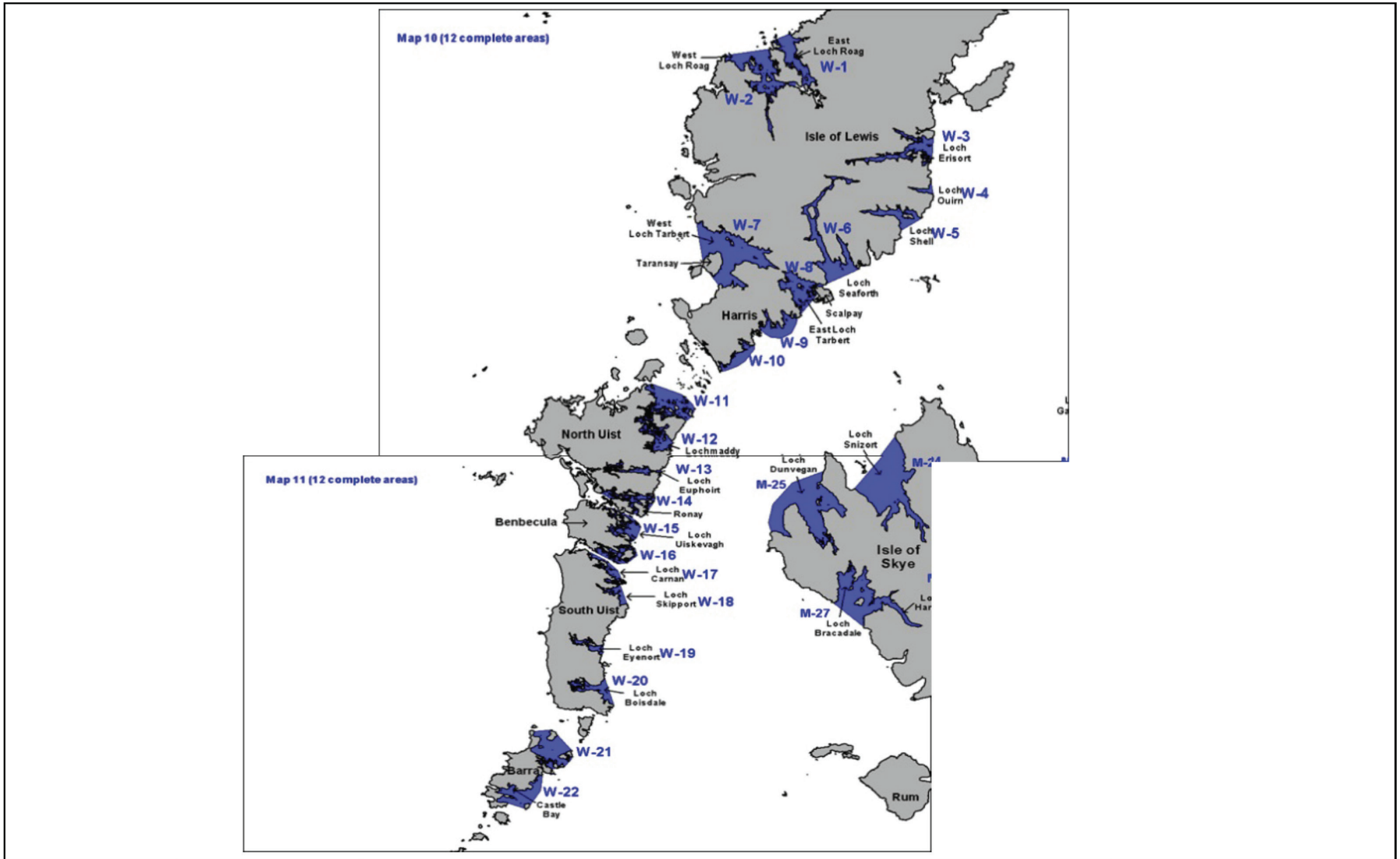
$$\boldsymbol{x}(t) = \boldsymbol{x}(t_n) + \int_{t_n}^{t} \boldsymbol{v}(x(t), \tau) d\tau \tag{5.2}$$



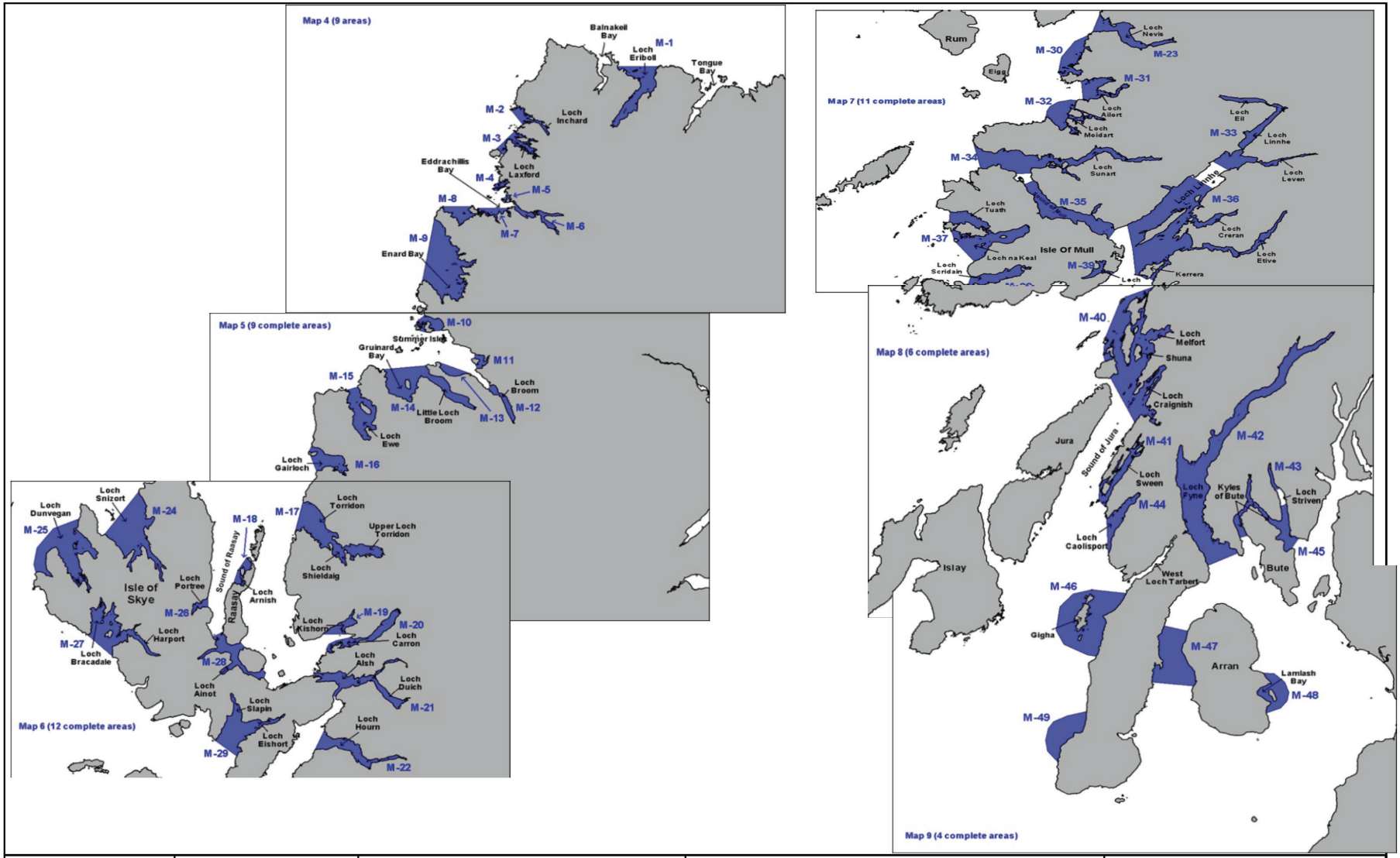
Client	Consulting Engineer	Project:	Figure Title:	Figure 5.1		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	Locations of Scottish FMA group maps	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



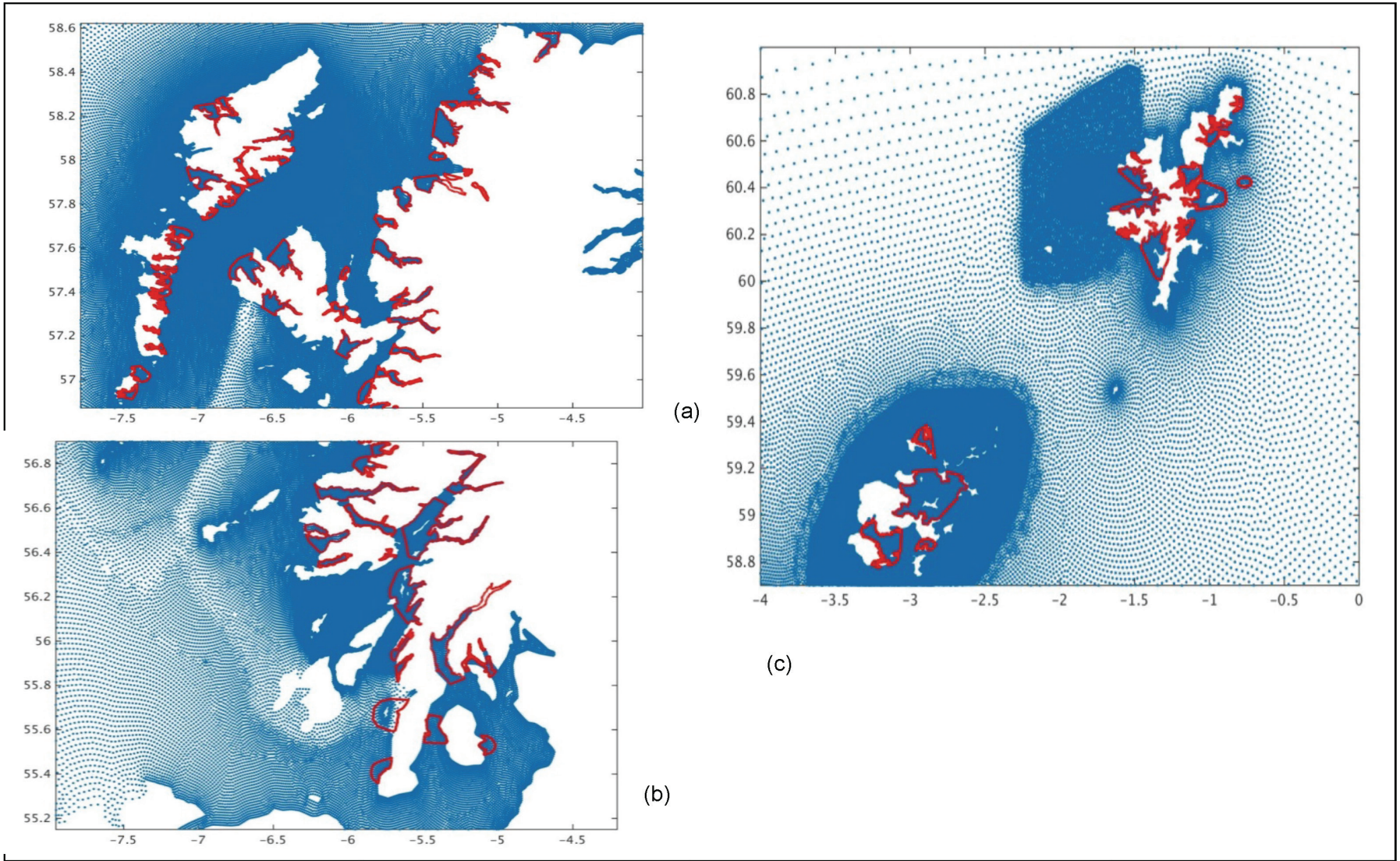
Client	Consulting Engineer	Project:	Figure Title:	Figure 5-2		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	FMAs in Shetland (left) and Orkney (right)	Checked: JW	Scale: Not to scale	Rev.: 0
				Designed:	Drawn:	Date: 21/11/2015



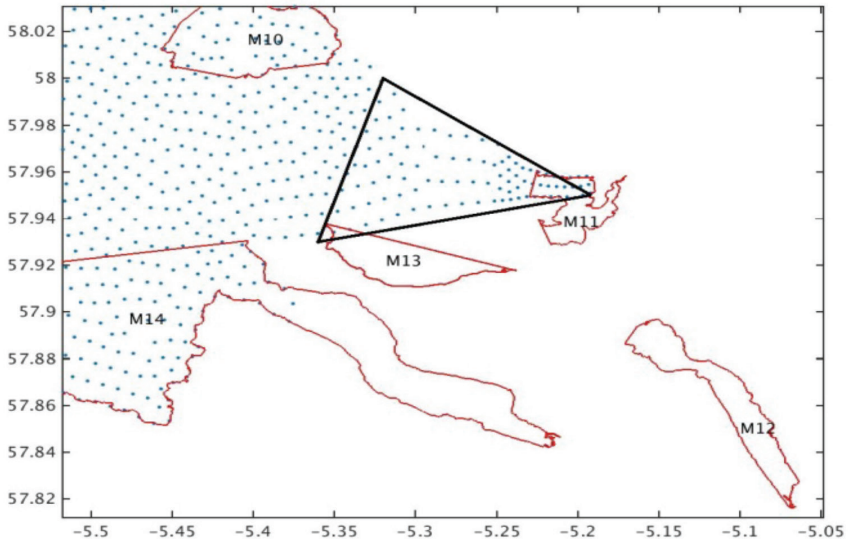
Client	Consulting Engineer	Project:	Figure Title:	Figure 5-3		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	FMAs in Western Isles	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



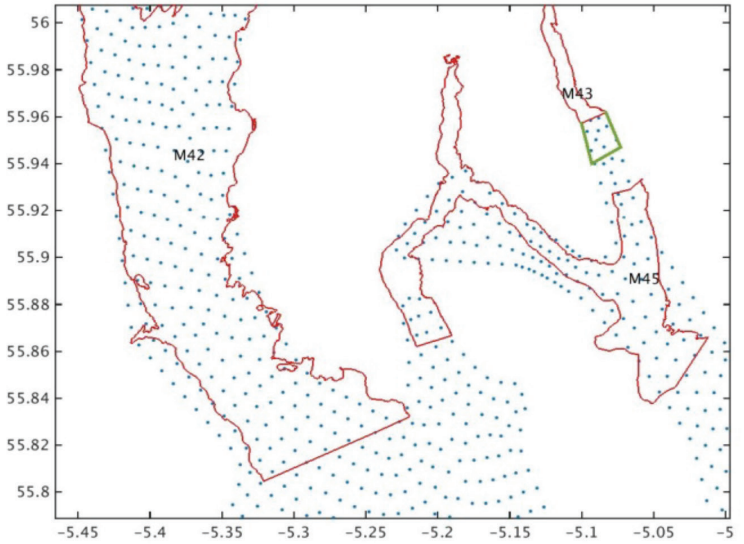
Client	Consulting Engineer	Project:	Figure Title:	Figure 5-4		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	FMAs on Mainland – North (left) and South (right)	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



Client	Consulting Engineer	Project:	Figure Title:	Figure 5-5		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	Plots of FMA shape files on combined model grid (a) northern mainland and Western Isles (b) southern mainland © Orkney and Shetland	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



(a)



(b)

Client	Consulting Engineer	Project:	Figure Title:	Figure 5-6		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	**Modifications to FMA's (a) Loch Broom (b) Loch Striven. Original FMA boundaries are in red, new boundaries in black; model nodes are blue dots**	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

Assume that $x_n = x(t_n)$ is the position of a particle at time $t=t_n$, then the new position $x_{n+1} = x(t_{n+1})$ of this particle at time $t = t_{n+1}$ $(= t_n + \Delta t)$ can be determined by the 4th order 4-stage ERK method where Δt is the time step. The dependence of the velocity field on time has been eliminated since the velocity field is considered stationary during the tracking time interval of Δt. It is important to understand that in a multidimensional system, the local functional derivative of v must be evaluated at the correct sub-stage point x in (x, y, z) space. On a 2-dimensional (x,y) plane, for example, a particle can be tracked by solving the x and y velocity equations given as

$$\frac{dx}{dt} = u, \quad \frac{dy}{dt} = v, \tag{5.3}$$

Many users have added a random walk-type process into this 3-D Lagrangian tracking code to simulate sub-grid-scale turbulent variability in the velocity field. In FVCOM version 2.5, only the advection tracking program was included as described above, however version 3.1.6 (as used here) includes an optional random walk, R (uniformly distributed within the domain [-1,1]), where the horizontal diffusivity D_h is specified as a constant and the vertical diffusivity D_v is provided from the circulation model.

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_n) + \int_{t_n}^{t} \boldsymbol{v}(x(t), \tau) d\tau + \sqrt{6RD_h\Delta t} \tag{5.4}$$

Some smoothing of the diffusivity may be required in the vertical (Brickman and Smith, 2002). A key property of a correct Lagrangian Stochastic Model is that it maintains an initially uniform concentration of particles uniform for all time. This is called maintaining the well-mixed condition (WMC). If the result does not conform to WMC this may be due to inadequate resolution of the hydrodynamic model. Ideally one should conduct statistical tests to ensure that the number of particles is sufficient for the investigation (Brickman and Smith, 2002).

The in-line particle tracking program can be run on both single and multi-processor computers. However, in the MPI parallel system, tracking many particles simultaneously with the model run on a multi-processor computer can significantly slow down computational efficiency, since particles moving from one sub-domain to another require additional information passing. Multiple runs of the particle tracking would also require re-running the hydrodynamic model. For this reason, it is suggested that users use the offline version of the particle tracking code.

5.2.2 Offline particle tracking code

The offline code is provided in the FVCOM package. This is not parallelised and runs on a single processor only. For large numbers of particles (O(100,000)) the calculations may be run on multiple processors by dividing the particles between processors, to speed up processing. Multiple runs can be carried out in parallel as long as the particles are from different spatial locations (multiple particles from one point may produce duplicate runs due to the nature of the random number generator).

Note that the supplied version of the offline particle tracking code had some software errors which have now been fixed. This code includes no biological behaviour, but particles can be released at different vertical levels and there are options for inclusion of a random walk diffusion term in the horizontal and vertical, as well as 3-dimensional advection. There is an option for a fixed level or a sigma-coordinate level for the release points.

The modules of the offline package are shown in Table 5-1. The main code is in **offlag.f90**, which includes the main program PARTICLE_TRAJ which in turn calls subroutines in **offlag.f90, alloc_vars.f90, data_run.f90, ncdio.f90** and **triangle_grid_edge.f90**. The other modules set array sizes, initialise arrays and provide certain utility subroutines and functions.

Table 5-1: Modules of Lagrangian off-line particle tracking program

Module	Purpose
alloc_vars.f90	Allocates and initialises most arrays
data_run.f90	Inputs parameters which control the model run
mod_inp.f90	Decompose input line into variable name and variable value(s)
mod_ncd.f90	NetCDF utilities
mod_prec.f90	Defines floating point precision using kind
mod_var.f90	Sets global limits and array sizing parameters
ncdio.f90	NetCDF I/O: input time and output surface elevation and bottom depth
offlag.f90	Lagrangian particle tracking off-line program
triangle_grid_edge.f90	Define the non-overlapped, unstructured triangular meshes used for flux computations
util.f90	Utilities, from Numerical Recipes

The important parts of the code deal with particle advection, then optional dispersion using a random walk method. The method of vertical diffusion is given in Visser (1997) and Ross and Sharples (2004).

The code as supplied worked for advection only and for Cartesian coordinates but not for lat/lon coordinates. The start-up time is quite long (~2 hours for the large combined model grid). A modified code which shortened this set-up time for subsequent runs, by saving metrics calculated within *triangle_grid_edge.f90* was provided (Pierre Cazenave, pers. comm.), however there was a bug in this code which has now been fixed. The code also did not work for horizontal and vertical dispersion, which is calculated using a random walk. The horizontal random walk had some errors, with some variable declarations needing to be corrected. Additionally, there was a problem with the vertical random walk: there was an error in the dimension of

the vertical diffusivity, which is read in at nodes but has to be interpolated to elements.

5.3 Particle Tracking in SSM

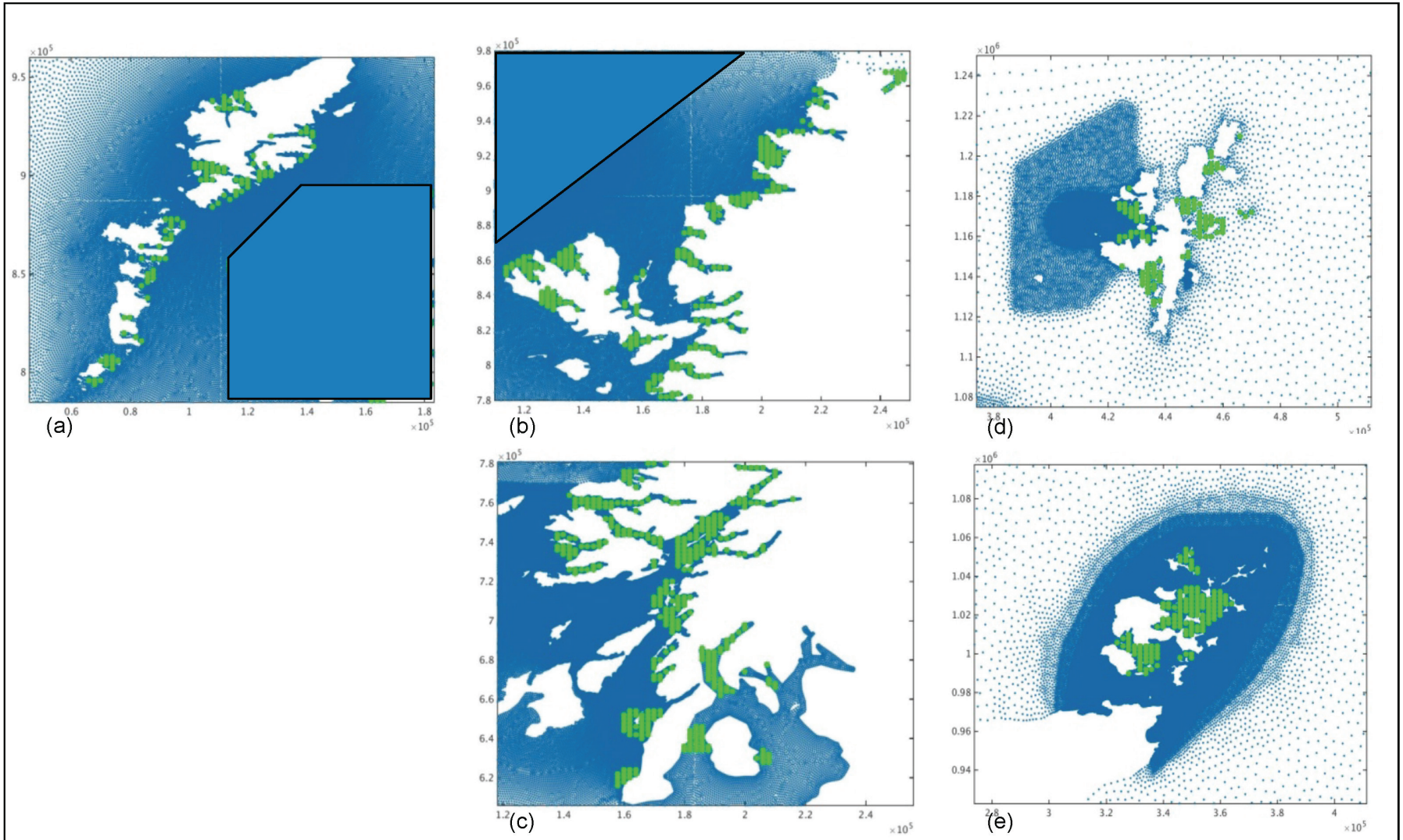
The particle release points were generated by generating a uniform 2kmx2km mesh extending over the whole model grid then selecting those points which lay within the FMAs. This produced at least 1 particle release point in each FMA, except for 3 locations where a particle release point had to be generated manually. The final selection was 977 release points with between 1 and 100 particle release points per FMA (Figure 5-7).

Multiple particles were released at each location, using a random walk to model the diffusion, checking that the result was not sensitive to the number of particles. 100 particles per release point seemed satisfactory. A limited number of particles were used due to computational constraints. The number of particles required is discussed by Brickman et al. in North et al., (2009) which also refers to Brickman and Smith (2002). In typical releases they tested 100-2000 particles, to ensure that the final result is not sensitive to the number of particles.

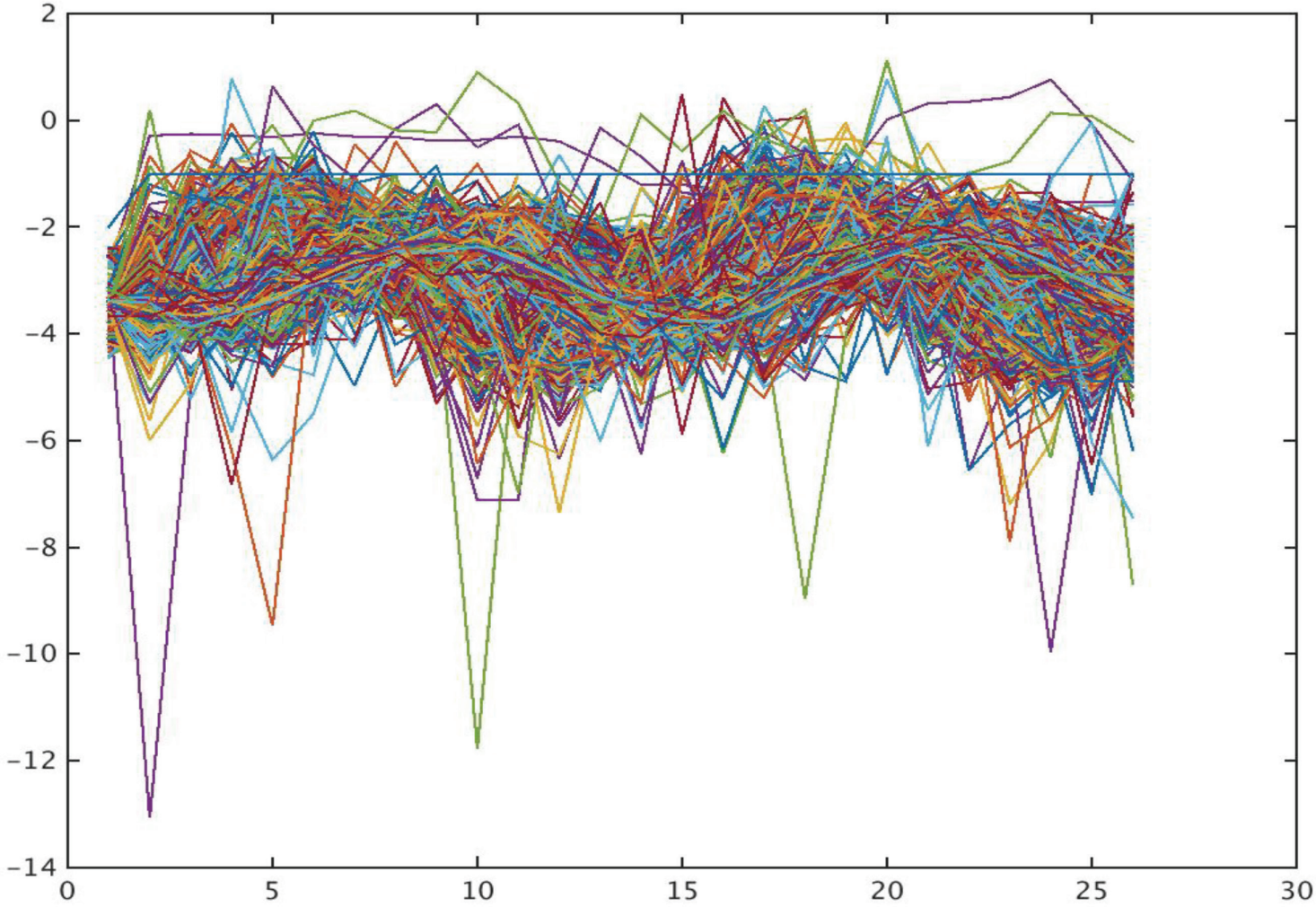
'Sea lice' particles are constrained to stay in the surface layer. For this it was found best to use the fixed depth option, with the initial depth below the surface as 3m and only horizontal diffusion. The particles do move in the vertical by advection, to some extent, but most particles stay within the surface layer (see Figure 5-8).

'Virus' particles were released at surface, mid-depth and bottom in the water column, using 50 particles at each level, which was a compromise from the ideal (100 particles at each of 10 levels) to avoid excessively long run times of the particle tracking code.

The particles were tracked for appropriate PLD periods for each season (see Table 5-2).



Client	Consulting Engineer	Project:	Figure Title:	Figure 5-7		
Marine Scotland	ch2m:	Scottish Shelf Waters Model	Particle tracking release points: (a)Western Isles (b) north mainland (c) southern mainland (d) Shetland (e) Orkney	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



Client	Consulting Engineer	Project:	Figure Title:	Figure 5-8		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	**Height above mean sea level for 1 particle from each release point tracked over 1 day – including 3D advection and horizontal diffusion, fixed depth (3m)**	Checked: JW	Scale: Not to scale	Rev.: 0
				Designed:	Drawn:	Date: 21/11/2015

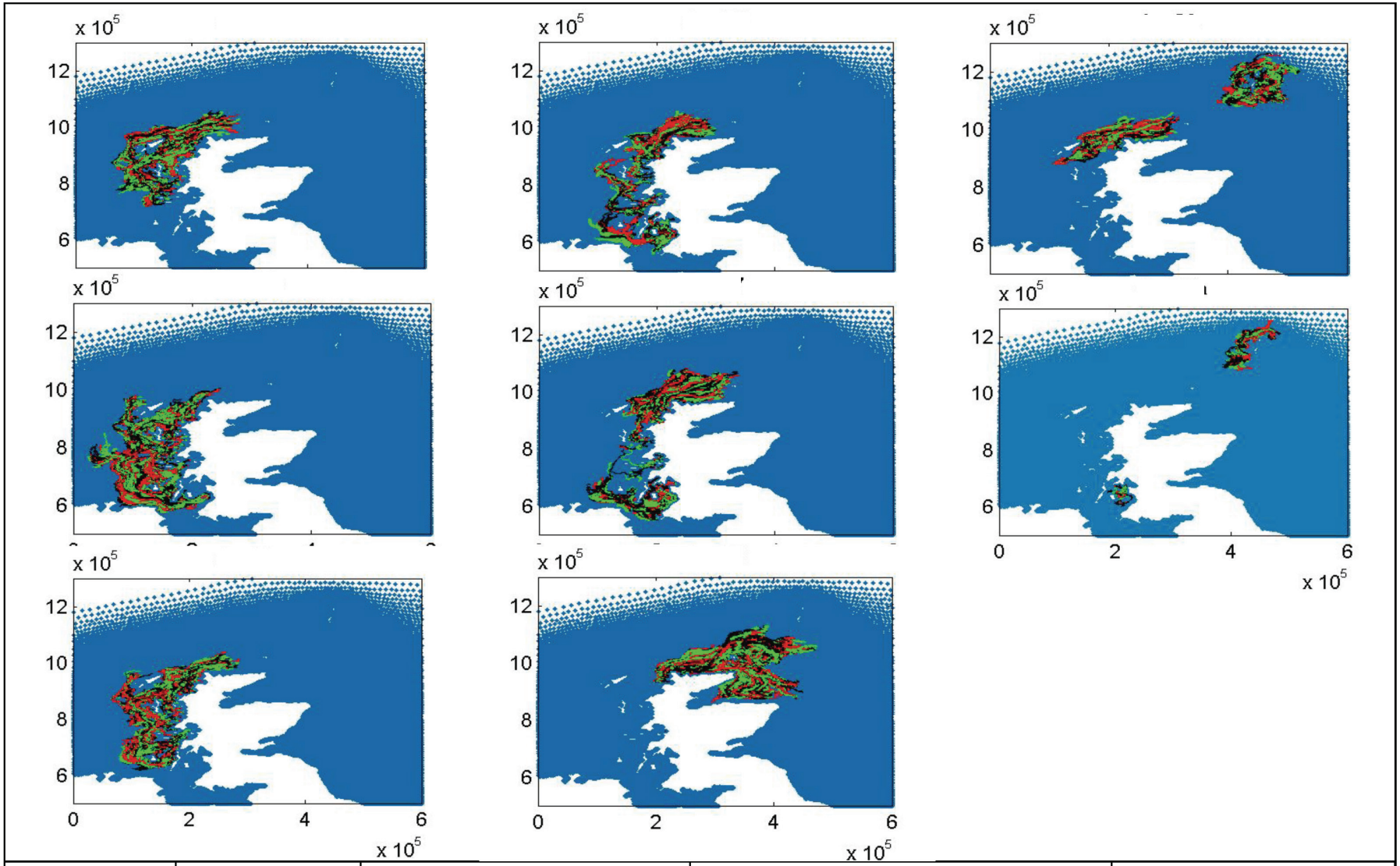
Table 5-2: Particle tracking runs

Biology	Season	Start date	Duration	Scoring	Number of particles (depth)	Physics
Sea-lice larvae	Spring	1 April	15 days	Hours 121-360	977 x 100 (3m)	Advection plus horizontal diffusion
"	Summer	1 July	10 days	Hours 81-240	977 x 100 (3m)	Advection plus horizontal diffusion
"	Autumn	1 October	15 days	Hours 121-360	977 x 100 (3m)	Advection plus horizontal diffusion
"	Winter	1 January	18 days	Hours 145-432	977 x 100 (3m)	Advection plus horizontal diffusion
Viruses ISAV + IPNV	Spring	1 April	35 days	All (1^{st} 3 days for ISAV)	977 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion
"	Summer	1 July	17 days	All (1^{st} 3 days for ISAV)	977 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion
"	Autumn	1 October	35 days	All (1^{st} 3 days for ISAV)	977 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion
"	Winter	1 January	35 days	All (1^{st} 3 days for ISAV)	977 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion

5.4 Results

The separation matrix for the 86 FMAs has been computed, taking a simple direct separation using plane geometry. The maximum separation between FMAs is 662 km, between the southernmost FMA on the mainland and the north of Shetland. From the climatology run the residual currents near the shelf edge are directed towards the NE and have a maximum velocity of 25cm/s, generally much smaller residual currents will be present nearshore, where the FMAs are located. At 25cm/s a distance of 324km could be covered in 15 days, however much smaller distances are more likely.

Figure 5-9 shows particle tracks for the January 35-day virus runs where the particles are released at surface, mid-depth and bottom. Each panel represents a sub-division of all the particles between 10 processors (as discussed in section 5.2.2). The first 9 processors have been used to each calculate 15,000 particle tracks; 150 particles released at 100 different release locations for each case. The 10th processor tracked the remaining released particles (making a total of 146,550 particles). A final run was carried out for 3 release points (450 particles) which were not moving within the grid. The surface releases are shown in red, mid-depth are green and bottom are black. The tracks for particles released at different levels do not differ substantially, apart from the random walk component, because the particles move freely through the water column, unlike the sea lice larvae which are constrained to stay in the surface layer.



Client	Consulting Engineer	Project:	Figure Title:	Figure 5-9		
Marine Scotland	ch2m.	Scottish Shelf Waters Model	**Particle Tracks for the January 35-day virus runs: red = surface release; green = mid-depth release; black = bottom release**	Checked: JW	Scale: Not to scale	Rev.: 0
				Designed:	Drawn:	Date: 21/11/2015

6. Connectivity Indices

6.1 Methodology

The final step is construction of Connectivity Indices between the FMAs. The likelihood of larval exchange between FMAs is represented using the following matrices:

- Distance matrix of the separation of individual Management Areas: this can be easily calculated as a straight line distance but will be less than the actual seaway distance that must be travelled.
- Transitional Probability Matrix P_{ij} (hereafter termed the Connectivity Matrix) representing the probability that an individual particle released at the source *i* will disperse to the destination *j*, over a given period of time.

The method of calculation of P_{ij} is as follows:

- Capture all particles which are 'infective' at each FMA downstream of original release FMA (includes self-recruitment). For sea lice this means capturing particles during the last 2/3 of the tracking period. For ISAV the capture period is the first 3 days of the virus run. For IPNV the whole of the virus tracking period is used. A 3-D array has been produced, named *inxy_<mmm>_<bb> (np,nf,nh),* for each month (*mmm*) and both sea lice and virus runs (*bb= sl* or *vr*). The dimensions are *np* (number of released particles), by *nf* (number of target FMAs) and *nh* (number of hours). From this matrix various outputs can be calculated.
- Sum over all particles starting in each origin FMA to get an 86x86 array containing numbers of particles, at each hour of the tracking period.
- Normalise by number of release points within each FMA to give a percentage of points released which are captured within any target FMA at any time.
- Finally, decide on how to plot array e.g. whole period, final destination. An alternative is to flag each FMA reached from origin FMA i.e. one or zero is recorded depending on whether a particle does or does not reach a given FMA from a specific starting FMA.

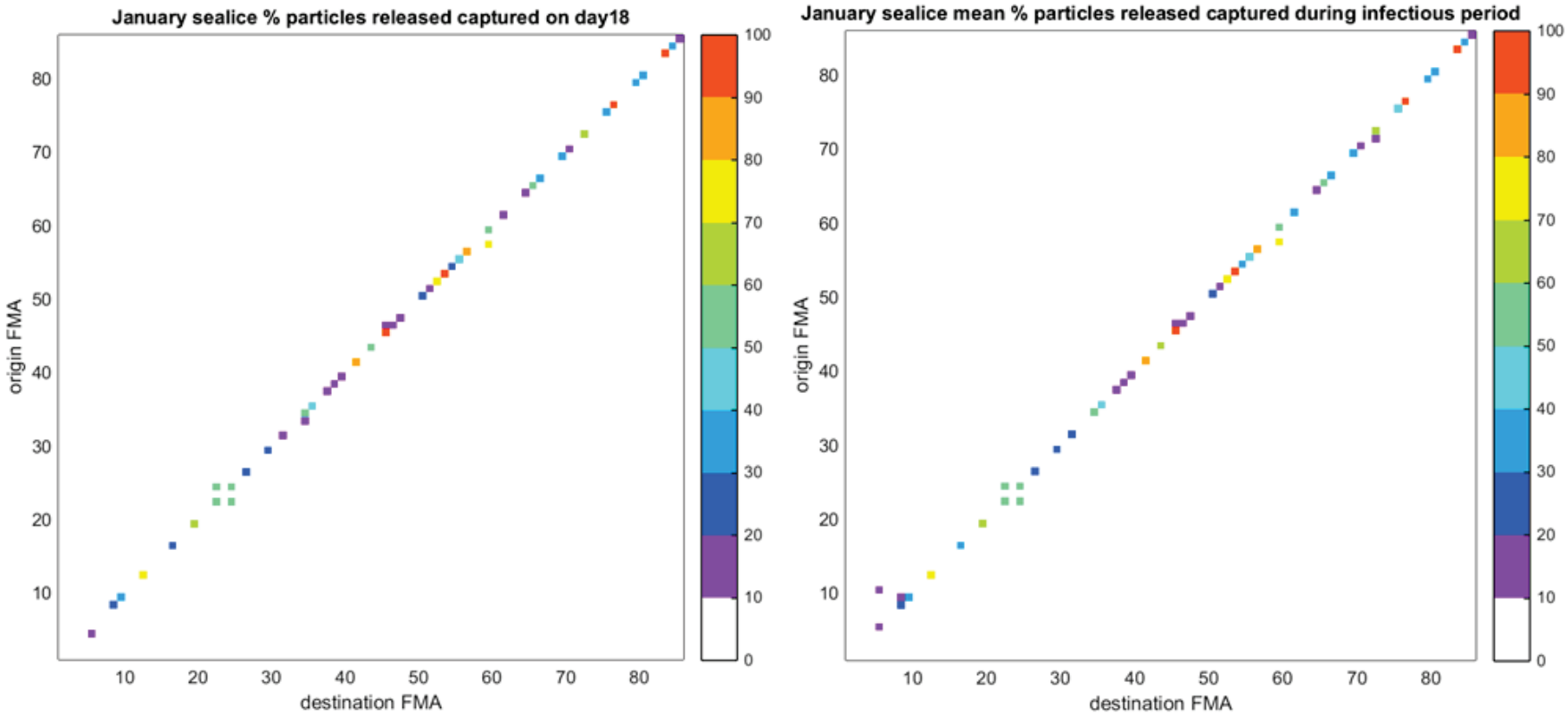
6.2 Sea Lice Connectivity

Figures 6-1 - 6-4 show different plots of the connectivity matrix for the sea lice runs for each season: January, April, June and October. The left hand panel plots the probability of a particle being found in FMA j, from original release at FMA i. The right hand size is the mean

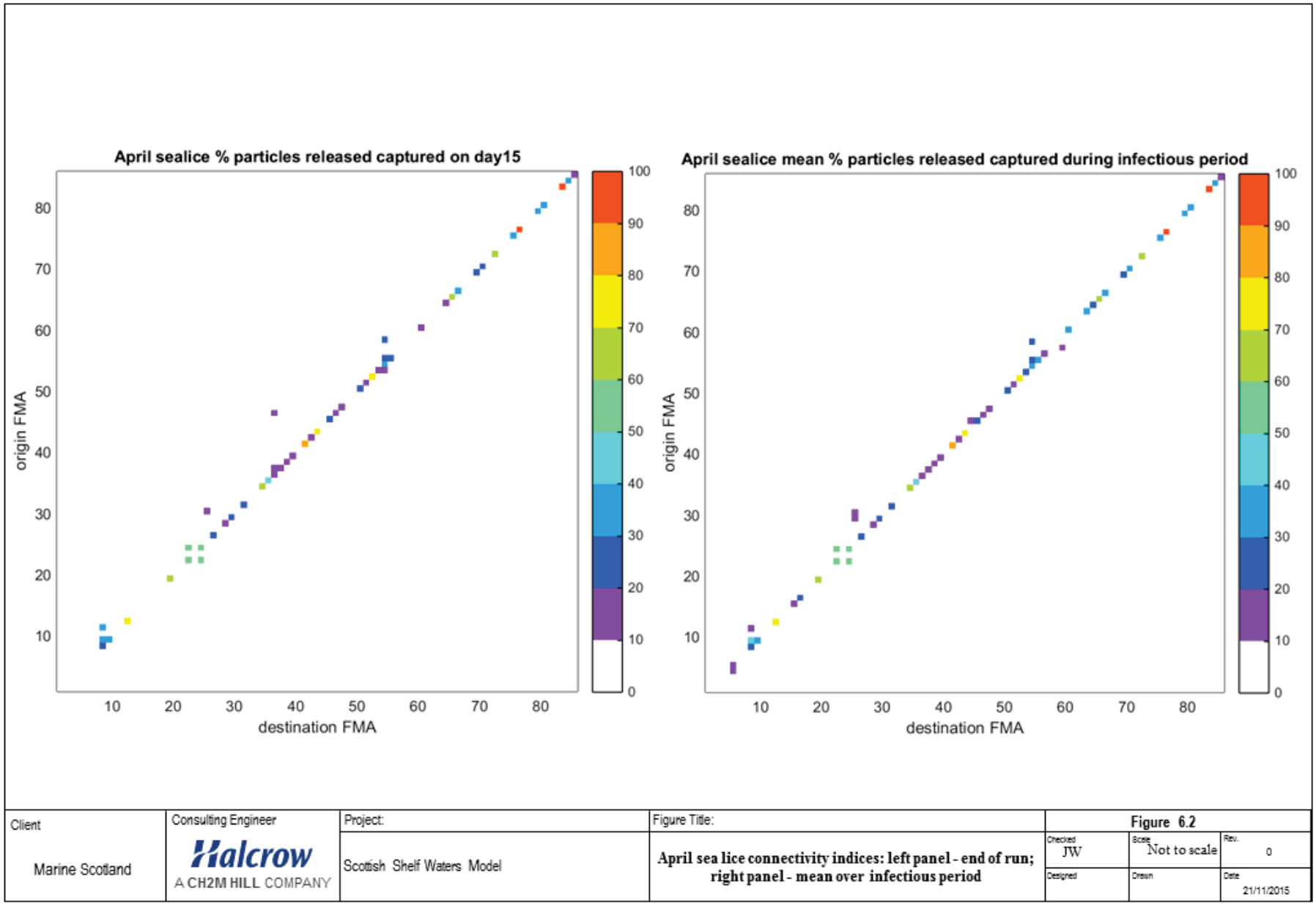
probability of capture over the whole infectious period. The colour bar is in 10% intervals. It may be seen that most coloured pixels lie on the diagonal, representing self-recruitment. A few particles move to an adjacent FMA.

Particles appear to move further from their original positions in July and least far in January, despite the fact that the January tracking period is longest and July the shortest.

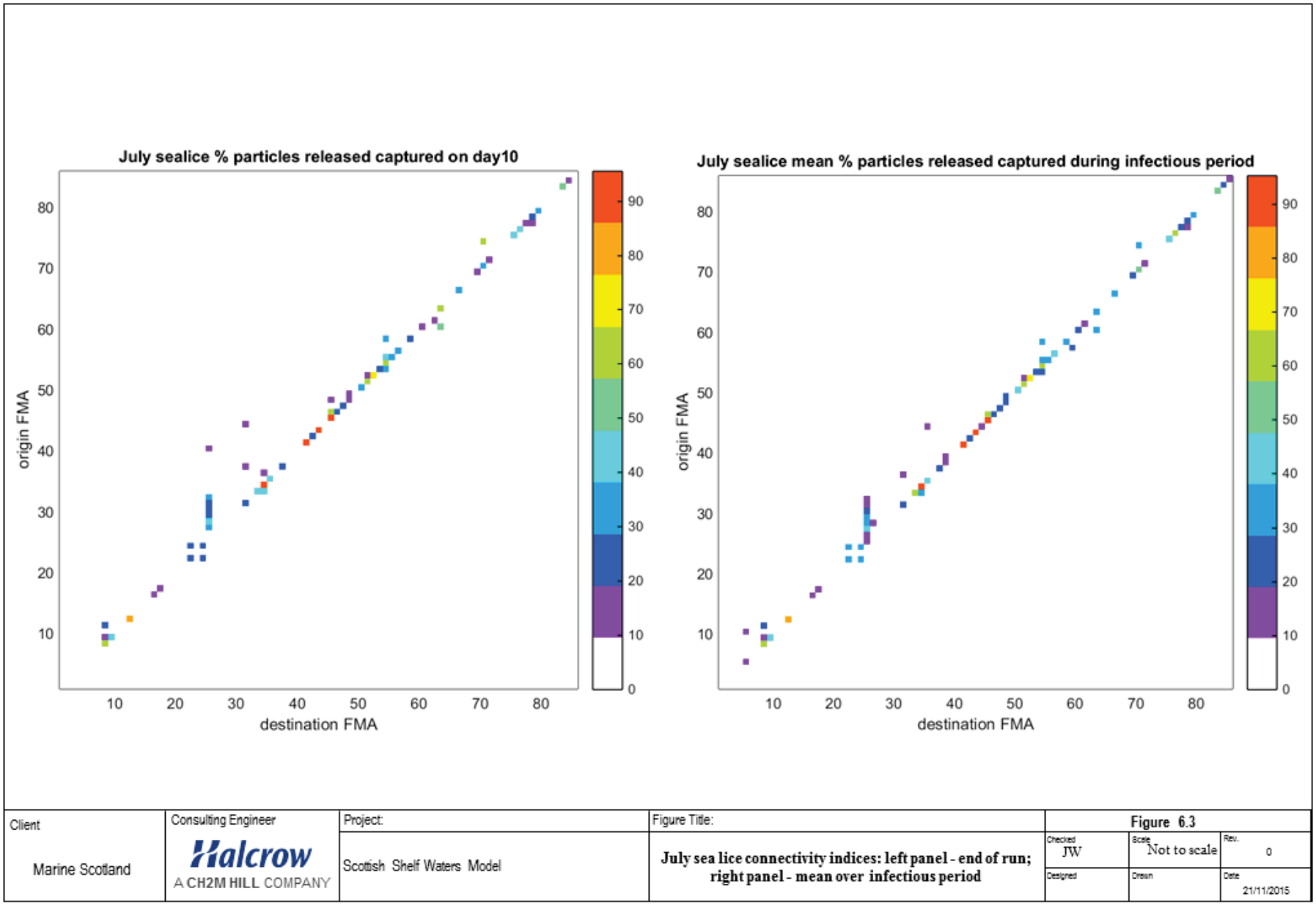
Figure 6-5 shows the 0/1 flags indicating whether there is at least one particle captured at the target from the origin FMA, over the whole period. This is more sensitive to only a few particles being captured than the previous figures so it can be seen that seen that there is some exchange between the Inner Hebrides (FMA numbers ~40-50) and the Western Isles (64-86) which are adjacent areas with similar latitude.



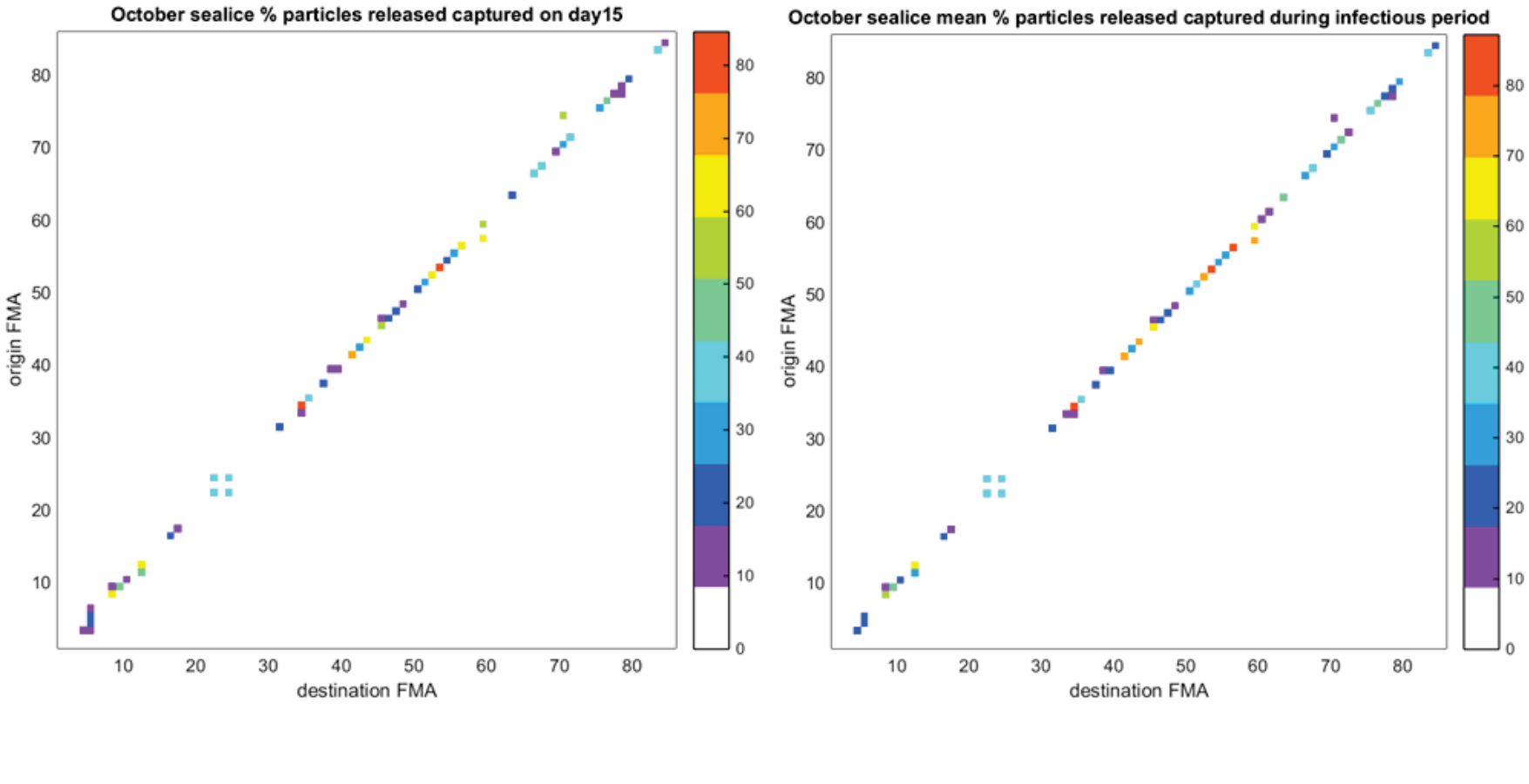
Client	Consulting Engineer	Project:	Figure Title:	Figure 6.1		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	January sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



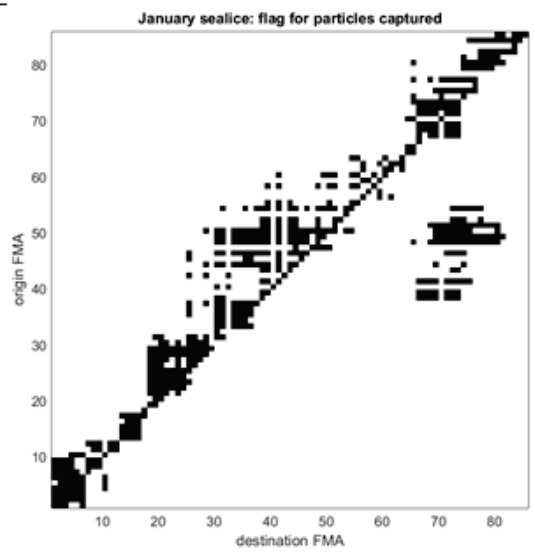
Client	Consulting Engineer	Project:	Figure Title:	Figure 6.2		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	April sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

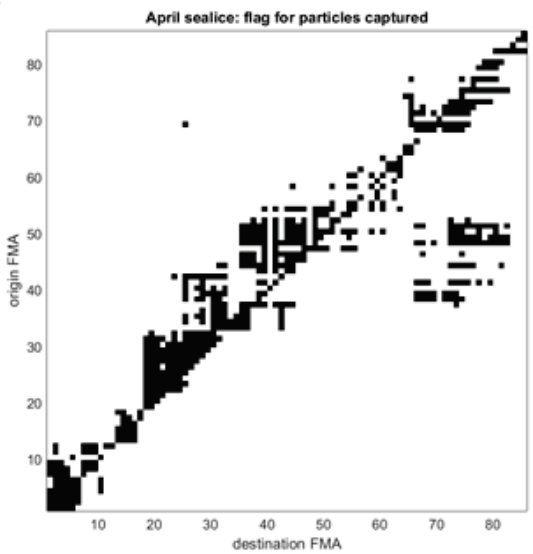


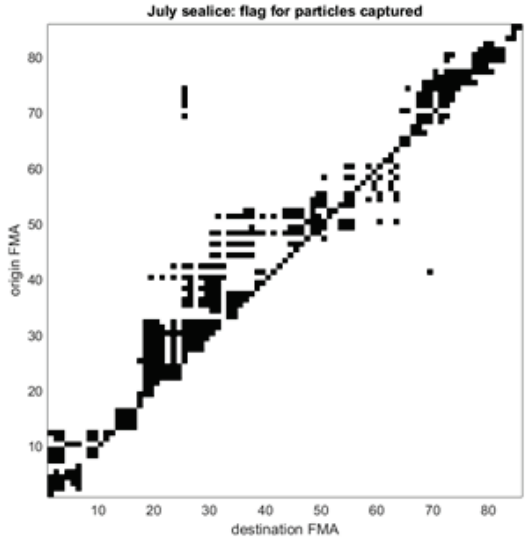
Client	Consulting Engineer	Project:	Figure Title:	Figure 6.3		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	**July sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period**	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

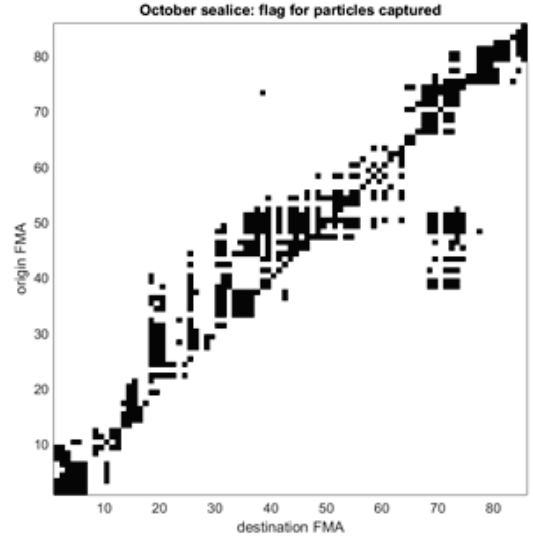


Client	Consulting Engineer	Project:	Figure Title:	Figure 6.4		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	October sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015





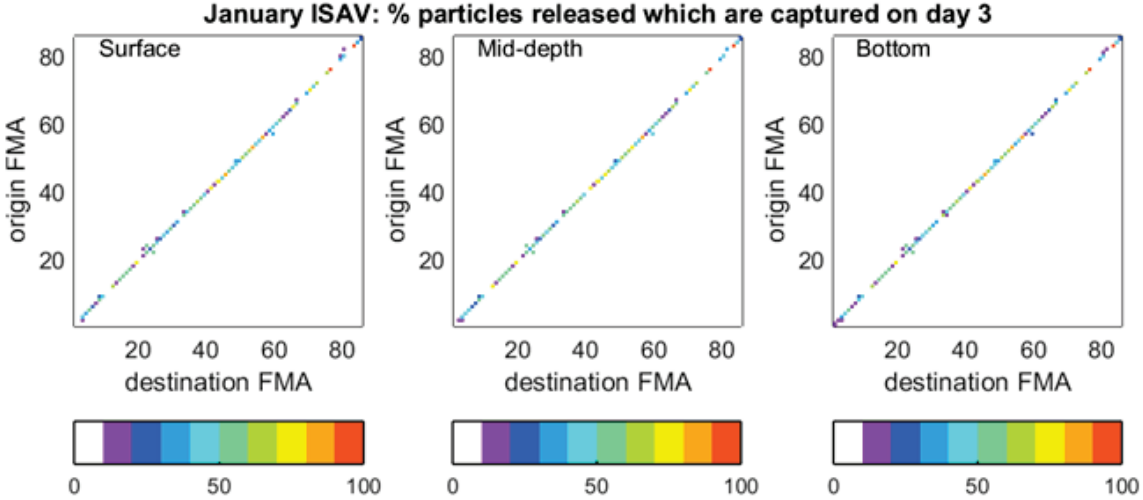


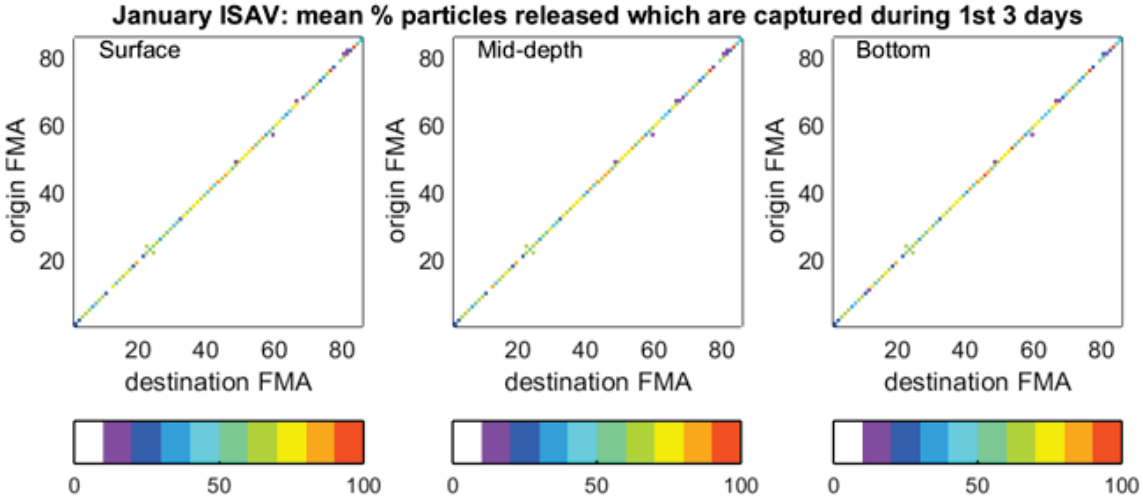


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-5		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	**Connectivity flags for sea lice: top left – January; top right – April; bottom left – July; bottom right - October**	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

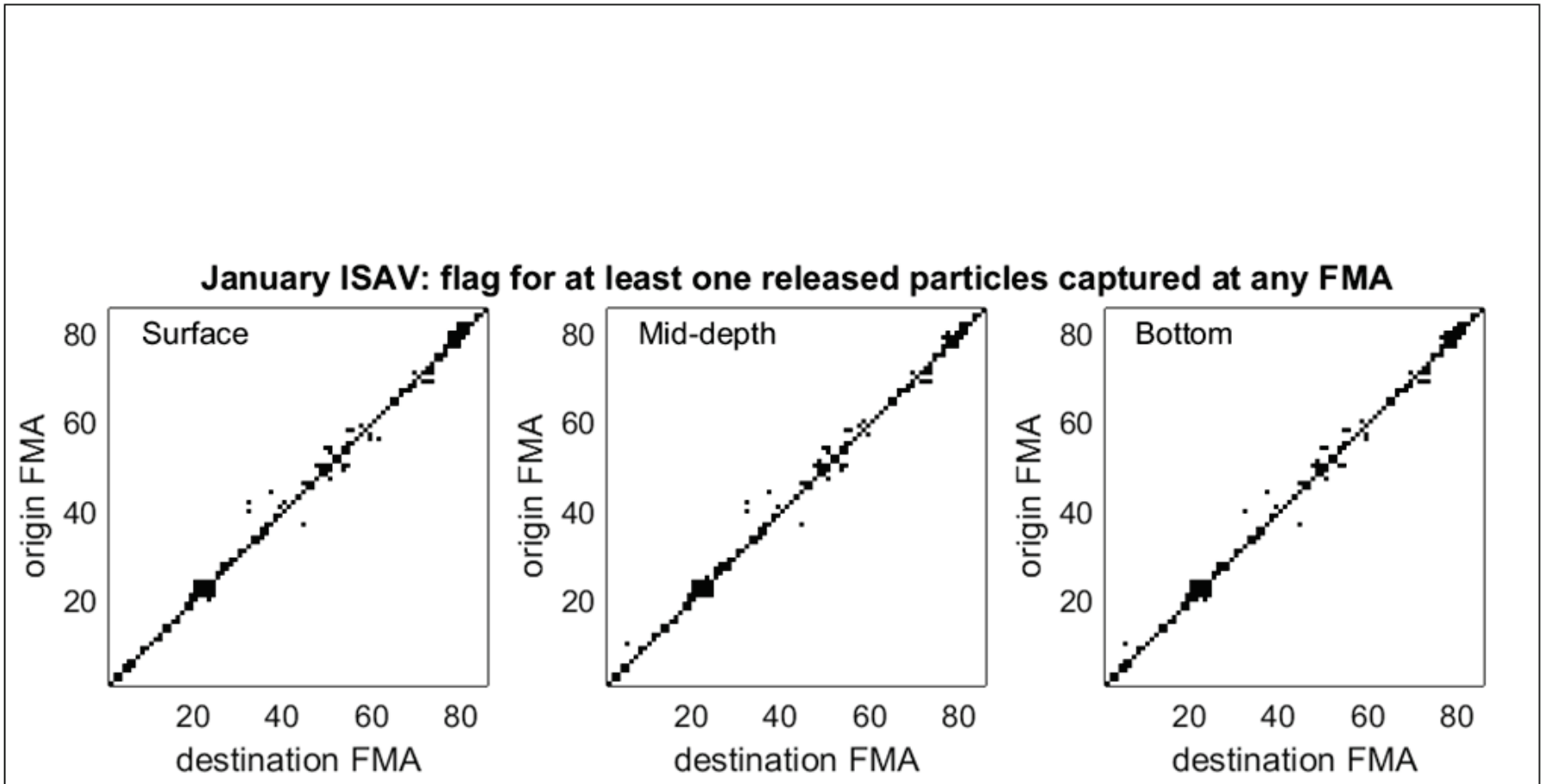
6.3 ISAV Connectivity

The following figures (6-6 – 6-13) show results for the 1st 3 days of the virus-tracking period, representing the viable infective period of the ISA virus. This is a very short duration virus so less connectivity between adjacent areas is seen.

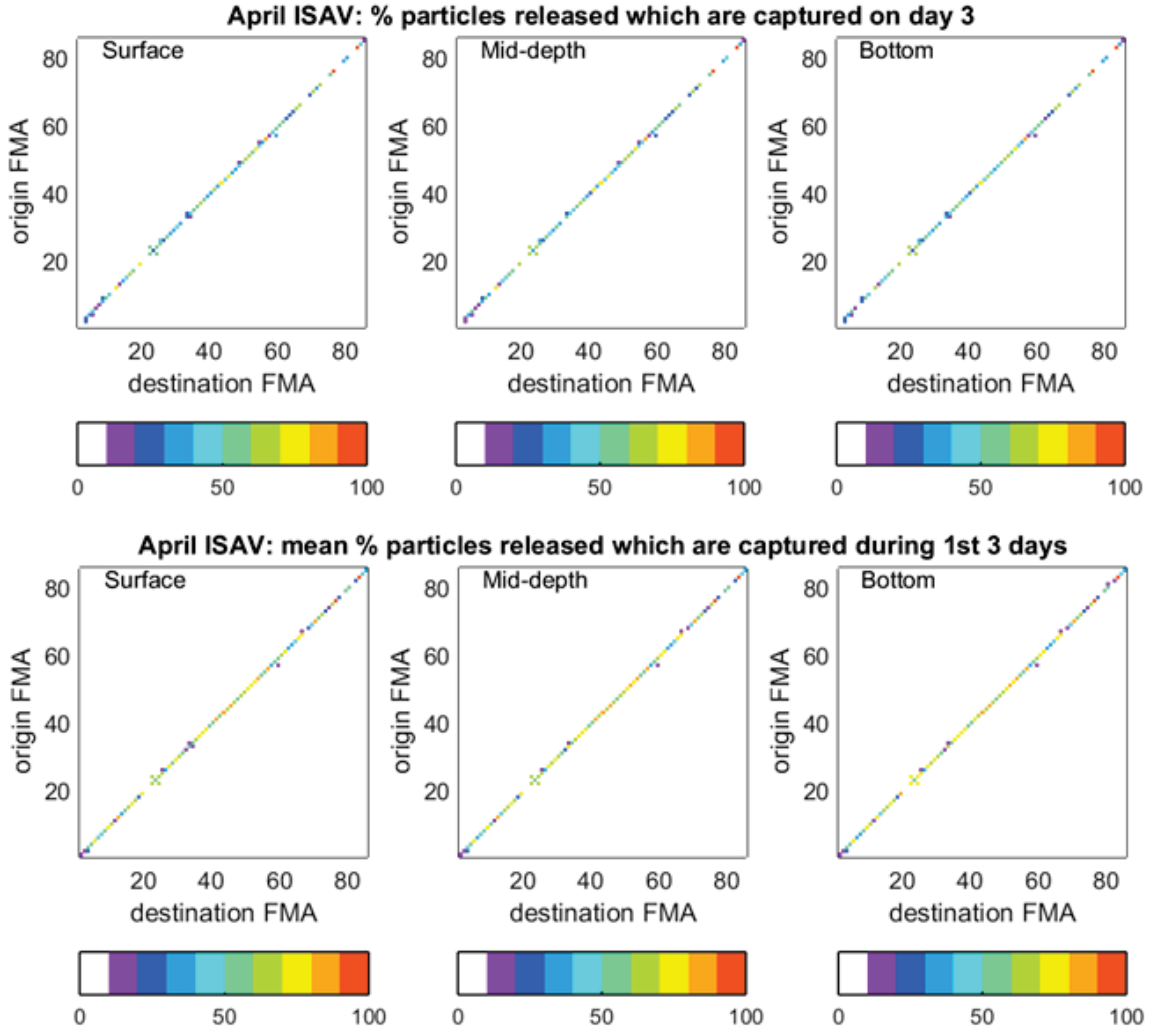




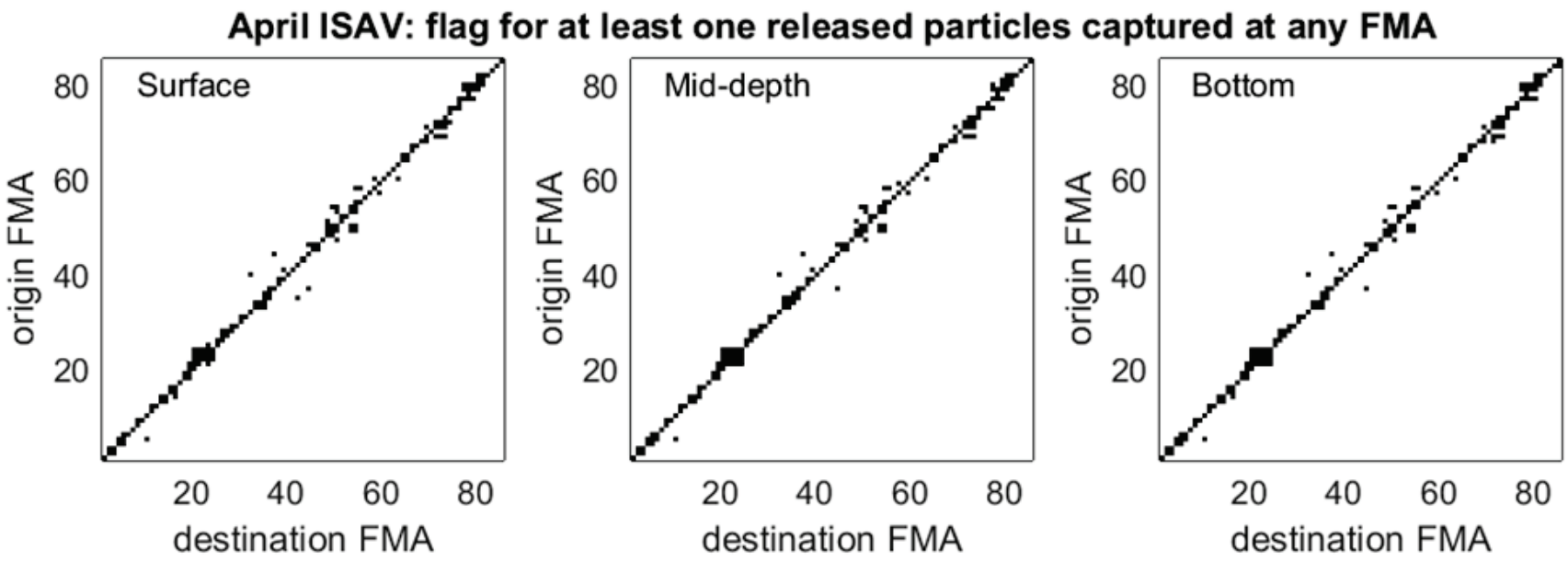
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-6		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	January ISAV connectivity indices: left panel – surface; centre - mid-depth; right – bottom; upper - %capture on day 3; lower - % captured 1st 3 days	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



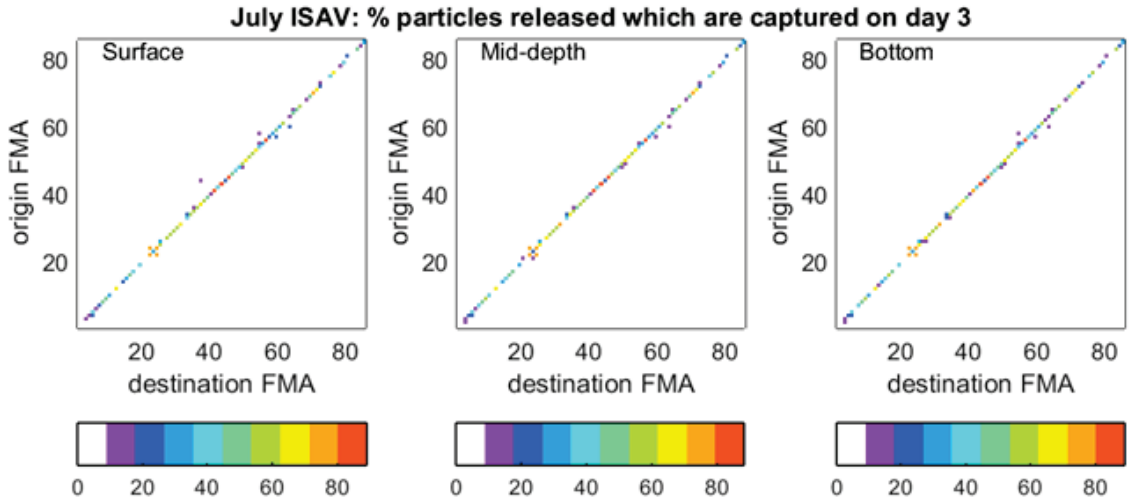
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-7		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	January ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

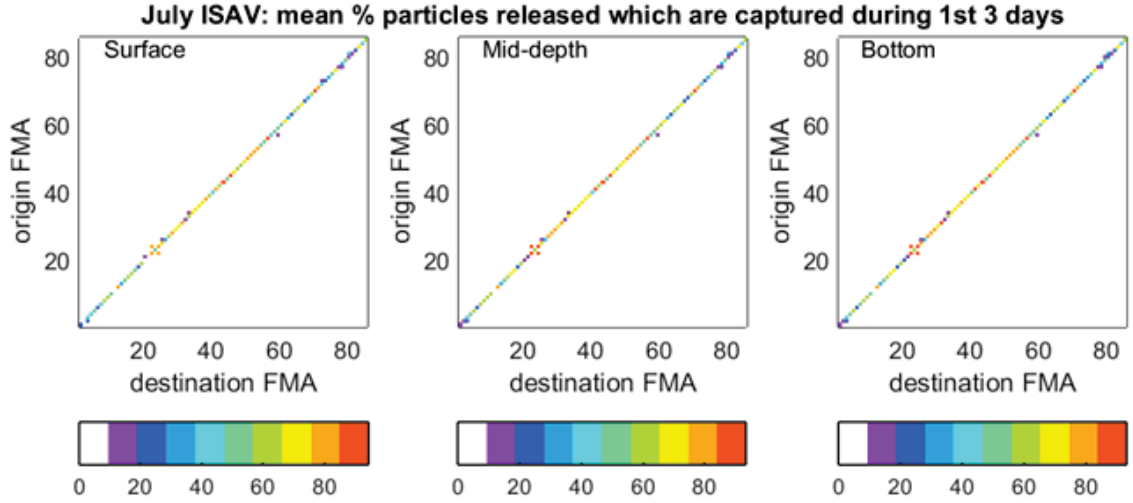


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-8		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	April ISAV connectivity indices: left – surface; centre - mid-depth; right – bottom; upper - %capture on day 3; lower - % captured 1st 3 days	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

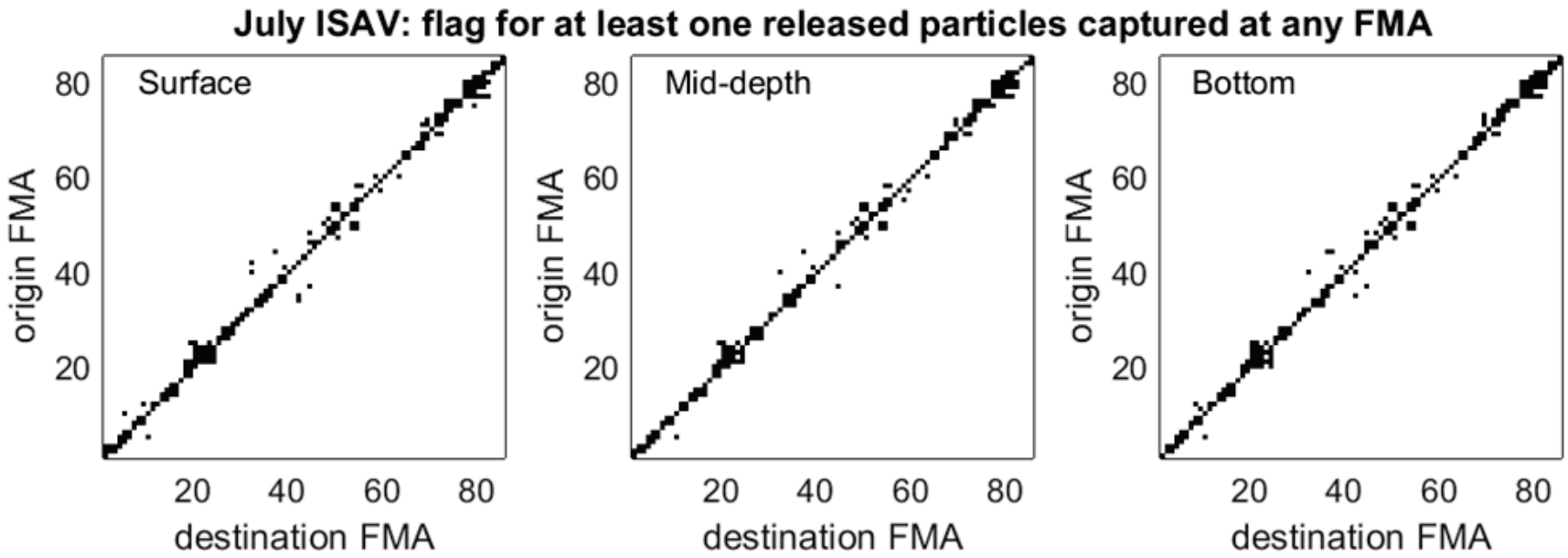


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-9		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	April ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

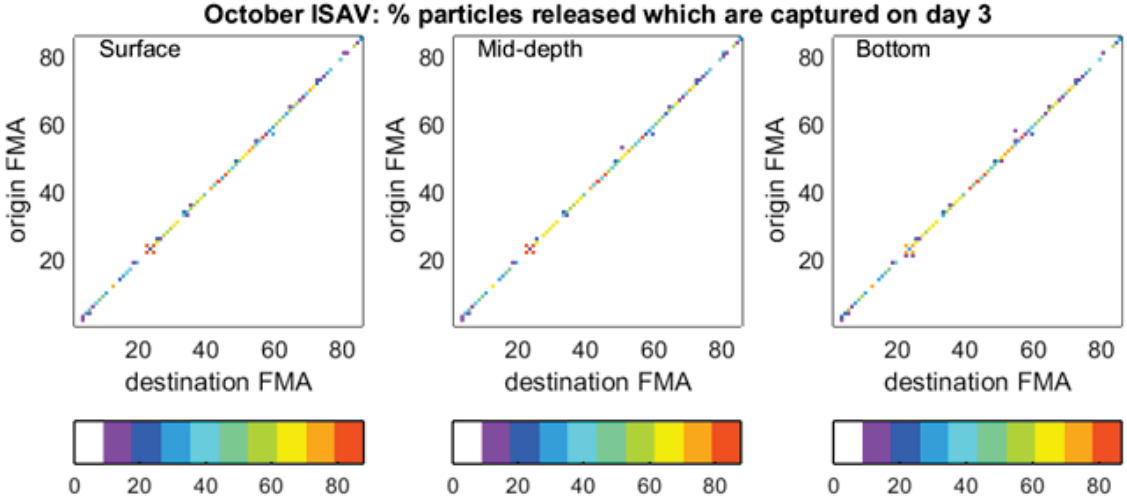


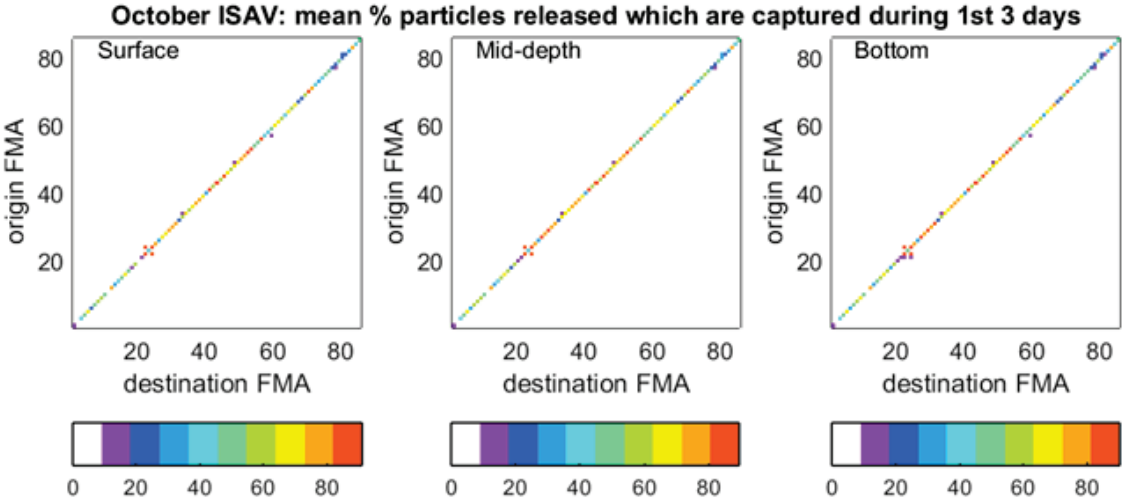


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-10		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	July ISAV connectivity indices: left – surface; centre - mid-depth; right – bottom; upper - %capture on day 3; lower - % captured 1st 3 days	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

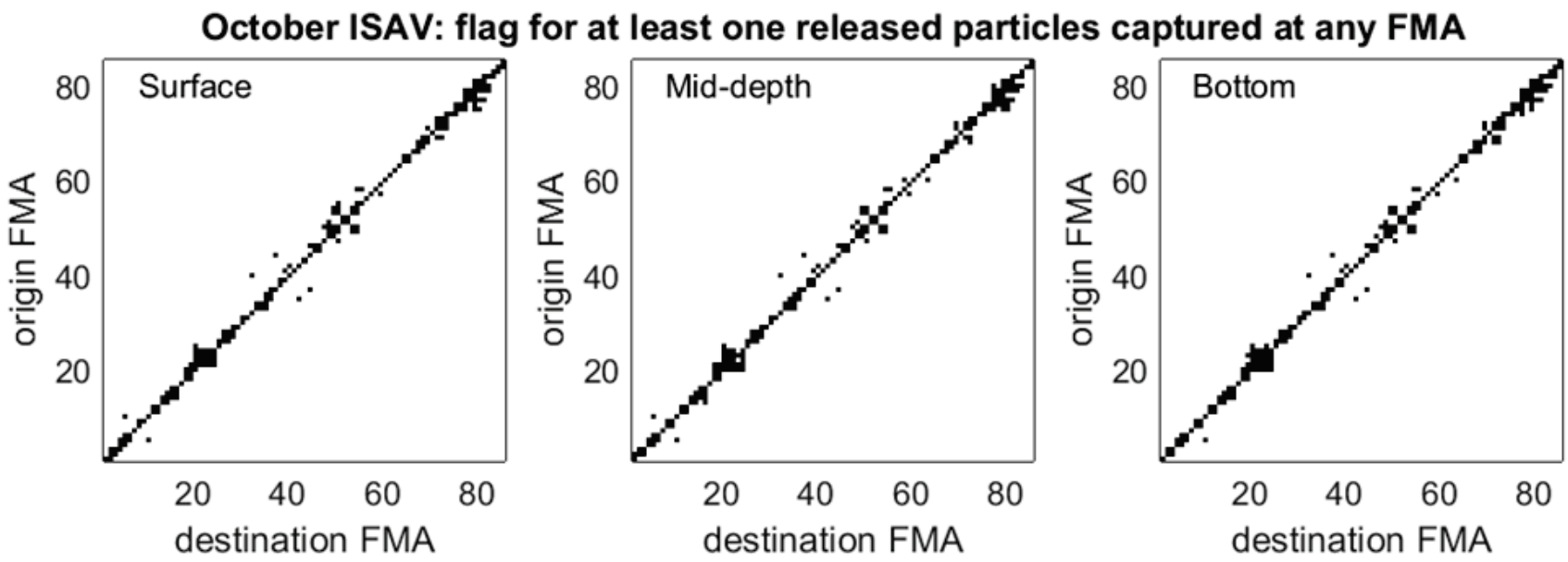


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-11		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	July ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015





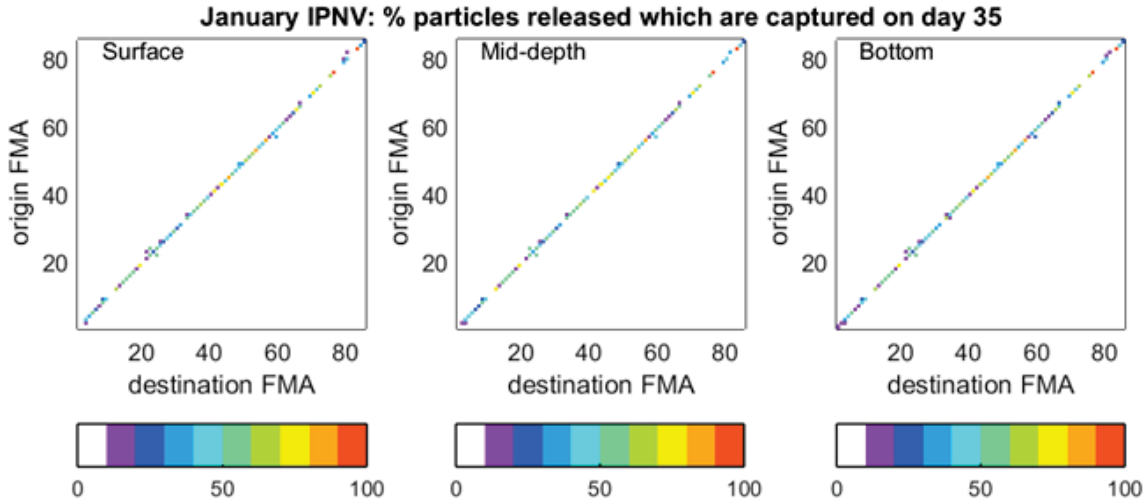
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-12		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	October ISAV connectivity indices: left – surface; centre - mid-depth; right – bottom; upper - %capture on day 3; lower - % captured 1st 3 days	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

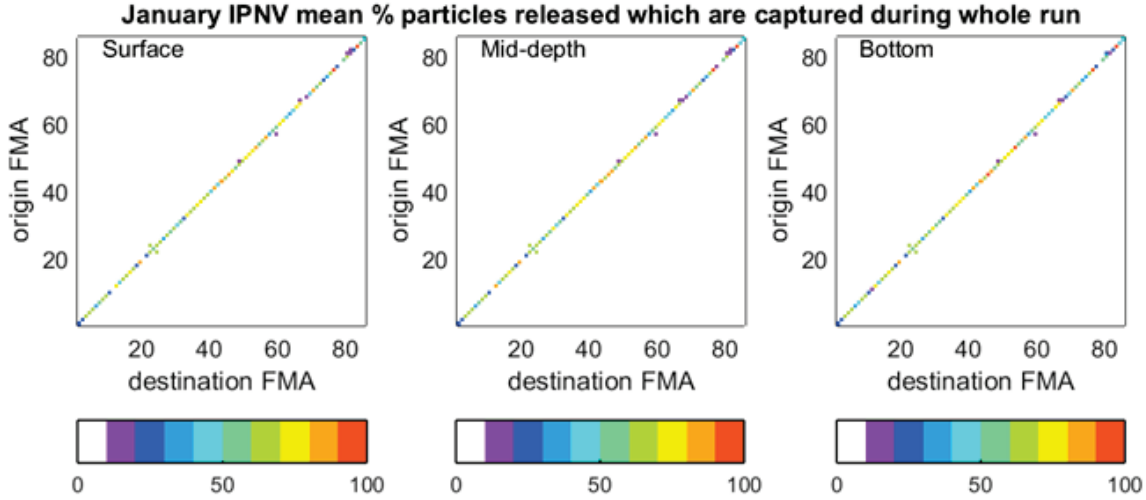


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-13		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	October ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

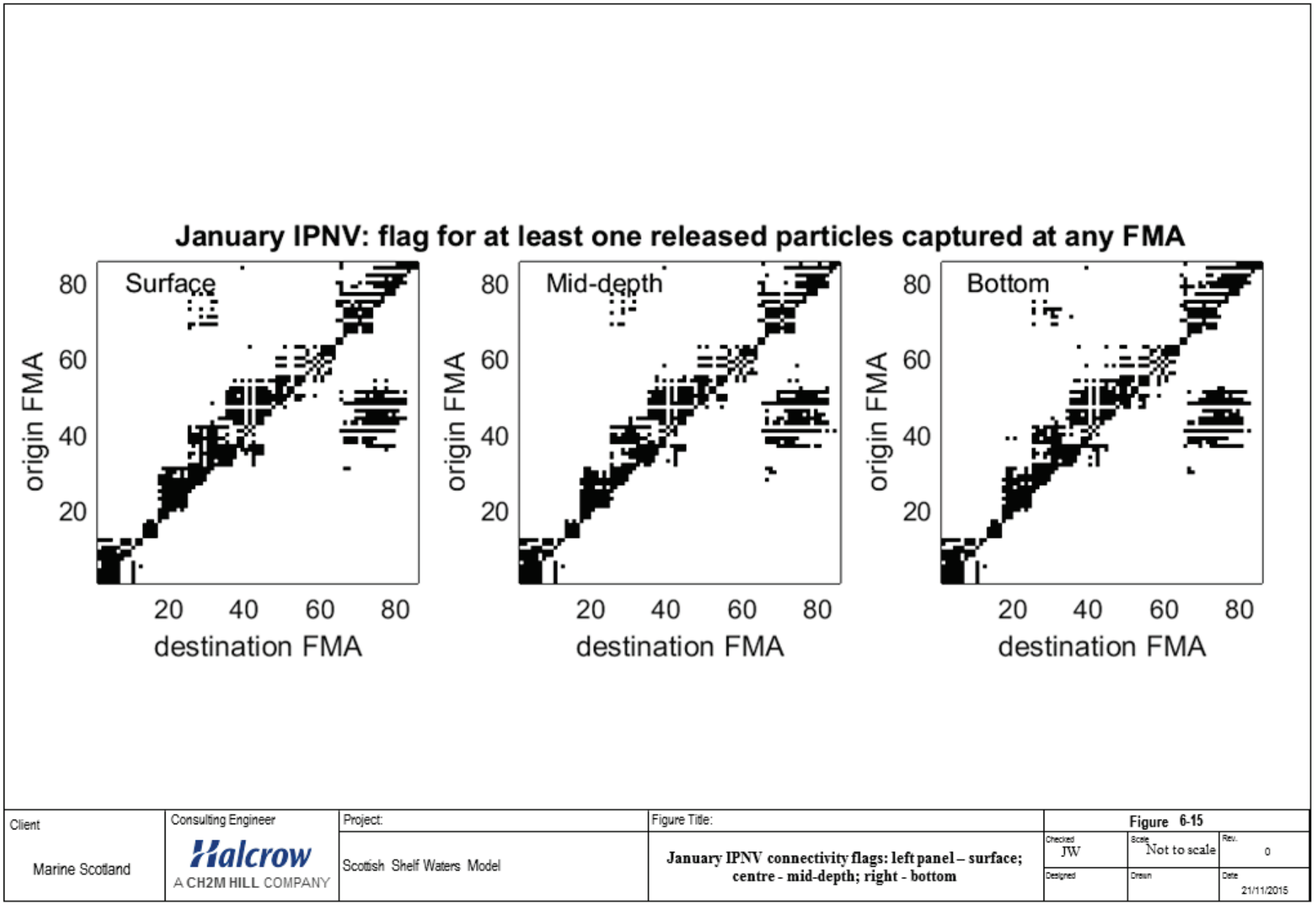
6.4 IPNV Connectivity

The following figures (6-14 – 6-21) show results for the whole of the virus-tracking period, representing the viable infective period of the IPN virus. Due to the longer duration there is more connectivity, similar to the sea lice tracks. It may be seen that there is little difference between particle releases at surface, mid-depth or bottom.

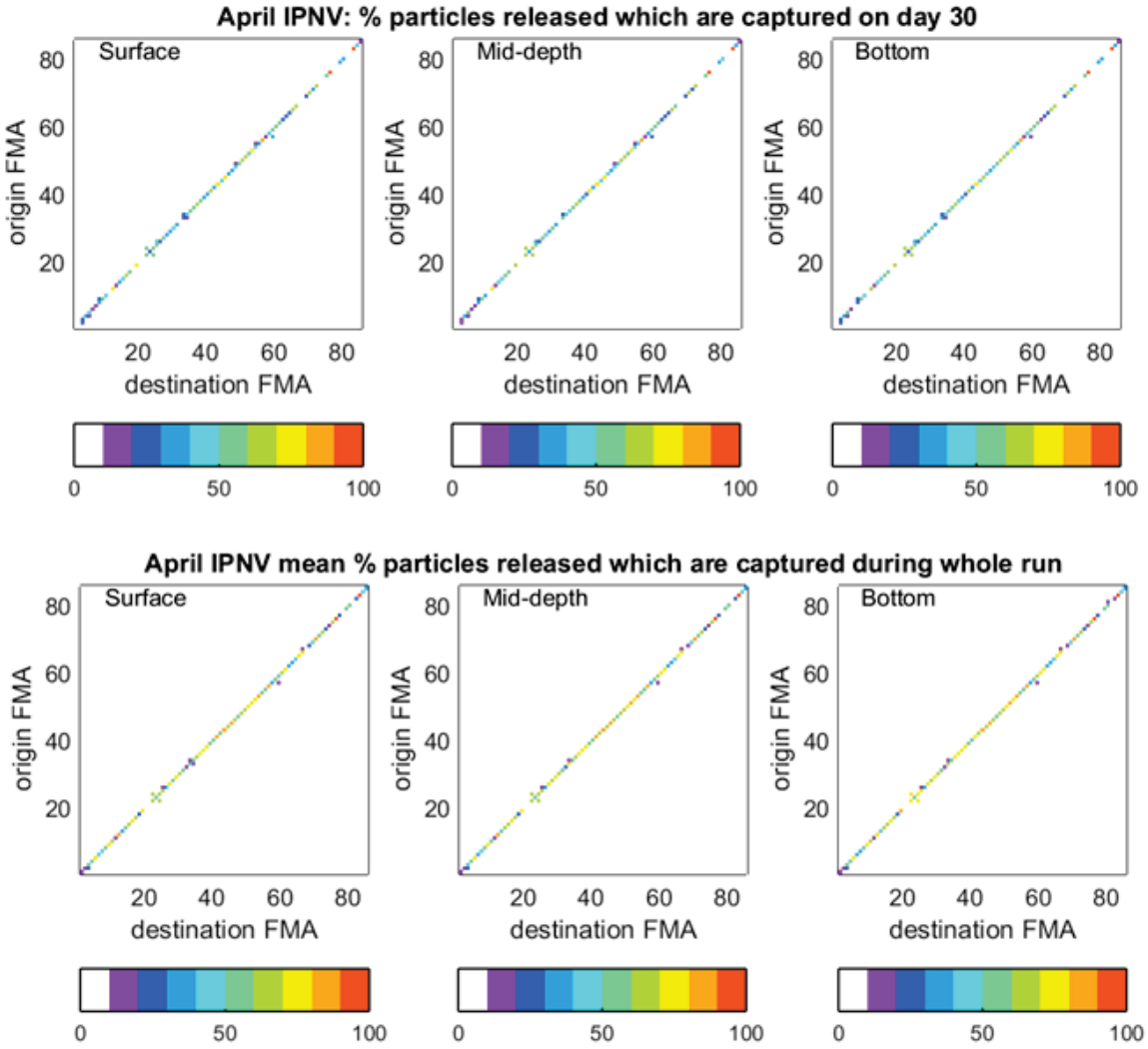




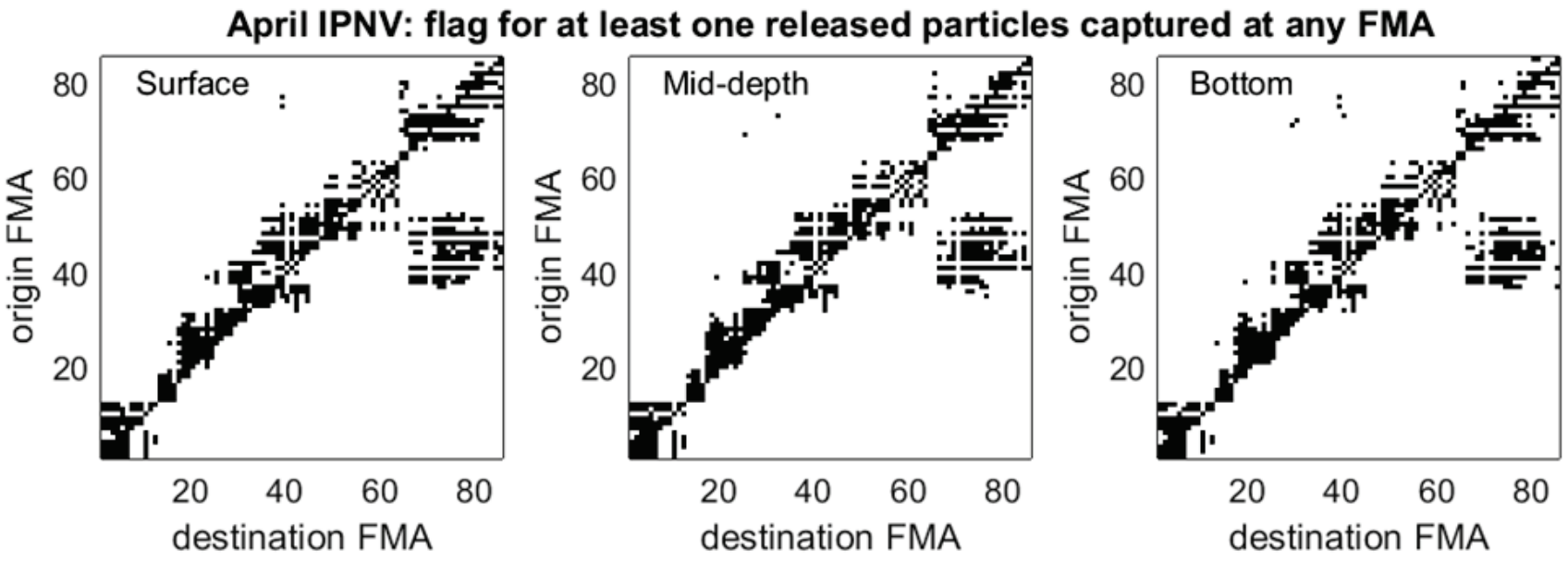
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-14		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	**January IPNV connectivity indices: left panel – surface; centre - mid-depth; right – bottom; upper - %capture on day 35; lower - % captured whole run**	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



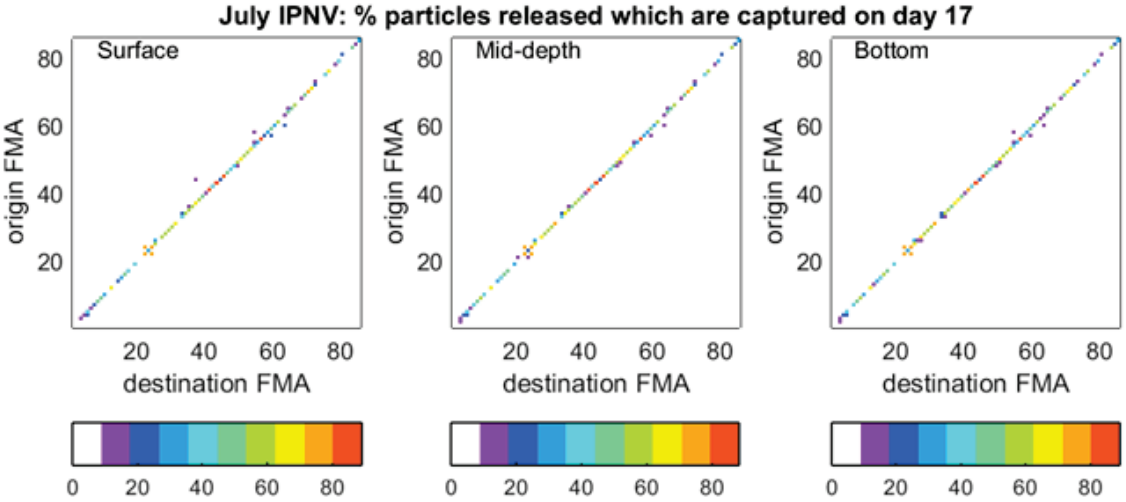
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-15		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	January IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



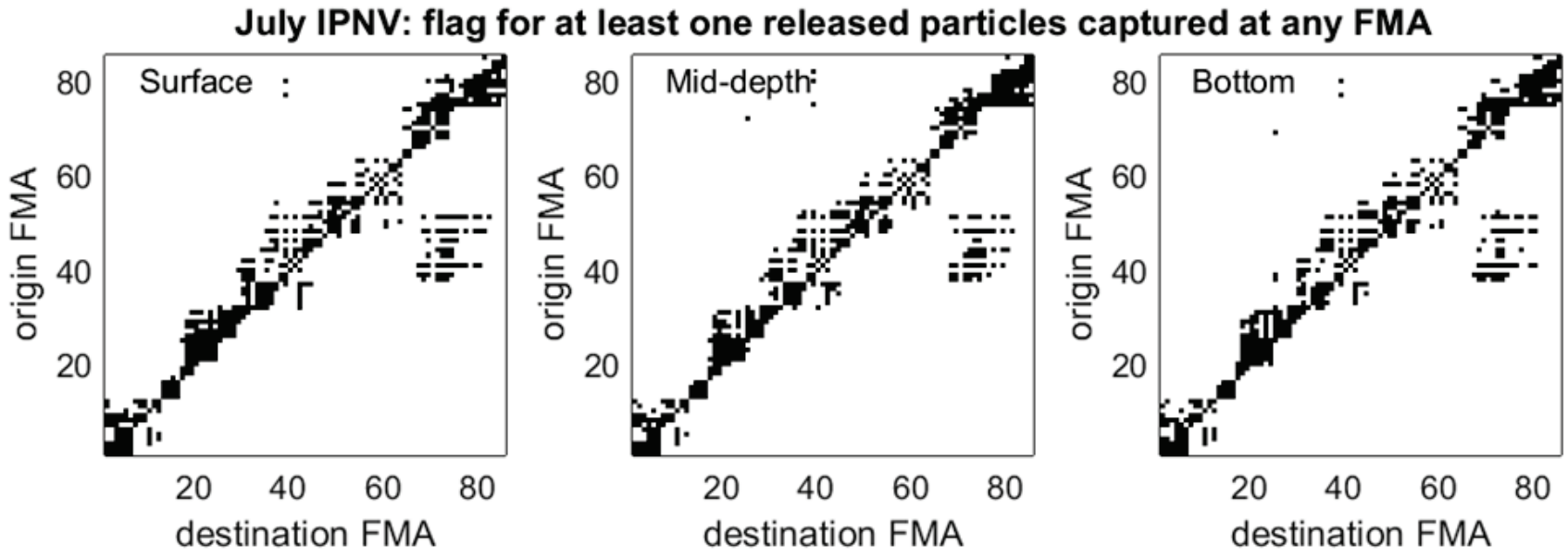
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-16		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	April IPNV connectivity indices: left panel – surface; centre - mid-depth; right – bottom; upper - %capture on day 30; lower - % captured whole run	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



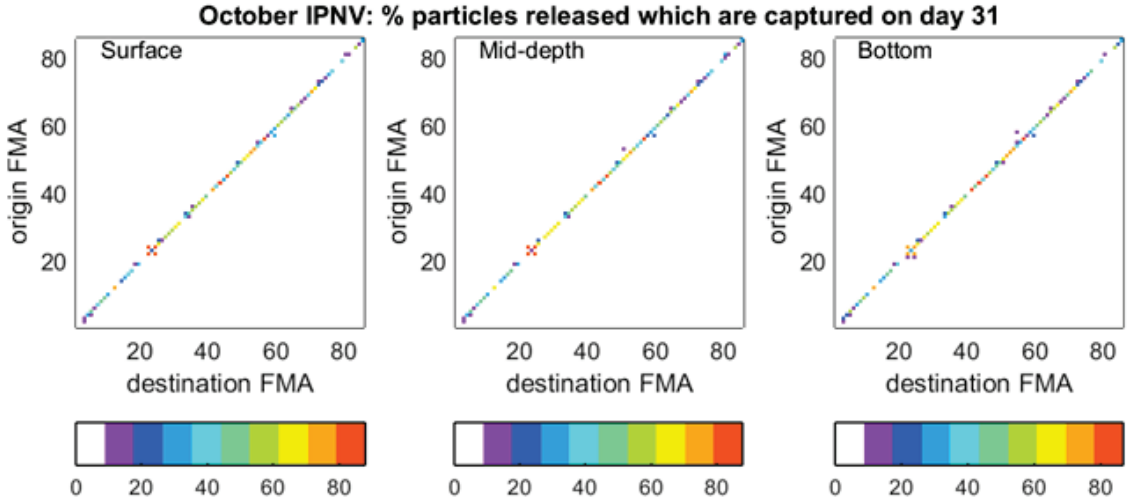
Client	Consulting Engineer	Project:	Figure Title:	Figure 6-17		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	April IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

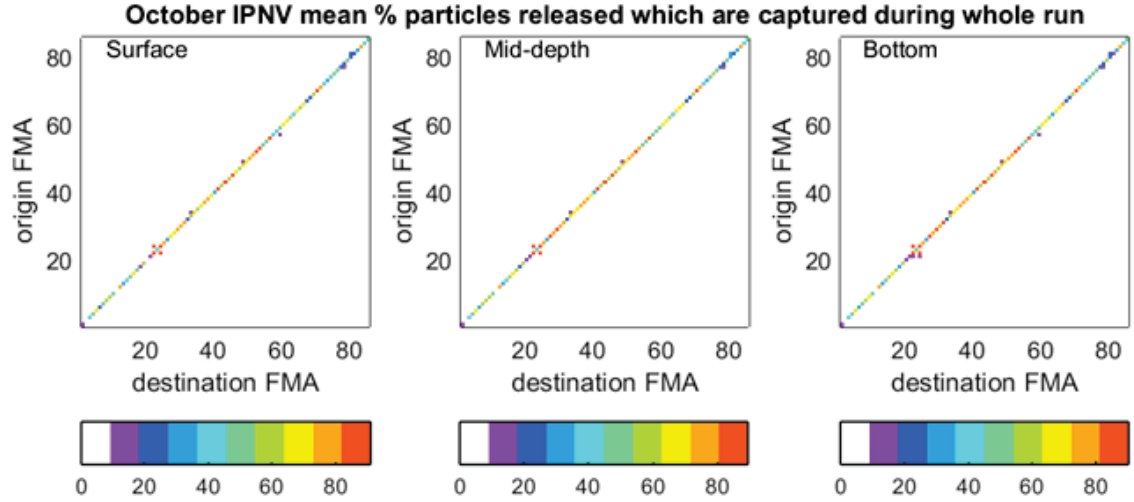


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-18		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	July IPNV connectivity indices: left panel – surface; centre - mid-depth; right – bottom; upper - %capture on day 17; lower - % captured whole run	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

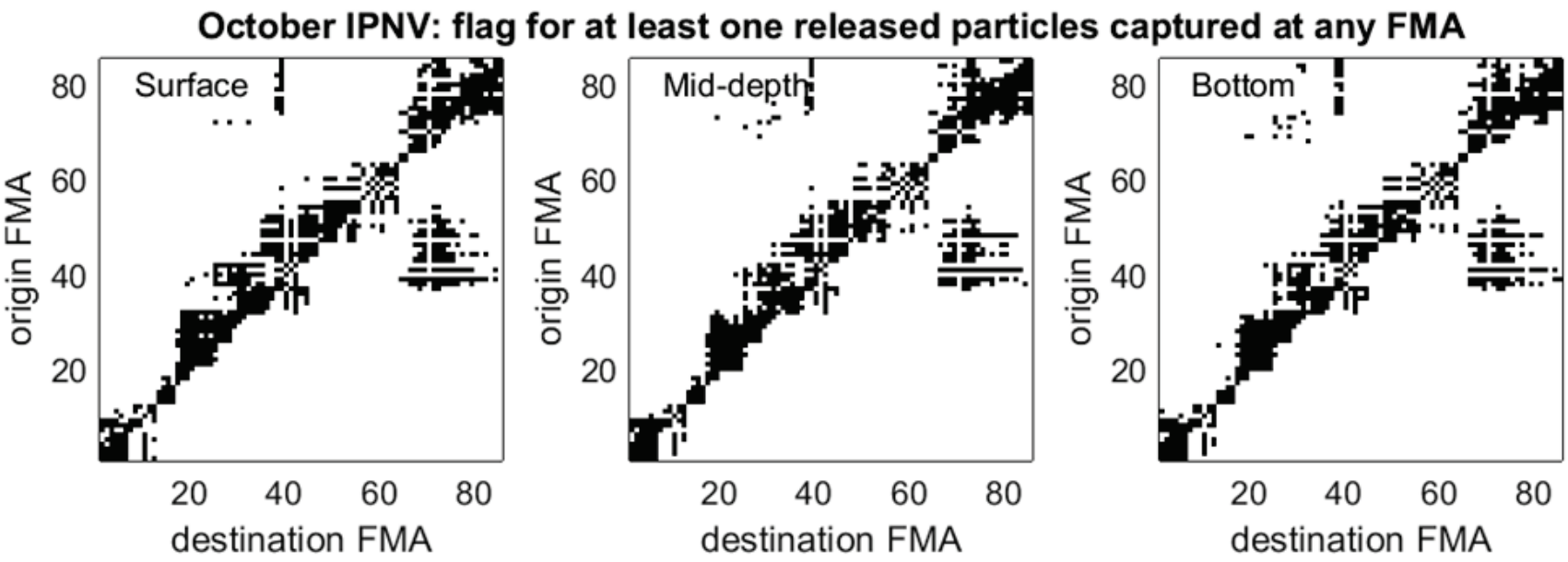


Client	Consulting Engineer	Project:	Figure Title:	Figure 6-19		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	July IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015





Client	Consulting Engineer	Project:	Figure Title:	Figure 6-20		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	October IPNV connectivity indices: left panel – surface; centre - mid-depth; right – bottom; upper - %capture on day 31; lower - % captured whole run	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015



Client	Consulting Engineer	Project:	Figure Title:	Figure 6-21		
Marine Scotland	Halcrow A CH2M HILL COMPANY	Scottish Shelf Waters Model	October IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom	Checked JW	Scale Not to scale	Rev. 0
				Designed	Drawn	Date 21/11/2015

7. Summary and Conclusions

Stage 3 of the Scottish Shelf waters project focusses on integration of the case study sub-models into the wider domain shelf model and the application of the combined model to calculate connectivity indices between fish farms for the study of disease transmission by sea lice and viruses. This report presents this final piece of work.

In order to combine the shelf model and nested model outputs an interpolation method was developed. This method utilised the results produced in Stage 1 and Stage 2 of the project. Two integrated meshes were produced. The first is used to integrate the results from all four case study sub-models and the shelf model from May to October. The second is used to integrate the results from two case study sub-models (PFOW & WLLS) and the shelf model only for November to February. The integrated meshes were developed to ensure the best mesh resolution was preserved. Results were interpolated using Matlab to produce daily output files with an hourly timestep for use in the particle tracking model.

The FVCOM offline particle tracking code as supplied had some bugs in the diffusion part of the code which had to be fixed. We decided to implement a version of the code developed by Pierre Cazenave (Plymouth Marine Laboratory) which saved the grid metrics calculated after the first run of the code, allowing a saving of about 2 hours in run time on subsequent runs and much quicker debugging, as the particle tracking starts immediately. This code also had some initial bugs which had to be fixed.

The particle tracking runs were time-consuming in that 97,700 particles were tracked for the sea lice setup and 146,550 for the virus setup and each run took several days to weeks. This was speeded up by dividing the particles between several processors. Although the code is not parallelised, multiple runs can be carried out in parallel as long as the particles are from different spatial locations (multiple particles from one point may produce duplicate runs due to the nature of the random number generator).

8. Recommendations for future work

Here are some suggestions for improvements to the particle tracking code which could be made relatively easily

1. Implement the option for lat/lon model output (Dmitry Aleynik has already produced code with this fix, which could be adopted).
2. Jim Clark (Plymouth Marine Laboratory) has provided a modified code in September 2015 – adding a local search for velocity elements to yield a substantial speed up in run times.
3. Another suggestion is to speed up the I/O by reading a whole daily file at once rather than hour by hour (this will have memory implications however).
4. Remove the hard-coded year number of *offlag.f90*.
5. Allow particle tracking to go beyond the year end and cross boundaries between April/May and October/November (latter is due to only 2 nested models being run for whole year so combined grid changes size).

9. References

Brickman, D., and Smith, P. (2002) Lagrangian stochastic modeling in coastal oceanography. Journal of Atmospheric and Oceanic Technology, 19, 83 – 99.

Chen, C, R. C. Beardsley, G. Cowles, J. Qi, Z. Lai, G. Gao, D. Stuebe, Q. Xu, P. Xue, J. Ge, S. Hu, R. Ji, R. Tian, H. Huang, L. Wu, H. Lin, Y. Sun and L. Zhao, 2013. An unstructured grid, finite-volume community ocean model: FVCOM User Manual. SMAST/UMASSD Technical Report-13-0701.

Halcrow, 2014. Model documentation report. Hydrodynamic Model of the Wider Loch Linnhe System, December 2014.

Halcrow, 2014. Model documentation report. Hydrodynamic Model of St Magnus Bay, December 2014.

Halcrow, 2014. Model documentation report. Hydrodynamic Model of Scottish Shelf Waters, December 2014.

Halcrow, 2015. Model documentation report. Hydrodynamic Model of the Pentland Firth and Orkney Waters., January 2015.

Halcrow, 2015. Model documentation report. Hydrodynamic Model of the East Coast of Lewis and Harris, February 2015.

North, E.W., Gallego, A. and Petitgas, P. (eds) (2009) Manual of recommended practices for modelling physical−biological interactions during fish early life. ICES Coop Research Report 295

Price, D., Stuiver, C., Johnson, H., Gallego, A., O'Hara Murray, R. 2015a. The Scottish Shelf Model. Part 2: Pentland Firth and Orkney Waters Sub-Domain. Scottish Marine and Freshwater Science Vol 7 No 4. Prepared by CH2M on behalf of Marine Scotland. Edinburgh: Scottish Government, 359pp.

Price, D., Stuiver, C., Johnson, H., Gallego, A., O'Hara Murray, R. 2015b. The Scottish Shelf Model. Part 3: St Magnus Bay Sub-Domain. Scottish Marine and Freshwater Science Vol 7 No 5. Prepared by CH2M on behalf of Marine Scotland. Edinburgh: Scottish Government, 197pp.

Price, D., Stuiver, C., Johnson, H., Gallego, A., O'Hara Murray, R. 2015c. The Scottish Shelf Model. Part 4: East Coast of Lewis and Harris Sub-Domain. Scottish Marine and Freshwater Science Vol 7 No 6. Prepared by CH2M on behalf of Marine Scotland. Edinburgh: Scottish Government, 149pp.

Price, D., Stuiver, C., Johnson, H., Gallego, A., O'Hara Murray, R. 2015d. The Scottish Shelf Model. Part 5: Wider Loch Linnhe Sub-Domain. Scottish Marine and Freshwater Science Vol 7 No 7. Prepared by CH2M on behalf of Marine Scotland. Edinburgh: Scottish Government, 292pp.

Ross, O. N. and Sharples, J. (2004) Recipe for 1-D Lagrangian particle tracking models in space-varying diffusivity. Limnology and Oceanography: Methods, 2, 289-302.

Visser, A. W. (1997) Using random walk models to simulate the vertical distribution of particles in a turbulent water column. Marine Ecology Progress Series, 158, 275-281.

Wolf, J. 2015. Particle Tracking and Connectivity: Methodology, November 2015.

Wolf, J., Yates, N., Brereton, A., Buckland, H., De Dominicis, M., Gallego, A., O'Hara Murray, R. 2015. The Scottish Shelf Model. Part 1: Shelf-Wide Domain. Scottish Marine and Freshwater Science Vol 7 No 3. Prepared by CH2M on behalf of Marine Scotland. Marine Scotland Science, 151pp.

Appendix A

Particle Tracking and Connectivity Methodology

Particle Tracking and Connectivity Methodology

Judith Wolf, NOC

November 2015

Contents

Particle Tracking and Connectivity: Methodology 94

1 Introduction 97

1.1 Calculation of Connectivity Indices among Aquaculture Management Areas in Scotland 97

1.2 Background 99

1.3 Sea Lice 100

1.4 Infectious Salmon Anaemia 101

1.5 Infectious Pancreatic Necrosis 102

1.6 Scottish Aquaculture Management 103

1.6.1 Farm Management Areas (FMAs) 103

1.6.2 Disease Management Areas (DMAs) 104

2 Particle Tracking in FVCOM 110

2.1 Method 110

2.2 Offline particle tracking code 111

2.3 Fixing the code 113

2.4 Input output files 113

2.5 Output files 118

2.6 Compiling and running particle tracking 118

3 Methodology for Scottish Waters Model 120

3.1 Model output preparation 120

3.2 Particle tracking 120

3.3 Post-processing of particle tracking output 125

3.4 Connectivity Indices 127

4 Results 128

4.1 FMA separation and connectivity matrices 128

4.2 Sea Lice Connectivity 130

4.3 Virus Connectivity 132

4.3.1 ISA Virus 132

4.3.2 IPN Virus 137
5 Summary 142
6 Recommendations for future work 142
References 143
Appendix: Particle Tracking code 145

Introduction

This report provides the methodology used to calculate connectivity indices between Scottish aquaculture Farm Management Areas, using 3D currents from climatology-forced output of the Scottish Shelf Model and the FVCOM offline particle tracking model.

○ Calculation of Connectivity Indices among Aquaculture Management Areas in Scotland

Within the Scottish Shelf Model project there is a requirement to deliver “Connectivity indices (which may be defined as the degree of dynamic interactions between geographically separated populations via the movement of individuals), such as transition probability matrices between (finfish aquaculture) Farm Management Areas (FMA).” Further background has been provided in a note prepared by Alejandro Gallego (AG) of Marine Scotland, including the statement that “If the spatial scale of specific FMAs is not adequate (e.g. too small or too large) for a tractable analysis, connectivity indices may be produced for alternative oceanographically-coherent areas.” Some decisions about this have been made, in order to proceed, as discussed below. The note also provided relevant biological and aquaculture management information and information on appropriate connectivity timescales, which is summarised here.

The aim is the computation of connectivity indices in the form of transition probability matrices identifying the proportion (and number) of Lagrangian particles released from each individual (“source”) FMA which reach any other (“target”) FMA (including self-recruitment). This was to be carried out by tracking artificial (neutrally buoyant) particles introduced into the Scottish Waters model, with embedded high-resolution sub-areas. These particles represent individual organisms or groups of organisms which are advected and dispersed by the flow. It was proposed that the relevant Lagrangian simulations to be carried out fulfil the following characteristics:

1. The simulations are to be carried out off-line from the FVCOM hydrodynamic model runs, using the FVCOM particle tracking software.
2. The simulations are to be carried using a combined mesh in which the sub-domain models will be merged into the Scottish Shelf Waters (SSW) model so that the highest available resolution will be used in all areas. If the resolution is still not sufficient for aquaculture management, there is a need to agree with MSS the provision of connectivity matrices between oceanographically-coherent areas, as mentioned above.
3. The simulations are to be carried out using the climatology output of the hydrodynamic model and sub-models. The basic time step is to be one hour, which is the output time-step of the Climatology run. There is a sub-time-step within the particle model, typically a few minutes, to interpolate the flow to

provide a reasonable trajectory within each advection time step e.g. not crossing land. There is a further sub-division of the time step for the random walk component of the trajectory, representing sub-grid-scale diffusion.

4. Given the year-round prevalence of diseases and parasites and the likely seasonal oceanographic variability, these simulations should ideally be carried out for 4 seasons (e.g. using a single mid-season starting point).
5. Particles are to be released from “wet” (water depth > 0 m) points covering the entirety of each FMA.
6. The number of particles per start position and their horizontal (and, where relevant, vertical) spacing are to be sufficient to achieve numerical stability, accounting for stochastic processes (diffusion).

Three types of biological organism are to be considered as follows:

1. Sea-lice larvae - representative species *Lepeophtheirus Salmonis* (Leps): these will be modelled as particles with a fixed position in the vertical (3m constant depth) with passive horizontal drift (including horizontal diffusion). The pelagic larval duration (PLD) is temperature-dependent so, based on some generalisations, this could be approximated to 18 days (winter), 15 days (spring and autumn) or 10 days (summer), comprising a 5-day non-infectious period + 10-day infectious period (spring and autumn), or the approximate pro-rata equivalent for the remaining seasons. All “target” FMAs reached within the infectious part of the PLD will be scored.
2. Infectious Salmon Anaemia Virus (ISAV - representative short-persistence pathogen): Whole water column releases and passive vertical and horizontal drift (including diffusion) will be used. Pelagic duration = 3 days. All “target” FMAs reached within this period are to be scored.
3. Infectious Pancreatic Necrosis Virus (IPNV; representative long-persistence pathogen): Whole water column releases and passive vertical and horizontal drift (including diffusion). Pelagic duration = 35 days (autumn to spring) and 17 days (summer), respectively. All “target” FMAs reached within this duration are to be scored.

A first draft of this methodology report was reviewed by Prof Christina Sommerville (CS, Institute of Aquaculture, University of Stirling) in March 2014. Her response focussed on the sea lice life cycle and behaviour (her area of expertise) rather than particle tracking modelling and connectivity. Details of the implemented methodology are described in section 3 below, after being fully discussed and agreed with Marine Scotland (AG) prior to carrying out the simulations. The following section provides some definitions and references to recent work on hydrodynamic modelling, dispersion, particle tracking and sea lice dispersal in particular.

Background

Population connectivity is often used to explore the viability of populations recruiting individuals from neighbouring habitats of varying separation distance (e.g. Phelps et al., 2014; Phelps, 2015). However here we are looking at another aspect – the likelihood of parasites and disease spreading to adjacent populations of farmed salmon in Scottish Waters. We look at two issues: dispersal of sea lice larvae and dispersal of viruses. For sea lice, connectivity depends on pelagic larval duration (PLD) as well as other factors, such as the survival and behaviour of larvae, and the fecundity of adults. Gallego et al. (2013) state that the mean transport distance was mostly related to the duration of the pelagic larval phase, although season of spawning and distance to shore were also important factors. The mean straight distance between start and end positions at the end of the PLD can only give an approximation of the actual transport. The actual particle trajectories will always be longer due to tidal and random (diffusion) effects, in addition to the circulation around land masses.

Definitions:

Connectivity, in marine ecology, is the exchange of individuals among marine populations (Cowen and Sponaugle, 2009). Connectivity can refer to the flux of any material (e.g., organisms, gametes, genes, disease vectors, nutrients) between locations. In their paper they focus explicitly on the movement of individuals within and among local or subpopulations, assuming that the level of exchange, when referring to population connectivity, must be sufficient to impact the demographic rates of the local population(s).

A **Connectivity matrix** (Cowen and Sponaugle, 2009) provides the probability of exchange of individuals between patches; if the matrix is normalized with respect to the number of individuals in population *i*, then the matrix element P_{ij} gives the probability that an individual in population *i* came from population *j*. We wish to calculate the relative connectivity between origin and destination FMAs, based on the percentage of all particles released at each origin FMA (Gallego et al., 2013).

Larval dispersal is the intergenerational spread of larvae away from a source to the destination or settlement site by the end of the larval stage.

Pelagic Larval Duration is the time that larvae can persist in the water column

Larval Behaviour

Many larvae are able to regulate their position in the water column. This normally involves active vertical swimming to either maintain a desired depth throughout the planktonic phase or migrate vertically in response to physical and biological cues such as light intensity, tidal state or larval stage (Kingsford et al., 2002). Diurnal migration is common, moving vertically in the water column between night and day. Yet another relatively common vertical migration scheme is circatidal migration,

which is characterised by swimming vertically in synchronisation with tidal state. For larvae aiming to reach inshore areas, this can allow them to avoid the ebbing tide (North et al, 2008; Adams et al., 2014b). Some larvae are able to exploit the vertical shear in tidal currents in order to manipulate their horizontal transport. This process is referred to as selective tidal stream transport (STST, Forward and Tankersley, 2001). It is not clear whether larvae that exhibit this type of migration respond to changes in pressure, salinity, turbulence or another physical cue (Kingsford et al., 2002).

Predation and mortality can also be important considerations. Not only does mortality reduce the overall number of larvae that survive through to adulthood, but if there are spatial variations to mortality, for example due to predator abundance, or food availability, then this can affect the overall spatial pattern of dispersal and connectivity.

Another common feature is the influence of physical properties, particularly temperature, upon larval growth. Typically warmer seawater temperatures lead to faster development, and therefore a shorter PLD and some larvae also develop at different rates according to seawater salinity. Shorter PLDs are typically associated with shorter dispersal distances. Other considerations include competition for resources, substrate availability and tolerances to physical properties such as temperature and salinity.

Larval swimming behaviour (even at small speeds) can influence dispersal and larvae may respond to physical cues such as a halocline (North et al., 2008) and migrate vertically. Horizontal swimming may also be relevant in some cases. Other elements of larval behaviour that have been successfully incorporated into numerical models include temperature-dependent larval development rates (e.g. Phelps et al., 2014).

○ Sea Lice

The sea louse *(Lepeophtheirus salmonis)* is a naturally occurring parasite on wild salmonids. Infestations of this sea louse pose a major economic burden to the Atlantic salmon aquaculture industry in Scotland and may be linked to the decline of wild salmonid populations (Amundrud and Murray, 2007) although this is still hotly debated. Fish farms can be areas of high concentration of sea lice and may represent infectious sources which provide a significant threat to wild stocks of migratory fish as they come into contact with the fish farm areas, although the source of the lice in any Farm Management Area (FMA) is not exclusive to fish farms. Utilising a particle tracking model, we can study the movement of a ‘modelled louse’ between FMAs and the connectivity of these areas with respect to the transmission of infection.

Attempts at modelling to date have made suggestions as to the dispersal of larval lice over varying distances of up to 30km, 75 km and even 100km from source (CS,

pers. comm.). Other predictions suggest that the louse larvae could disperse an average of 27 km (range 11 to 45 km) over 5 to 15 days. Predicted averages for dispersal of sea lice larvae range from 12 km (range 5 -17 km) in low currents (~5 cm s^{-1} to 47 km (range 23 - 70 km) in higher currents (~ 20 cm s^{-1}).

L. salmonis has three free-swimming planktonic larval stages: two (non-infective) nauplii and an infective copepodid (see Murray and Gillibrand, 2006, with further references therein). These non-feeding larval stages rely on yolk reserves to survive, and drift with the prevailing current until the copepodid encounters a host fish to attach to, whereupon it begins feeding and development progresses through a further 7 stages on the host (Fig. 1).

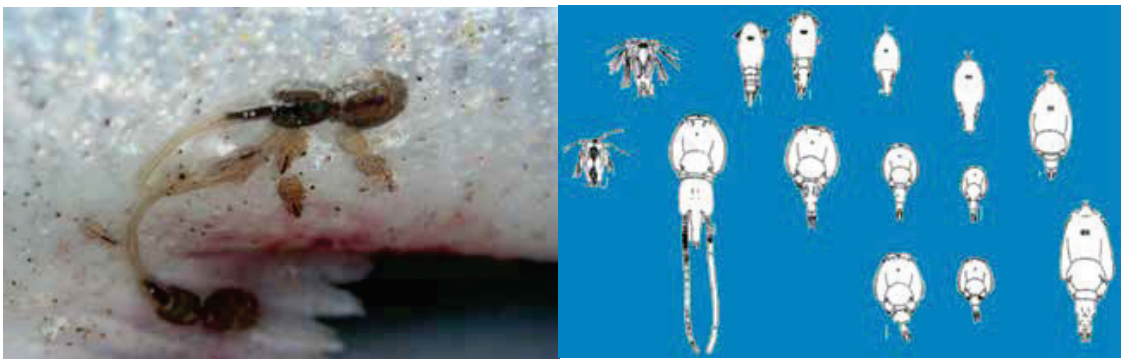


Figure 1: (a) Sea louse on host (b) Life cycle of Lepeoptheirus salmonis commonly called LEPS (from Marine Scotland Topic Sheet no 91 v1 Sea Lice: Control & Regulation)

They are not entirely passive, tending to keep in surface waters so that most infection occurs at depths of 0–4 m below the surface. Nauplii and copepodids are naturally buoyant owing to the lipid gut content. The copepodid hops upwards and then sinks downwards for longer, but the distance gained in upward swimming is greater than the distance sinking. e.g. a hop distance 1.43 cm; a sink 0.05cm. Swimming is halted at salinities 21-23 psu. They move up in the day and down at night e.g. from ~2m to 3.5m below the surface. Sea lice life cycles are entirely driven by temperature (CS, pers. comm.). Based on laboratory experiments, the optimum temperature for *L. salmonis* is 10°C and optimum salinity is 33 to 35 psu. Prof Sommerville notes that environmental temperature will determine the rate of usage of the yolk and therefore the PLD (pelagic larval duration). This may be a more significant effect of temperature than its impact on developmental/maturation/growth rate of the larvae.

○ Infectious Salmon Anaemia

Infectious salmon anaemia (ISA) is a viral disease of Atlantic salmon (*Salmo salar L.*) that can cause severe losses to infected farms, caused by the ISA virus (ISAV). The disease was first reported in Norway in 1984, but has since been reported in Canada, the USA, the Faroe Islands, Ireland and Scotland. It causes severe anaemia of infected fish (unlike mammals, the red blood cells of fish have

DNA, and can become infected with viruses). The fish develop pale gills and may swim close to the water surface, gulping for air. However, the disease can also develop without the fish showing any external signs of illness, the fish maintain a normal appetite, and then they suddenly die. The disease can progress slowly throughout an infected farm and, in the worst cases, death rates may approach 100%.

ISA appears to be most like influenza viruses. Its mode of transfer and the natural reservoirs of ISAV are not fully understood. Apart from Atlantic salmon, both sea-run Brown trout (Salmo trutta) and Rainbow trout (*Onchorhyncus mykiss*) can be infected, but do not become sick, so it is thought possible that these species may act as important carriers and reservoirs of the virus

In May 1998, a salmon farm at Loch Nevis on the west coast of Scotland reported its suspicions of an outbreak of ISA. By the end of the year, the disease had spread to an additional fifteen farms not only on the Scottish mainland but also on Skye and Shetland. In 2008-9 there was another outbreak of ISA in Shetland. ISA was detected in fish from just one site, which was then harvested and left fallow. The disease was eradicated and no further outbreaks have occurred to date.

The virus can be transmitted through water, but the highest risk factors for spread of disease are movement of live fish, discharge of untreated blood and contact with infected vehicles and equipment. It is a notifiable disease in the EU and control measures are: compulsory slaughter and disinfection of infected farms, strict movement controls on suspect farms and placing farms in the vicinity of an outbreak under surveillance. ISA has a "weak" external protective capsid so it is unlikely to be viable any longer than 3 days in the water (AG, pers. comm.).

○ Infectious Pancreatic Necrosis

Infectious pancreatic necrosis (IPN) is a severe viral disease of salmonid fish, caused by infectious pancreatic necrosis virus (IPNV). This disease mainly affects young salmonids, such as trout or salmon, of less than six months, although adult fish may carry the virus without showing symptoms. Resistance to infection develops more rapidly in warmer water. It is highly contagious and found worldwide, but some regions have managed to eradicate or greatly reduce the incidence of disease. The disease is normally spread horizontally via infected water. Clinical disease is particularly important in farmed Atlantic salmon and Rainbow trout.

A sharp rise in mortality is often seen (depending on the virulence of the disease). Other clinical signs include abdominal swelling, anorexia, abnormal swimming, darkening of the skin, and trailing of the faeces from the vent. Surviving fish should recover within one to two weeks. Currently, no treatment is available.

Good husbandry measures, such as high water quality, low stocking density, and no mixing of batches, help to reduce disease incidence. To eradicate the disease, very strict protocol with regards to movement, water sources and stock replacement must be in place – this is difficult to achieve and very expensive. IPNV degrades with temperature, taking about 17 days to be inactivated at 15°C and 14 days at 20°C. A standard inactivation period of 35 days in autumn, winter and spring is assumed here (AG, pers. comm.).

○ Scottish Aquaculture Management

Marine fish farms typically consist of net pens that exchange their contents easily with the environment. Released material includes nutrients, organic waste, pathogens (including sea lice and viruses) and medicines used to treat those pathogens. The number of 'particles' released will vary according to season/water temperature; age/size of fish and management practice i.e. the number of particles released at a fixed time point depends on:
a) The management practice i.e. whether the management adhere to treatment regulations which specify the number of allowable adult females per fish before treatment.
b) Size/age of fish. Lice burdens will be heavier in larger fish in year two of the production cycle than in year one fish, unless no fallowing has been carried out, in which case smaller year one stocked fish will also carry a heavy burden of lice.

The amount of dispersal of sea lice and their contribution to the decline in wild Atlantic salmon and sea trout has been debated over the years. A great deal of recent work has been carried out in Loch Torridon, on the west coast of Scotland. The biannual cycle of louse abundance along the shoreline at the head of Loch Shieldaig matched the production cycle of the local salmon farms, with the appearance of louse copepodids lagging behind farm louse burdens by 1 to 3 weeks (McKibben and Hay 2004). They found that the infectious stage could be located close to river mouths, using plankton sampling. Copepodids were present in high numbers over a sustained period and were abundant in the early spring at times when salmon and sea trout smolts go to sea. Such high levels of copepodids have not been recorded previously outside fish farm cages.

Although there are no FMAs on the east coast of Scotland, lice are present on the east coast with no apparent genetic differentiation from those on the west coast.

○ Farm Management Areas (FMAs)

These describe defined areas in which farmers undertake farming activities at one or more farm sites and plan and synchronise production in order to reduce and manage risks posed by infectious agents and parasites which can be present in the environment, in wild and farmed fish, and in other naturally occurring biota. FMA

policies will, in some cases, focus mainly on stocking and production cycles, fallowing arrangements and sea lice management, while in others, they will relate to other issues which have a potential to affect fish health. N.B. not all designated SMAs will contain a fish farm.

A very simplified production cycle is as follows:

Fish are stocked in year one of the production cycle and grow on for up to 18 to 22 months. They may be stocked at different times depending on the age of the smolts. The fish are harvested in year two and a fallow period is used before the site is restocked. Only one year class at a time is stocked in any one site to avoid the heavier burdens found on year two fish infecting the newly stocked year one fish i.e. Single Year Class stocking, which is now universal in Scotland. The fallow period is varied but the Scottish Salmon Producers Code of Practice recommends a minimum of four weeks and an average of 21 weeks was recorded in 2013. It has many values but is also intended to empty the site of any mobile lice (larvae, pre adults and adults). It doesn't take into account any resident fish which may be infected e.g. sea trout, escaped fish or migrating salmon. However this procedure should ensure that sea lice infection should not spread to more distant FMAs by infecting intermediate locations, over several seasons.

- Disease Management Areas (DMAs)

These describe areas that are designated by Marine Scotland for the purpose of statutory controls for the management of fish diseases. They include areas defined in relation to the control of a range of listed diseases of fish. Notable examples are the control and surveillance zones, based on a tidal excursion model, established in relation to the management of ISA. FMAs may be smaller than, identical to, or larger than DMAs.

In Fig. 2, the Scottish Shelf Waters area is subdivided into several maps, which are shown in detail in Figs. 3 - 6, showing the individual FMA's, with a total of 87 management areas. We wish to know whether sea lice and viral dispersal can occur between these FMA's.

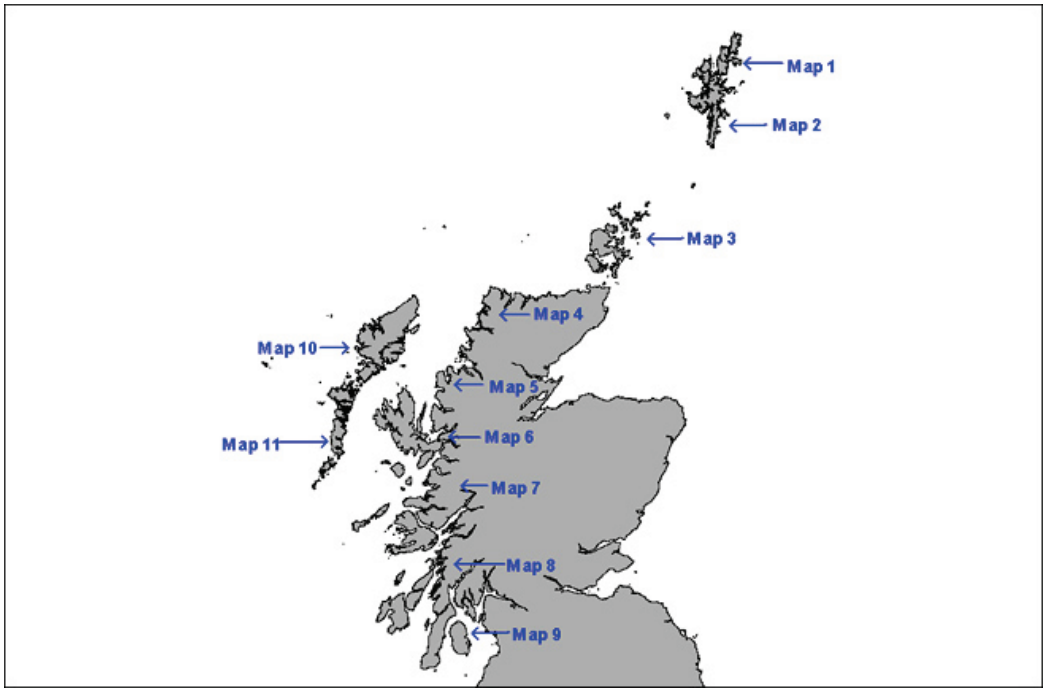


Figure 2: Map of locations of Scottish FMA group maps

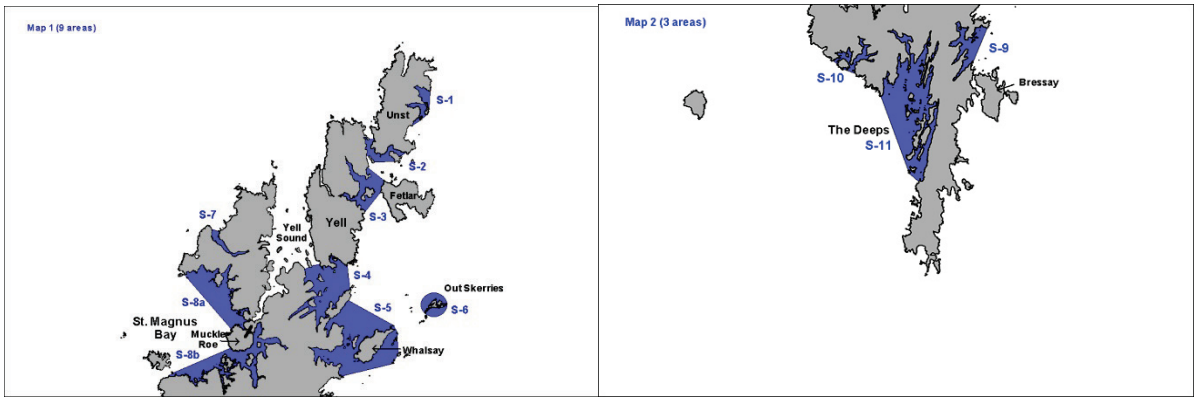


Figure 3: Shetland (12 management areas)

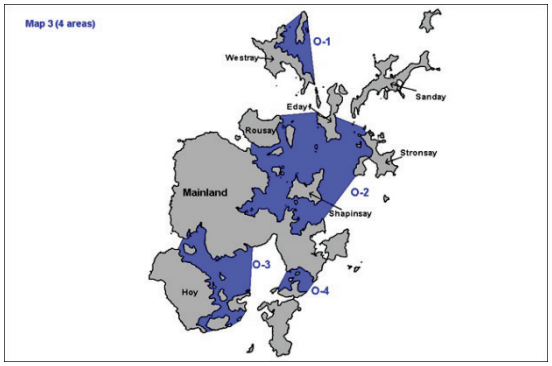


Figure 4: Orkney (4 management areas)

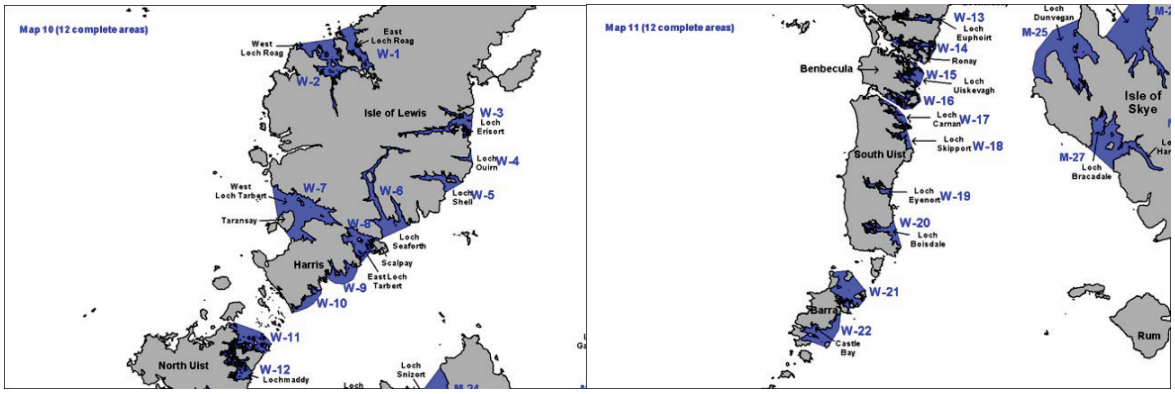


Figure 5: Western Isles (22 management areas)

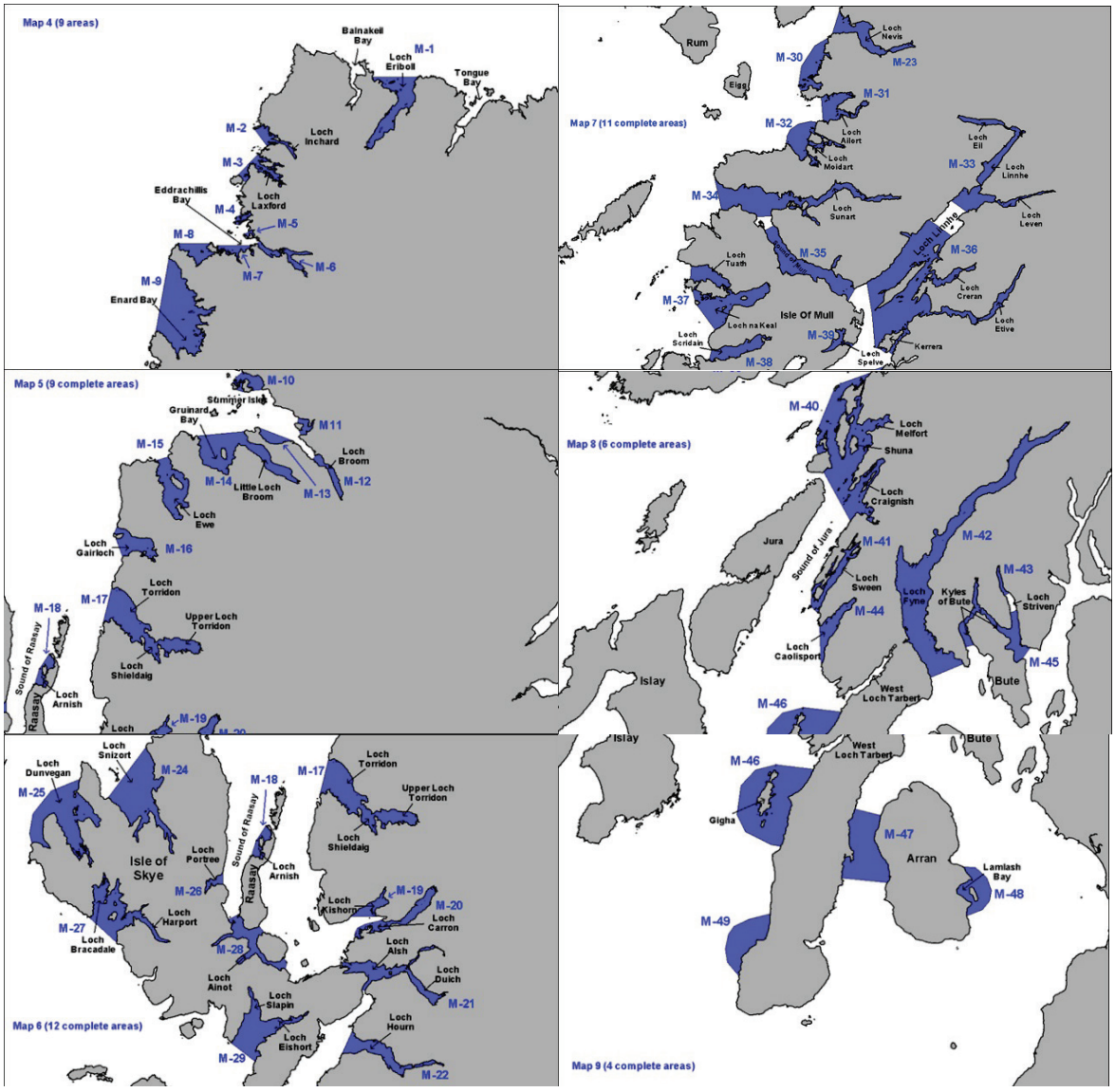
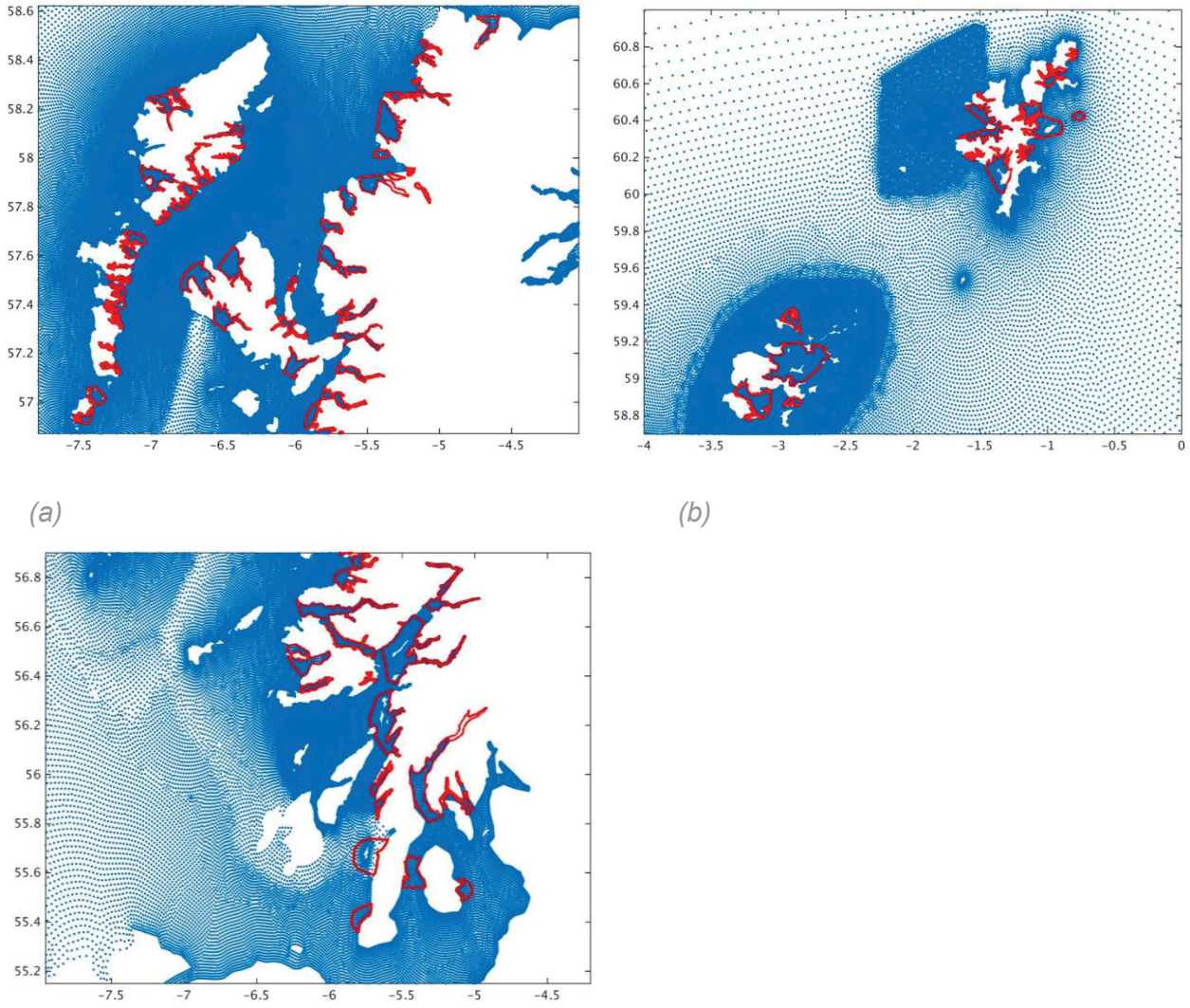


Figure 6: Mainland (49 management areas)

The nomenclature used in Figs. 3-6 is adopted for the rest of this report i.e. S1-S11 (Shetland, including S8a and S8b), O1-O4 (Orkney), M1-M49 (Mainland) and W1-

W22 (Western Isles). GIS shape files (89 shape files), for the polygons giving the boundaries of these areas, have been provided through Marine Scotland Science (Fig. 8). Of these 89 areas, one represents a tiny extension of M13 (only 0.008km^2) and another is a westward extension of W14. Most of the FMAs are well-resolved in the combined shelf model mesh, however there are some that do not include any nodes of the model (M12, inner Loch Broom and M43, inner Loch Striven) and some that are only partially resolved (e.g. S10 and M13). The FMAs numbered M11, M12 and M13 have therefore been combined within a boundary further out into the estuary and called LB (Loch Broom), see Fig. 9a. The inner FMA in Loch Striven (M43) has been extended south in order to enclose some model nodes (Fig. 9b). The resulting 86 polygons have been used to define the areas of sources and sinks for particle tracking.



(a) *(b)*

(c)

Figure 8: Plots of FMA shape files

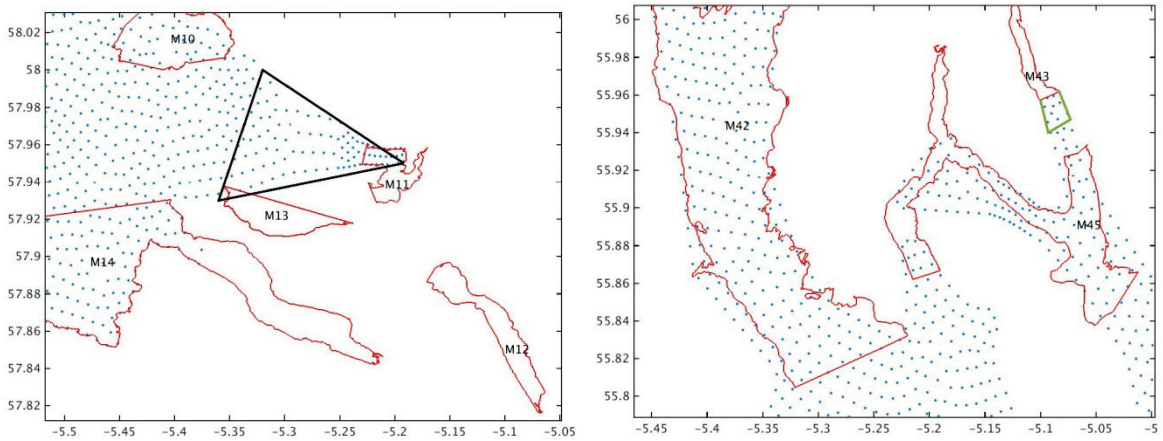


Figure 9: Modifications to FMA's (a) Loch Broom (left) (b) Loch Striven. Original FMA boundaries are in red, new boundaries in black; model nodes are blue dots

Various previous studies have been made of the hydrodynamic circulation, dispersion and particle tracking in the west of Scotland, related to sea lice dispersion. Dmitry Aleynik has built a Scottish West Coast FVCOM model, forced by a high-resolution WRF atmospheric model and shown excellent validation at high resolution in sea lochs (personal communication, UK FVCOM workshop, 2015). Other modelling work has validated the ability of high-resolution modelling to predict dispersion. For example Stashchuk et al. (2014) looked at horizontal dye dispersion in the Celtic Sea using a high resolution (50m), non-hydrostatic implementation of the MITgcm model, finding the dispersion is related to inertial oscillations and vertical shear. The most relevant work to this study is Adams et al. (2014a) which looked at larval dispersal of intertidal organisms in the Firth of Lorn on the west coast of Scotland, and found that meteorological variation and broad scale current patterns interact strongly with local geography to determine connectivity in coastal areas. They studied a range of larval durations (1–28 days), and two different meteorological forcing scenarios. They found that particles released from regions of high current velocity, open coastline and low local habitat availability travelled furthest but were less likely to disperse successfully to other coastal site. Adams et al. (2014b) considered whether renewable energy devices might act as stepping stones for the spread of intertidal marine organisms with pelagic larvae (such as barnacles), providing intermediate habitats, but this is not relevant to sea lice or virus transmission.

Murray and Gillibrand (2006) carried out particle tracking, using advection and turbulent diffusion for a structured grid model of Loch Torridon, forced by tides and winds. Inter-farm site exchange in Loch Torridon may occur under suitable winds. However, most lice remain in the basin that they are released in, even under these

winds. Amundrud and Murray (2007; 2009) carried out further modelling of sea lice dispersal in Loch Torridon. They found that simulated dispersal patterns of viable sea lice demonstrate a high dependence on wind and freshwater forcing, such that validation must be carried out under a range of environmental conditions. The complex coastlines of Scottish fjords mean that wall parameterisations can have significant influence on individual particle tracks. In the first paper they examined the impact of varying wall parameterisations and found that a discrepancy in trajectories due to wall interactions will not greatly affect the dispersion pattern of a large number of particles. However, specific implementations of particle tracking models where diffusion is low, or not present, must consider the impact of wall interactions and experimental design should be robust enough to avoid allowing this feature to influence results. Another example of modelling of sea lice spread in Norway is given in Aldrin et al. (2013).

In the next section we introduce the FVCOM offline particle tracking model: this includes no biological behaviour, but particles can be released at different vertical levels and there are options for inclusion of a random walk diffusion term in the horizontal and vertical, as well as 3-dimensional advection. In section 3 we apply this using the SSM climatology-forced output (3D currents).

Particle Tracking in FVCOM

Method

From the FVCOM manual (Chen et al., 2013) the Lagrangian particle tracking module consists of solving a nonlinear system of ordinary differential equations (ODE) as follows

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}(\boldsymbol{x}(t), t) \qquad (2.1)$$

where $\boldsymbol{x}$ is the particle position at a time t, $d\mathbf{x}/dt$ is the rate of change of the particle position in time and $\mathbf{v}(\mathbf{x},t)$ is the 3-dimensional velocity field generated by the model. This equation can be solved using any method suitable for solving coupled sets of nonlinear ODE's such as the explicit Runge-Kutta (ERK) multi-step methods which are derived from solving the discrete integral:

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_n) + \int_{t_n}^{t} \boldsymbol{v}(x(t), \tau) d\tau \qquad (2.2)$$

Assume that $x_n = x(t_n)$ is the position of a particle at time $t=t_n$, then the new position $x_{n+1} = x(t_{n+1})$ of this particle at time $t = t_{n+1}$ $(= t_n + \Delta t)$ can be determined by the 4th order 4-stage ERK method where Δt is the time step. The dependence of the velocity field on time has been eliminated since the velocity field is considered stationary during the tracking time interval of Δt. It is important to understand that in a multidimensional system, the local functional derivative of v must be evaluated at the correct sub-stage point x in (x, y, z) space. On a 2-dimensional (x,y) plane, for example, a particle can be tracked by solving the x and y velocity equations given as

$$\frac{\mathrm{dx}}{\mathrm{dt}} = \mathrm{u}, \quad \frac{\mathrm{dy}}{\mathrm{dt}} = \mathrm{v},$$

Many users have added a random walk-type process into this 3-D Lagrangian tracking code to simulate sub-grid-scale turbulent variability in the velocity field. In FVCOM version 2.5, only the advection tracking program was included as described above, however version 3.1.6 (as used here) includes an optional random walk, R (uniformly distributed within the domain [-1,1]), where the horizontal diffusivity D_h is specified as a constant and the vertical diffusivity D_v is provided from the circulation model.

$$\boldsymbol{x}(t) = \boldsymbol{x}(t_n) + \int_{t_n}^{t} \boldsymbol{v}(x(t), \tau) d\tau + \sqrt{6RD_h\Delta t} \qquad (2.3)$$

Some smoothing of the diffusivity may be required in the vertical (Brickman and Smith, 2002). A key property of a correct Lagrangian Stochastic Model is that it maintains an initially uniform concentration of particles uniform for all time. This is called maintaining the well-mixed condition (WMC). If the result does not conform to

WMC this may be due to inadequate resolution of the hydrodynamic model. Ideally one should conduct statistical tests to ensure that the number of particles is sufficient for the investigation (Brickman and Smith, 2002).

The in-line particle tracking program can be run on both single and multi-processor computers. However, in the MPI parallel system, tracking many particles simultaneously with the model run on a multi-processor computer can significantly slow down computational efficiency, since particles moving from one sub-domain to another require additional information passing. Multiple runs of the particle tracking would also require re-running the hydrodynamic model. For this reason, it is suggested that users use the offline version of the particle tracking code.

○ Offline particle tracking code

The offline code is provided in the FVCOM package (under 'root'/output/FVCOM_particle_tracking). This is not parallelised and runs on a single processor only. For large numbers of particles (O(100,000)) the calculations may be run on parallel processors by dividing the particles between processors, which is what has been done here. Note that the supplied version had some software errors which have now been fixed. This code includes no biological behaviour, but particles can be released at different vertical levels and there are options for inclusion of a random walk diffusion term in the horizontal and vertical, as well as 3-dimensional advection. There is an option for a fixed level or a sigma-coordinate level for the release points.

The modules of the offline package are shown in Table 1. The main code is in **offlag.f90**, which includes the main program PARTICLE_TRAJ which in turn calls subroutines in **offlag.f90, alloc_vars.f90, data_run.f90, ncdio.f90** and **triangle_grid_edge.f90**. The other modules set array sizes, initialise arrays and provide certain utility subroutines and functions.

Table 1: Modules of Lagrangian off-line particle tracking program (more details of the various subroutines in each module are given in Appendix)

Module	Purpose
alloc_vars.f90	Allocates and initialises most arrays
data_run.f90	Inputs parameters which control the model run
mod_inp.f90	Decompose input line into variable name and variable value(s)
mod_ncd.f90	NetCDF utilities
mod_prec.f90	Defines floating point precision using kind
mod_var.f90	Sets global limits and array sizing parameters
ncdio.f90	NetCDF I/O: input time and output surface elevation and bottom depth
offlag.f90	Lagrangian particle tracking off-line program
triangle_grid_edge.f90	Define the non-overlapped, unstructured triangular meshes used for flux computations
util.f90	Utilities, from Numerical Recipes

The steps in the particle tracking code are as follows:

1. CALL GETARG (implicit function) to read command line input: 'runname' and output stream
2. CALL DATA_RUN – reads 'basename'_run.dat for control parameters
3. CALL NCD_READ_GRID – reads model grid data from 1st daily file
4. CALL NCD_READ_SHAPE – reads model bathymetry, sigma levels and grid coefficients from 1st daily file
5. CALL NCD_READ_METRICS – reads 'runname'_metrics.nc file if it exists (output from TRIANGLE_GRID_EDGE)
6. CALL TRIANGLE_GRID_EDGE – calculates grid metrics (NTVE, NBVE, NBVT, ISBCE, ISONB) if 'runname'_metrics.nc does not exist
7. CALL NCD_WRITE_METRICS – writes 'runname'_metrics.nc if does not exist
8. CALL SET_LAG – calculate initial particle positions in model grid
    a. Reads initial particle positions from file
    b. CALL FHE_ROBUST – determine element containing each particle

   c. CALL NCD_READ – read model data from daily files
   d. CALL INTERP_ELH – linear interpolation of surface elevation
   e. CALL NCD_WRITE – write initial particle positions to file
9. CALL LAG_UPDATE – updates particle positions
   a. CALL NCD_READ - read next hourly data
   b. CALL TRAJECT – calculates particle position due to advection by velocity field
      i. CALL INTERP_V – interpolates velocity
      ii. CALL INTERP_ELH
      iii. CALL FHE_QUICK/ FHE_ROBUST – locate particles in grid
      iv. CALL INTERP_ELH
   c. If IRW>=1 CALL RAND_WALK – calculates turbulent diffusion using random walk
      i. Smooth vertical eddy diffusivity (KH) from model (in vertical), referring to Visser (1997) and Ross and Sharples (2004)
      ii. Calculate 2nd derivative of KH using spline
      iii. Calculate horizontal random walk (if IRW = 2 or 3)
      iv. Calculate vertical random walk (if IRW = 1 or 3)
   d. CALL NCD_WRITE – write particle positions to file – in ncdio.f90

Fixing the code

1. The code as supplied does work for advection only and for Cartesian coordinates but not for lat/lon coordinates.
2. The start-up time is quite long (~2 hours for the large combined model grid). Pierre Cazenave at PML provided a modified code which shortened this set-up time for subsequent runs, by saving metrics calculated within *triangle_grid_edge.f90*. However there was a bug in this code.
3. Horizontal random walk – some variable declarations had to be corrected from integer to real in RAND_WALK.
4. There was a problem with the vertical random walk: there was an error in the dimension of the vertical diffusivity, which is read in at nodes but has to be interpolated to elements and this wasn't being done.

Input output files

The necessary input files are: (i) a control file; (ii) one or more daily model output files; and (iii) an initial particle release location file.

The particle tracking configuration is controlled by the file ‘runname’_run.dat, which is in the ‘root’/output/FVCOM_particle_tracking/run/’basename’/ directory (for the combined climatology output ‘basename’=combined). An example of this file is given below:

```
!==============================================================================!
```

```
! INPUT FILE FOR PARAMETERS CONTROLLING EXECUTION OF OFF-LINE PARTICLE TRACKING     !
! DESCRIPTION OF VARIABLES AND SUGGESTED PARAMETERS CAN BE FOUND AT BOTTOM           !
!                                                                                   !
!        FORMAT:                                                                    !
!       1.) VARIABLE  = VALUE  (EQUAL SIGN MUST BE USED)                            !
!       2.) FLOATING POINT VARIABLES MUST CONTAIN A PERIOD "." EX: 1.3, 2.,etc      !
!       3.) BLANK LINES ARE IGNORED AS ARE LINES BEGINNING WITH ! (F90 COMMENT)     !
!       4.) COMMENTS CAN FOLLOW VALUES IF MARKED BY !                               !
!       5.) ORDER OF VARIABLES IS NOT IMPORTANT                                     !
!       6.) FOR MULTIPLE VALUE VARIABLES FIRST ENTRY IS NUMBER OF VARIABLES         !
!           TO FOLLOW (OR 0 IF NONE)                                                !
!       7.) DO NOT USE COMMAS TO SEPARATE VARIABLES                                 !
!       8.) DO NOT EXCEED EIGHTY CHARACTERS PER LINE                                !
!       9.) FOR LINE CONTINUATION ADD \\ TO END OF LINE TO FORCE CONTINUE           !
!           TO NEXT LINE.  MAXIMUM 4 CONTINUATIONS                                  !
!       10.) TRUE = T, FALSE = F                                                    !
!                                                                                   !
!===================================================================================!
!=========Parameters Controlling Time Integration===================================!
DTI      = 300.0 ! Time step for scheme resolution. mod(INSTP/DTI) should be 0
INSTP    = 3600  ! INPUT time step (s).
DTOUT    = 1     ! output time step in hour
TDRIFT   = 432   ! Drift duration (hours) = 18 days
!=========Parameters Controlling Starting Tracking Date=============================!
YEARLAG   = 1993 ! Year of tracking start (corresponds to climatological year)
MONTHLAG  = 1    ! Month of tracking start
DAYLAG    = 1    ! Day of tracking start
HOURLAG   = 0    ! Hour of tracking start
!=========Parameters Controlling Input/Output LOCATION==============================!
INPDIR   = ../../input/combined
GEOAREA  = Scottish_Waters
OUTDIR   = ../../output/combined/Jan01
INFOFILE = screen
LAGINI   = January01   ! Input file with particle location
!=========Parameters Controlling SIGMA/CARTESIAN====================================!
F_DEPTH    = T            ! Cartesian depth is kept constant if T.
P_SIGMA    = F            ! Input particle depth in sigma if T.
OUT_SIGMA  = F            ! Output particle depth in sigma if T.
!=========Parameters Controlling Random Walk========================================!
IRW   = 1   ! IRW (0-w/o rw; 1-hor rw; 2-vert rw; 3:hor+vert rw)
DHOR  = 10. ! DHOR (horizontal diff coeff m^2/s, miller 10^6m^2/day~11.57m^2/s)
DTRW  = 60.  ! time step (s) for RW (from Visser's criterion). mod(DTI/DTRW) should
be 0
```

The following parameters are set in this file:

1. **Time steps:**
   DTI – advection time-step (seconds): this must be divisible into INSTP – 300 seconds has been chosen as a compromise between a shorter time step which will take more computational time and a longer time step which would possibly allow particles to jump across cells or across land;
   INSTP – input time step (seconds): here we use 1 hr which is the output time-step of the model;
   DTOUT – output time step (hours): 1 hour has been chosen;
   TDRIFT – the total tracking time (hours): this is defined for different seasons and different representative particles.

2. **Date parameters:**
   YEARLAG, MONTHLAG, DAYLAG and HOURLAG are the start time of particle tracking (year, month, day and hour).
   Although YEARLAG is defined in this control file, the source code currently has hardcoded values for the year, so you need to edit the first line of **offlag.f90** (after INTEGER declarations) to use the correct year for your model run, i.e. set YEAR0='YYYY'. For the climatology run an arbitrary year of 1993 is used.

3. **Input and output file and directory names:**
   INPDIR is the input directory where output from the FVCOM model run is located - convention is for this to be the 'root'/output/FVCOM_particle_tracking/input/'basename'/ directory (maybe using a softlink – see below);
   GEOAREA is not used, so can be set to any value;
   OUTDIR is the output directory for the particle tracking output - here we use a sub-directory of 'root'/output/FVCOM_particle_tracking/output/'basename'/ e.g. Jan01, Jan02…for multiple runs of 'runname'= January (standard files 'runname'_LAG.nc and 'runname'_diag.dat are written to this directory);
   INFOFILE is where the particle tracking progress reports are sent, default = screen; this may be re-directed at run-time;
   LAGINI.dat is the file containing the initial particle positions, which must be in the input directory 'INPDIR'.

4. **Options for vertical coordinate:**
   F_DEPTH, P_SIGMA, OUT_SIGMA are logical variables (T or F).
   F_DEPTH = T indicates the particle is released at a fixed Cartesian depth (in LAGINI.dat); P_SIGMA = T means the input particle coordinate is in σ-coordinates;
   OUT_SIGMA = T gives the output particle coordinate in σ-coordinates.

5. **Random walk settings:**
   IRW = 0 - no random walk (or turbulent diffusion); 1 - horizontal random walk only; 2 - vertical random walk only; 3 - both horizontal and vertical random walk;
   DHOR is the (constant) horizontal diffusivity (m^2s^{-1});
   DTRW is the time-step for the random walk (seconds), which must be divisible into DTI.

Model data input file name format: The model output netCDF files (input to particle tracking) must be in a separate directory for each year, since the naming of the model output files must be 'runname'_dddd.nc where dddd is the Julian day number, starting from 0001. In the following runs we have used 'runname' = 'month'. So for

example the first day in April is day 0091 (assuming it is not a leap year) and the filename looked for is April_0091.nc. This file (in the nominated input directory) is soft-linked to the actual model output which is in ‘root’/output/FVCOM_output/output/combined.

In the supplied code there is presently no support for spherical coordinates, either the FVCOM model should be run in Cartesian coordinates, or enable FLAG_6 = -DPROJ when compiling FVCOM (and subsequently set the PROJECTION_REFERENCE in the ‘basename’_run.nml file). In this case the model had been run in spherical coordinates, without using this option, so the output had to be converted to Cartesian (the OS coordinate system was used). This was done by running a Matlab script

Table 2: Model output variables used in particle tracking

Variable name	Long name	Dimensions	Units
x	nodal x-coordinate	Node	metres
y	nodal y-coordinate	Node	metres
nv	nodes surrounding element	three, nele	--
h	bathymetry	node	metres
siglev	sigma levels	siglev, node	--
a1u	a1u	three, nele	--
a2u	a2u	three, nele	--
aw0	aw0	three, nele	--
awx	awx	three, nele	--
awy	awy	three, nele	--
time	time	time	days since 1858-11-17 00:00:00
zeta	water surface elevation	time, node	metres
u	eastward water velocity	time, siglay, nele	ms^{-1}
v	northward water velocity	time, siglay, nele	ms^{-1}
omega	vertical sigma coordinate velocity	time, siglev, node	s^{-1}
km	turbulent eddy viscosity for momentum	time, siglev, node	m^2s^{-1}

Particle initial position file

The offline code requires only a single file to define the release sites for the particles (LAGINI.dat). An example is given below:

```
3
1 510876 6555485 5.0 !5m depth
2 500064 6563972 0.0 !Surface
3 530350 6561007 10.0! 10m depth
```

The first line defines the number of particles to track (this is read in with a DO loop in **offlag.f90**, so if you have a long list of positions but only wish to use the first few, set the header number to the number you wish to read in, leaving the remaining points defined in the list; the code will ignore them).

The definition of each point is ID XPOS YPOS DEPTH !NAME with DEPTH being positive downwards (for Cartesian option this is the depth in metres below surface). ID (integer) is not used and can be an arbitrary number, but is useful to keep track of the particle release locations. !NAME is optional to label the releases particle. Set the name of this file to match the LAGINI value in the 'basename'_run.dat file.

○ Output files

The particle tracking generates 3 output files: (i) an asci text file reporting progress, reported to the screen or redirected to an output file if desired; (ii) the particle position file ('runname'_LAG.nc) and (iii) a diagnostic file ('runname'_DIAG.nc). The latter 2 files are written into OUTDIR as specified in the control file.

○ Compiling and running particle tracking

Edit the *makefile* to point to your netCDF library paths and compile the code with *make*. Some commands to load the necessary compiler may be required in advance. The output executable file is then called *ptraj*. Re-compile for different architecture or if any changes are made to the code. For ease of use on the NOCL system the following commands are used:

Linux workstation:

```
module load intel/12.0.2
cd 'root'/output/FVCOM_particle_tracking/source
make clean
make
mv ptraj ptraj_linux
cd ../run/'basename'/
../../ptraj_linux 'runname >output.txt
```

Mobius cluster (but run on single processor):

```
module add intel/compiler/64/14.0/2013_sp1.3.174
cd 'root'/output/FVCOM_particle_tracking/source
make clean
make
mv ptraj ptraj_mobius
cd ../run/'basename'/
../../ptraj_linux 'runname >output.txt
```

STEP-BY-STEP RUNNING PTRAJ

STEP 1: Create directory 'root'/output/FVCOM_particle_tracking/input/'basename'/

STEP 2: Copy particle_tracking.dat file into FVCOM_particle_tracking/input/'basename'/. from particle_tracking/ or other *.dat file, rename to 'runname'.dat

STEP 3: Change particle locations in 'runname'.dat from

```
    1
 1 1139800 2063300 0.0 !
          to
 NP
 1 x1 y1 z1 !name1 (NB 0=surface)
 2 x2 y2 z2 !name2
….
NP xNP yNP zNP !nameNP                    (where NP = number of particles)
```

N.B. It is only possible to use x/y coordinates – these arrays must be populated in model output or calculated from lat/lon – a script for this has been written

STEP 4: Use soft-link to link daily NetCDF FVCOM model output files to 'root'/output/FVCOM_particle_tracking /input/'basename'/'runname'_dddd.nc
N.B input to particle tracking is daily files of hourly data– convert 5-day (or other length) files to daily – a shell script has been written to do this

STEP 5: Create output directories 'root'/output/FVCOM_particle_tracking/output/'basename'/run_num$_1$…run_num$_{NP}$ e.g. Apr01..Apr20

STEP 6: Copy 'runname'_run.dat to 'root'/output/FVCOM_particle_tracking/run/'basename'/'runname'_run.dat

STEP 7: Edit 'runname'_run.dat for each run to point to new OUTDIR and LAGINI files, for multiple runs using different particle release points during same tracking period

STEP 8: Compile code (see above)

STEP 9: Run code: ptraj 'runname' >output.txt

STEP 10: Check results /output/'basename'/run_num/'runname'_LAG.nc

Methodology for Scottish Waters Model

Model output preparation

We have produced a set of FVCOM model results from the combined shelf and case study models to be used by the particle tracking model, using the Climatology run. The chosen approach is as follows:

1. Create a single mesh combining the shelf model and the four case study meshes using methodology developed by CH2M (Darren Price and Caroline Stuiver).
2. Run each of the case study models using nested boundaries obtained from the Shelf Model.
3. Interpolate results from each of the models (starting with Shelf model) onto this new mesh.
4. Use the new mesh result file with the particle tracking model.
5. Data must be provided as daily files of hourly data so the original SSW output files were split up into daily data, using a Linux shell script. Then the combined daily files were constructed.
6. The particle tracking code only works in Cartesian coordinates. The Climatology and other Scottish Waters model runs were done in spherical polar coordinates so a necessary step is to convert the model lat-lon grid to x-y coordinates and copy the *x* and *y* arrays back into the model output NetCDF files (the OS grid convention was used). Then the particle tracking code was run using these modified model data files.

Particle tracking

The second step is to carry out the particle tracking, using the following experiment design:

1. Use the offline FVCOM particle tracking package (see above):
2. The particle release points were generated using a uniform 2kmx2km mesh then selecting those points which lie within the FMAs. This produced at least 1 particle release point in each FMA, except for 3 locations where a particle release point had to be generated manually. The final selection was 977 release points with between 1 and 100 particle release points per FMA (Figure 10). Scripts which are used for FMA manipulation are in directory ‘root’/output/FVCOM_particle_tracking/FMAs/scripts. Use plot_FMAs.m to generate the initial set of particle release points (1093), then run the particle tracking model for the initialisation stage to identify which particles are actually not within the model grid and eliminate these (some particles are on the

boundaries so will not move). The FMA names and locations are shown in Table 3.

3. Multiple particles were released at each location, using a random walk to model the diffusion, checking that the result was not sensitive to the number of particles. 100 particles per release point seemed satisfactory. A limited number of particles were used due to computational constraints. The number of particles required is discussed by Brickman et al. in North et al., (2009) which also refers to Brickman and Smith (2002). In typical releases they tested 100-2000 particles, to ensure that the final result is not sensitive to the number of particles.
4. 'Sea lice' particles are constrained to stay in the surface layer. For this it was found best to use the fixed depth option (F_DEPTH = T), with the initial depth below the surface as 3m and only horizontal diffusion. The particles do move in the vertical by advection, to some extent, but most particles stay within the surface layer (see Figure 11).
5. 'Virus' particles were released at surface, mid-depth and bottom in the water column, using 50 particles at each level, which was a compromise from the ideal (100 particles at each of 10 levels) to avoid excessively long run times of the particle tracking code.
6. The particles were tracked for appropriate PLD periods for each season (see Table 4).
7. Note that tracking cannot be done across the year end. Also the mesh changes size between April and May and between October and November as all 4 nested models were only run from May to October, with only 2 nests (PFOW and WLLS) for the whole year. Therefore the tracking cannot be run from April to May or October to November.

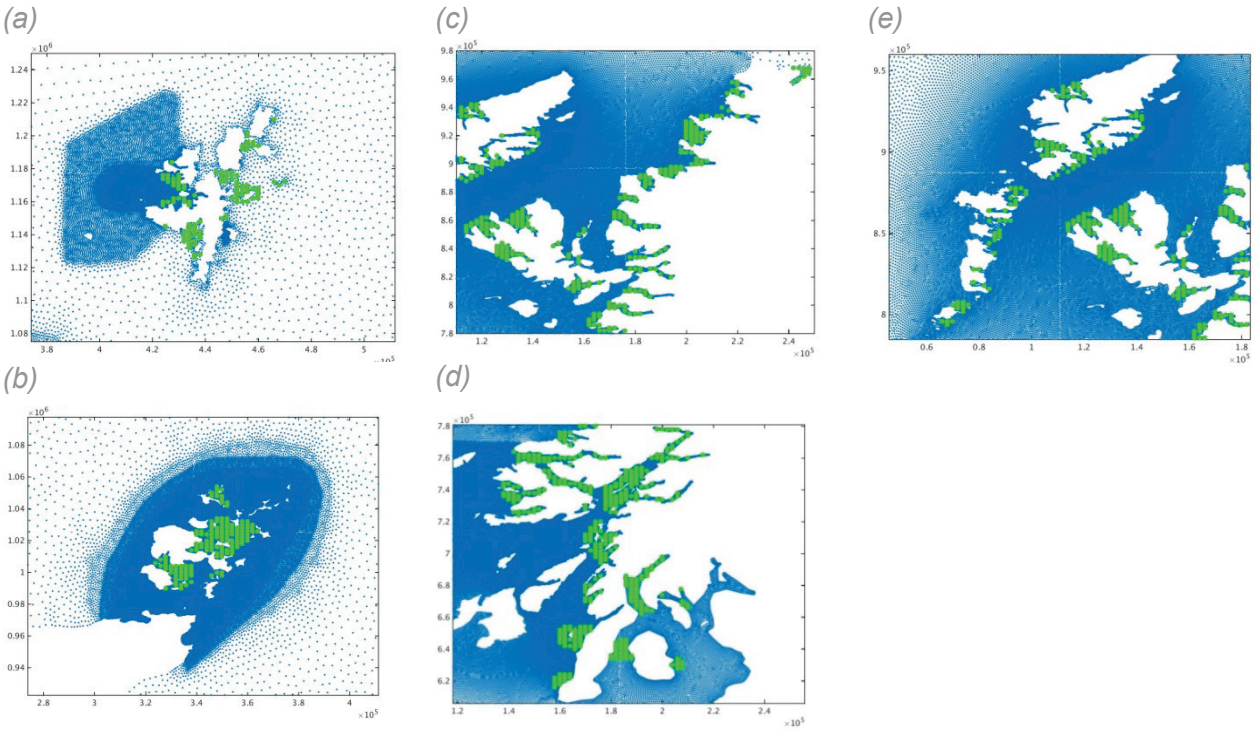


Figure 10: (a) Shetland release points; (b) Orkney release points; (c); N Mainland release points; (d) S Mainland release points; (e) Western Isles release points

Table 3: FMA names and locations

FMA no.	FMA name	Lon	Lat	FMA no.	FMA name	Lon	Lat	FMA no.	FMA name	Lon	Lat
1	'S1'	-0.82	60.76	30	'M16'	-5.75	57.72	59	'M45'	-5.13	55.91
2	'S2'	-0.93	60.68	31	'M17'	-5.67	57.58	60	'M46'	-5.72	55.67
3	'S3'	-0.98	60.63	32	'M18'	-6.02	57.49	61	'M47'	-5.42	55.6
4	'S4'	-1.16	60.44	33	'M19'	-5.65	57.39	62	'M48'	-5.07	55.53
5	'S5'	-1.04	60.37	34	'M20'	-5.57	57.37	63	'M49'	-5.78	55.41
6	'S6'	-0.77	60.42	35	'M21'	-5.56	57.27	64	'W1'	-6.81	58.24
7	'S7'	-1.46	60.53	36	'M22'	-5.55	57.12	65	'W2'	-6.91	58.18
8	'S8a'	-1.50	60.44	37	'M23'	-5.66	57.02	66	'W3'	-6.50	58.11
9	S8b'	-1.46	60.34	38	'M24'	-6.42	57.55	67	'W4'	-6.40	58.05
10	'S9'	-1.17	60.22	39	'M25'	-6.68	57.5	68	'W5'	-6.48	58
11	'S10'	-1.54	60.22	40	'M26'	-6.17	57.41	69	'W6'	-6.67	57.97
12	'S11'	-1.36	60.13	41	'M27'	-6.44	57.35	70	'W7'	-6.95	57.92
13	'O1'	-2.91	59.32	42	'M28'	-6.04	57.31	71	'W8'	-6.74	57.86
14	'O2'	-2.87	59.08	43	'M29'	-5.96	57.16	72	'W9'	-6.81	57.81
15	'O3'	-3.20	58.88	44	'M30'	-5.87	56.95	73	'W10'	-6.92	57.76
16	'O4'	-2.89	58.88	45	'M31'	-5.76	56.86	74	'W11'	-7.13	57.67
17	'M1'	-4.67	58.51	46	'M32'	-5.86	56.79	75	'W12'	-7.16	57.62
18	'M2'	-5.06	58.45	47	'M33'	-5.15	56.76	76	'W13'	-7.22	57.56
19	'M3'	-5.10	58.4	48	'M34'	-5.88	56.67	77	'W14a'	-7.21	57.5
20	'M4'	-5.16	58.32	49	'M35'	-5.85	56.54	78	'W14b'	-7.29	57.51
21	'M5'	-5.13	58.29	50	'M36'	-5.35	56.51	79	'W15'	-7.24	57.45
22	'M6'	-5.01	58.24	51	'M37'	-6.14	56.46	80	'W16'	-7.25	57.4
23	'M7'	-5.18	58.25	52	'M38'	-6.09	56.36	81	'W17'	-7.28	57.37
24	'M8'	-5.31	58.25	53	'M39'	-5.74	56.39	82	'W18'	-7.25	57.32
25	'M9'	-5.34	58.15	54	'M40'	-5.60	56.21	83	'W19'	-7.31	57.23
26	'M10'	-5.40	58.02	55	'M41'	-5.64	55.98	84	'W20'	-7.28	57.14
27	'LB'	-5.23	57.91	56	'M42'	-5.18	56.04	85	'W21'	-7.38	57.03
28	'M14'	-5.35	57.91	57	'M43'	-5.11	55.98	86	'W22'	-7.47	56.94
29	'M15'	-5.64	57.82	58	'M44'	-5.62	55.88				

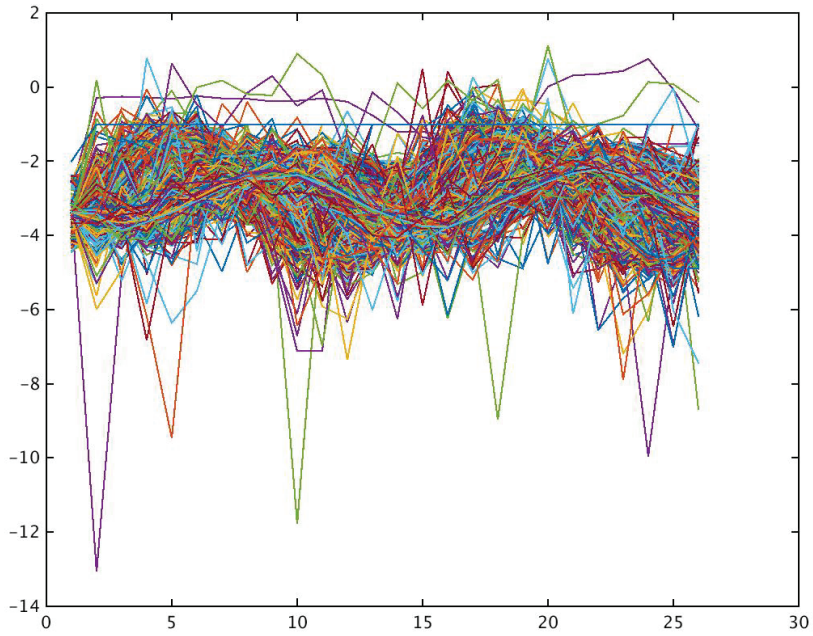


Figure 11: Height above mean sea level for 1 particle from each release point over 26 hours – including 3D advection and horizontal diffusion, fixed depth, no vertical diffusion (sea lice larvae behaviour)

Table 4: Particle Tracking Runs. Total run time (estimated) = 22.5 days

Biology	Season	Start date	Dura-tion	Scoring	Number of particles	Physics	Estimated run time (on 10 processors)
Sea-lice larvae	Spring	1 April	15 days	Hours 121-360	975 x 100 (3m)	Advection plus horizontal diffusion	1.4 days
"	Summer	1 July	10 days	Hours 81-240	975 x 100 (3m)	Advection plus horizontal diffusion	0.94 days
"	Autumn	1 October	15 days	Hours 121-360	975 x 100 (3m)	Advection plus horizontal diffusion	1.4 days
"	Winter	1 January	18 days	Hours 145-432	975 x 100 (3m)	Advection plus horizontal diffusion	1.7 days
Viruses ISAV + IPNV	Spring	1 April	30 days	All (1^{st} 3 days for ISAV)	975 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion	4.9 days
"	Summer	1 July	17 days	All (1^{st} 3 days for ISAV)	975 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion	2.4 days
"	Autumn	1 October	31 days	All (1^{st} 3 days for ISAV)	975 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion	4.9 days
"	Winter	1 January	35 days	All (1^{st} 3 days for ISAV)	975 x 150 (S, M, B)	Advection plus horizontal and vertical diffusion	4.9 days

○ Post-processing of particle tracking output

The output from the particle tracking (in 'runname'_LAG.nc) can be processed in various ways e.g. to plot tracks. The variables in this file are shown in Table 5. The dimensions of the main arrays are *nlag* (or *np* = number of particles) and time (or *nt* = number of output times). In general we just use *x, y* and *z* at each time to identify the particle location (in OS grid coordinates) and metres below the surface. In order to plot the particle tracks on the model grid use the following Matlab commands:

```
cd ‘run’\output\FVCOM_particle_tracking\output\combined
xp=ncread('Jan01\January_LAG.nc','x');
yp=ncread('Jan01\January_LAG.nc','y');
cd ../../../FVCOM_output/Combined
x=ncread('January/Jan_01.nc','x');
y=ncread('anuary/Jan_01.nc','y');
plot(x,y,'.')
hold on
np=size(xp,1);
nt=size(xp,2);
for n=1:np
   plot(xp(n,1:nt),yp(n,1:nt),'g-');
end
```

Table 5: Particle tracking output variables

Variable name	Long name	Dimensions	Units
time	Time	time	seconds
label	particle label	nlag	--
x	particle x position	nlag, time	metres
y	particle y position	nlag, time	metres
z	particle z position	nlag, time	metres
u	particle u velocity	Node	cm/s
v	particle v velocity	nlag, time	cm/s
omega	particle w velocity	nlag, time	mm/s
elev	surface elevation above particle	nlag, time	metres
depth	bottom depth at particle	nlag, time	metres
indomain	particle indomain (1)	nlag, time	--
inwater	particle inwater (1)	nlag, time	--

In the next section we discuss how to calculate the particle capture and connectivity indices.

○ Connectivity Indices

The final step is construction of Connectivity Indices between the FMAs. The likelihood of larval exchange between FMAs is represented using the following matrices:

- Distance matrix of the separation of individual Management Areas: this can be easily calculated as a straight line distance but will be less than the actual seaway distance that must be travelled.
- Transitional Probability Matrix P_{ij} (hereafter termed the Connectivity Matrix) representing the probability that an individual particle released at the source *i* will disperse to the destination *j*, over a given period of time.

The method of calculation of P_{ij} is as follows:

- Capture all particles which are 'infective' at each FMA downstream of original release FMA (includes self-recruitment). For sea lice this means capturing particles during the last ⅔ of the tracking period. For ISAV the capture period is the first 3 days of the virus run. For IPNV the whole of the virus tracking period is used. A 3-D array has been produced, named *inxy_<mmm>_<bb> (np,nf,nh),* for each month (*mmm*) and both sea lice and virus runs (*bb*= *sl* or *vr*). The dimensions are *np* (number of released particles), by *nf* (number of target FMAs) and *nh* (number of hours). From this matrix various outputs can be calculated.
- Sum over all particles starting in each origin FMA to get an 86x86 array containing numbers of particles, at each hour of the tracking period.
- Normalise by number of release points within each FMA to give a percentage of points released which are captured within any target FMA at any time.
- Finally, decide on how to plot array e.g. whole period, final destination. An alternative is to flag each FMA reached from origin FMA i.e. one or zero is recorded depending on whether a particle does or does not reach a given FMA from a specific starting FMA.

The scripts which have been used for the capture of particles and calculation of connectivity matrices are listed in Table 4. These are located in 'root'/output/FVCOM_particle_tracking /output/combined/scripts. The *inxy*.mat* files are located in the same directory.

Table 4: Scripts for particle connectivity calculations

Matlab Script	Purpose
FMA_capture_Jan_sl.m	Capture sea lice particles from January run
FMA_capture_Jan_vr.m	Capture virus particles from January run
FMA_capture_Apr_sl.m	Capture sea lice particles from April run
FMA_capture_Apr_vr.m	Capture virus particles from April run
FMA_capture_Jul_sl.m	Capture sea lice particles from July run
FMA_capture_Jul_vr.m	Capture virus particles from July run
FMA_capture_Oct_sl.m	Capture sea lice particles from October run
FMA_capture_Oct_vr.m	Capture virus particles from October run
Connectivity_sl.m	Calculate and plot connectivity matrices for sea lice runs
Connectivity_vr.m	Calculate and plot connectivity matrices for virus runs

• Results

This section presents plots of examples of the particle tracks and of the connectivity matrices.

○ FMA separation and connectivity matrices

Not all of the FMAs contain a salmon farm – some are historical and represent old/disused other marine sites – but have been kept in case the licences are re-established. The separation matrix is available as a spreadsheet.

The maximum separation between FMAs (taken as a simple direct separation using plane geometry) is 662 km, between the southern FMA on the mainland and the north of Shetland. From the climatology run the residual currents near the shelf edge are directed towards the NE and have a maximum velocity of 25cm/s, generally much smaller residual currents will be present nearshore, where the FMAs are located. At 25cm/s a distance of 324km could be covered in 15 days, however much smaller distances are more likely. At this time the results are for examined for the probability of a particle moving from one FMA to any other (including self-recruitment).

Figure 12 shows particle tracks for the January 35-day virus runs where the particles are released at surface, mid-depth and bottom. Each panel represents a sub-division of all the particles between 10 processors (as discussed in section 5.2.2). The first 9 processors have been used to each calculate 15,000 particle tracks; 150 particles

released at 100 different release locations for each case. The 10th processor tracked the remaining released particles (making a total of 146,550 particles). A final run was carried out for 3 release points (450 particles) which were not moving within the grid. The surface releases are shown in red, mid-depth are green and bottom are black. The tracks for particles released at different levels do not differ substantially, apart from the random walk component, because the particles move freely through the water column, unlike the sea lice larvae which are constrained to stay in the surface layer.

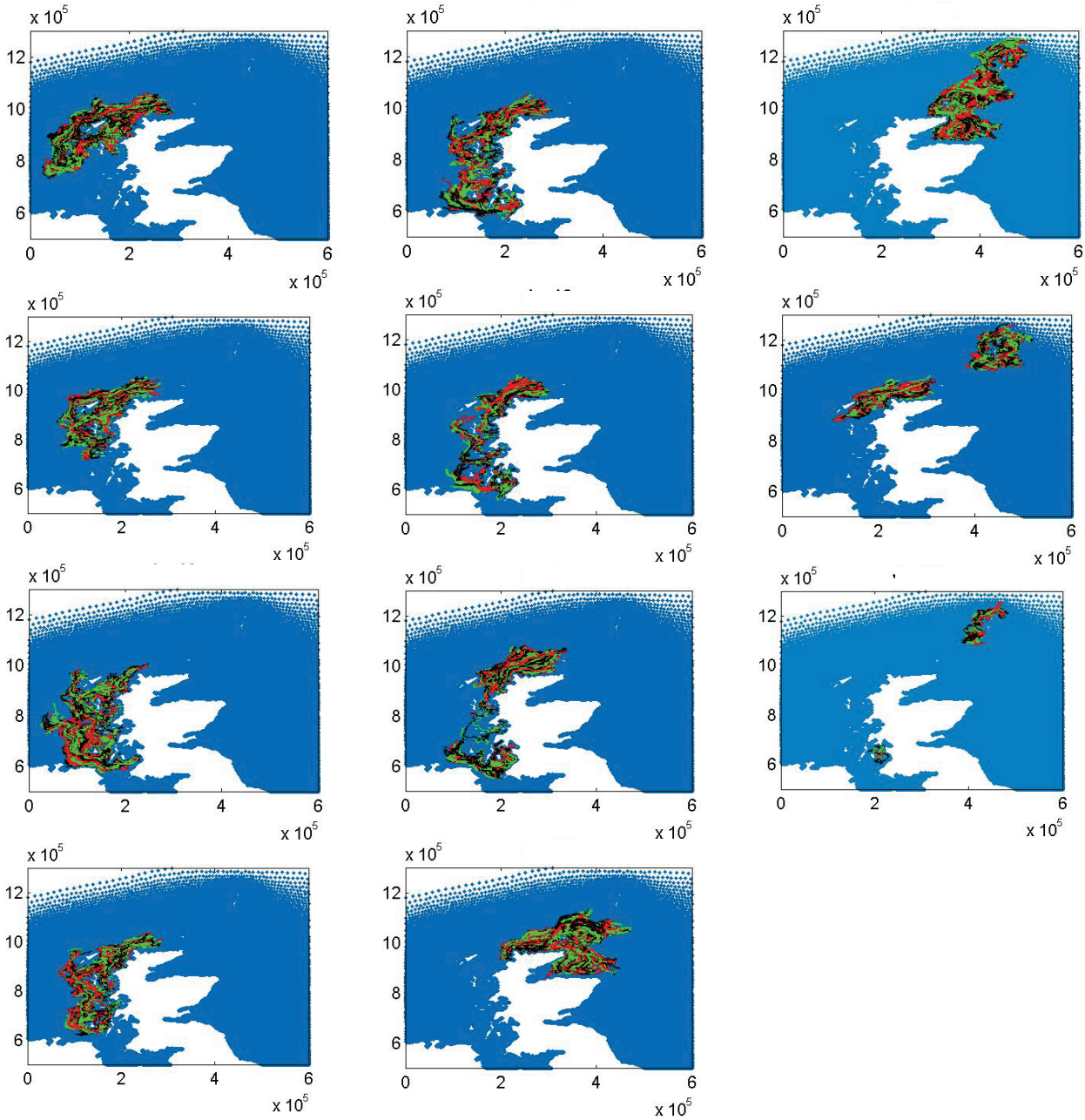


Figure 12: Particle Tracks for the January 35-day virus runs: red = surface release; green = mid-depth release; black = bottom release

○ Sea Lice Connectivity

Figures 13-16 show different plots of the connectivity matrix for the sea lice runs for each season: January, April, June and October. The left hand panel plots the probability of a particle being found in FMA j, from original release at FMA i. The right hand size is the mean probability of capture over the whole infectious period. The colour bar is in 10% intervals. It may be seen that most coloured pixels lie on the diagonal, representing self-recruitment. A few particles move to an adjacent FMA.

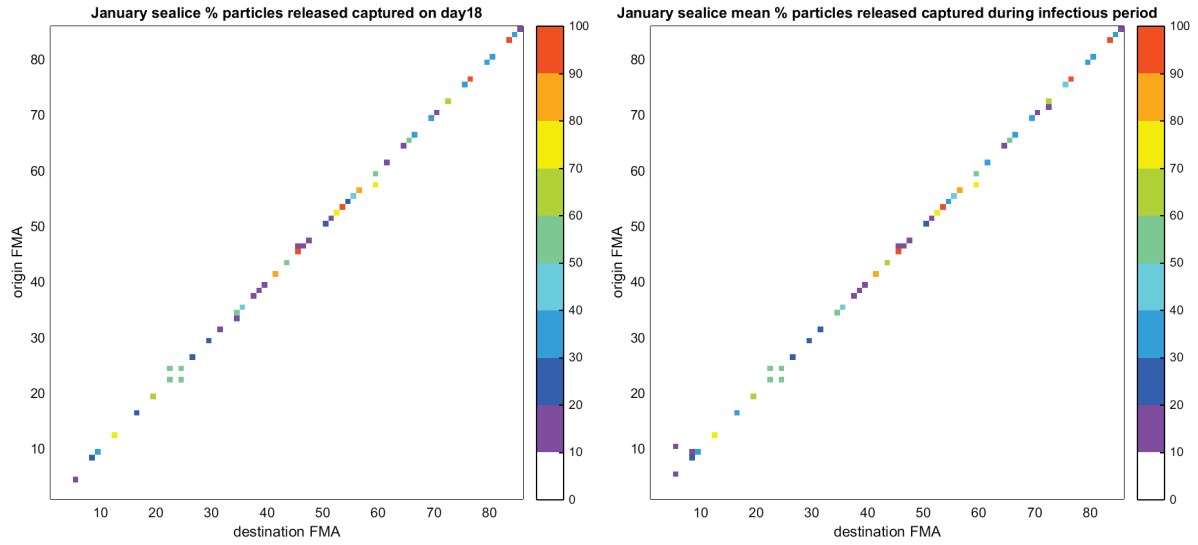


Figure 13: January sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period

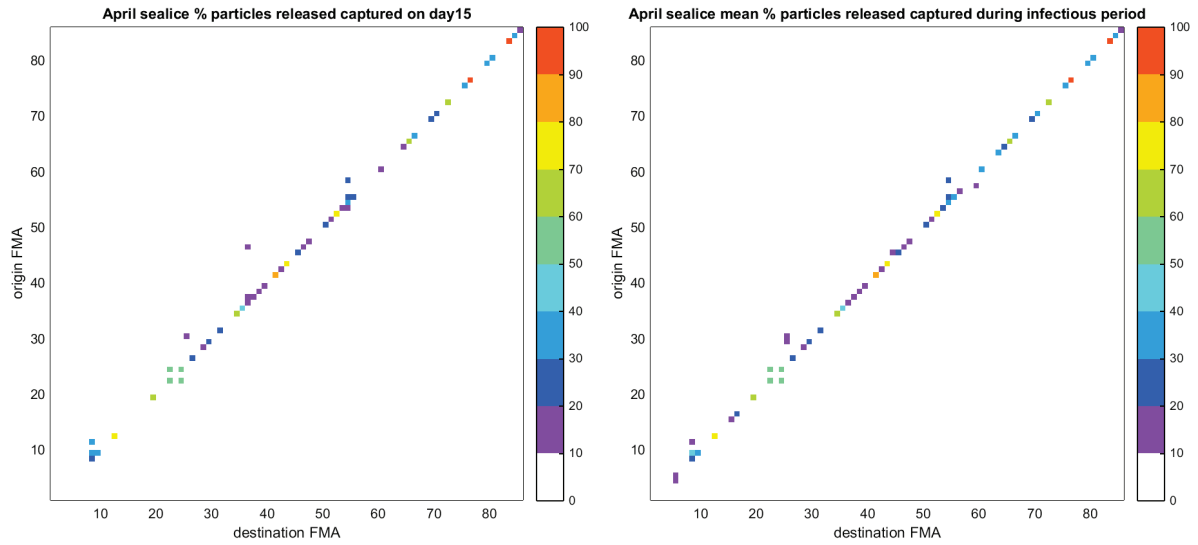


Figure 14: April sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period

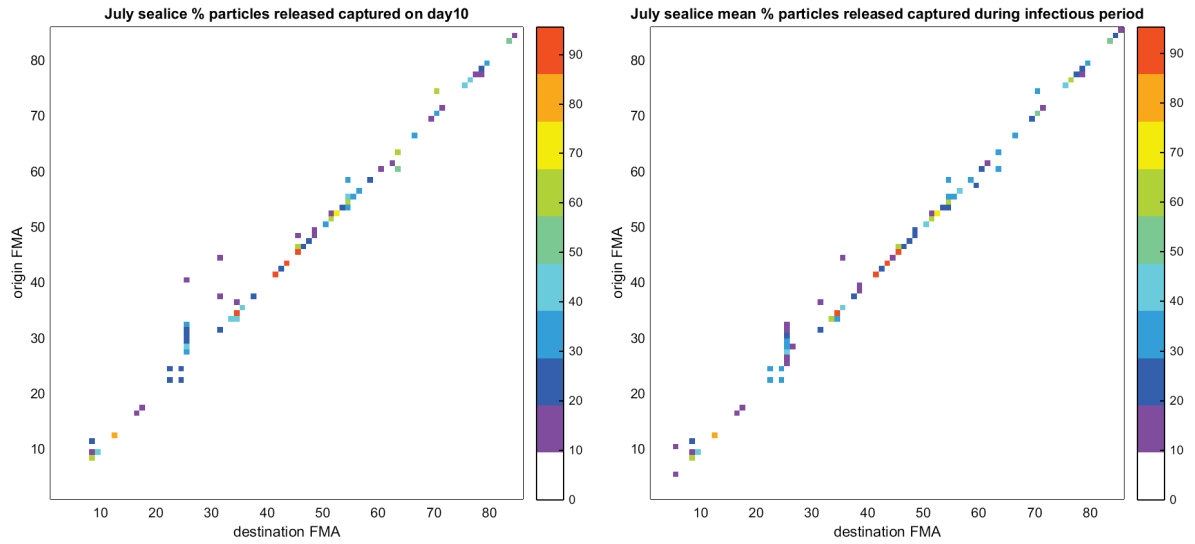


Figure 15: July sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period

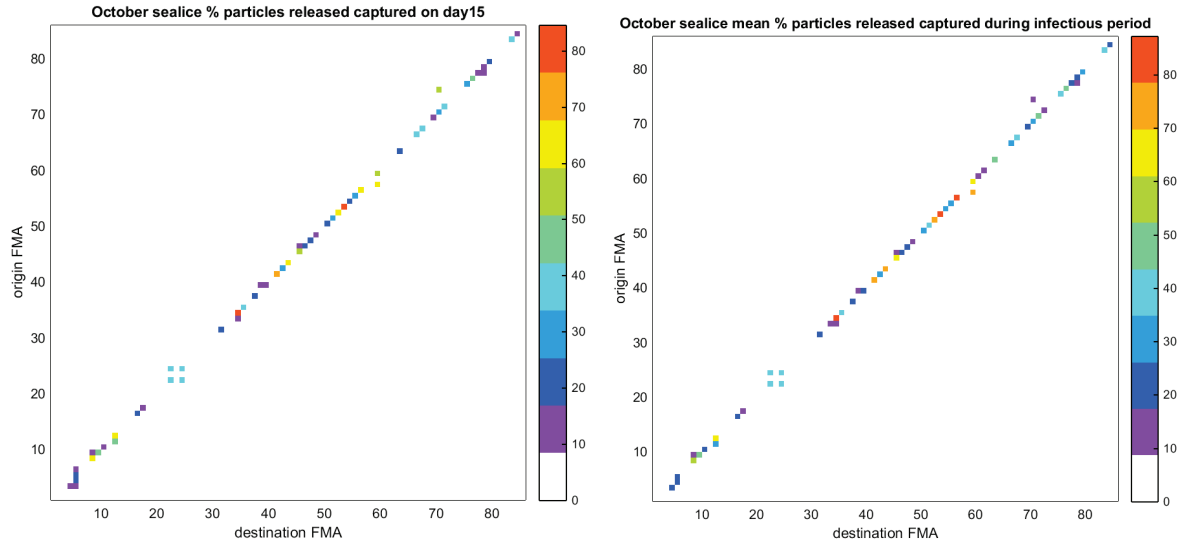


Figure 16: October sea lice connectivity indices: left panel - end of run; right panel - mean over infectious period

Particles appear to move further from their original positions in July and least far in January, despite the fact that the January tracking period is longest and July the shortest.

Figure 17 shows the 0/1 flags indicating whether there is at least one particle captured at the target from the origin FMA, over the whole period. This is more sensitive to only a few particles being captured than the previous figures so it can be seen that seen that there is some exchange between the Inner Hebrides (FMA numbers ~40-50) and the Western Isles (64-86) which are adjacent areas with similar latitude.

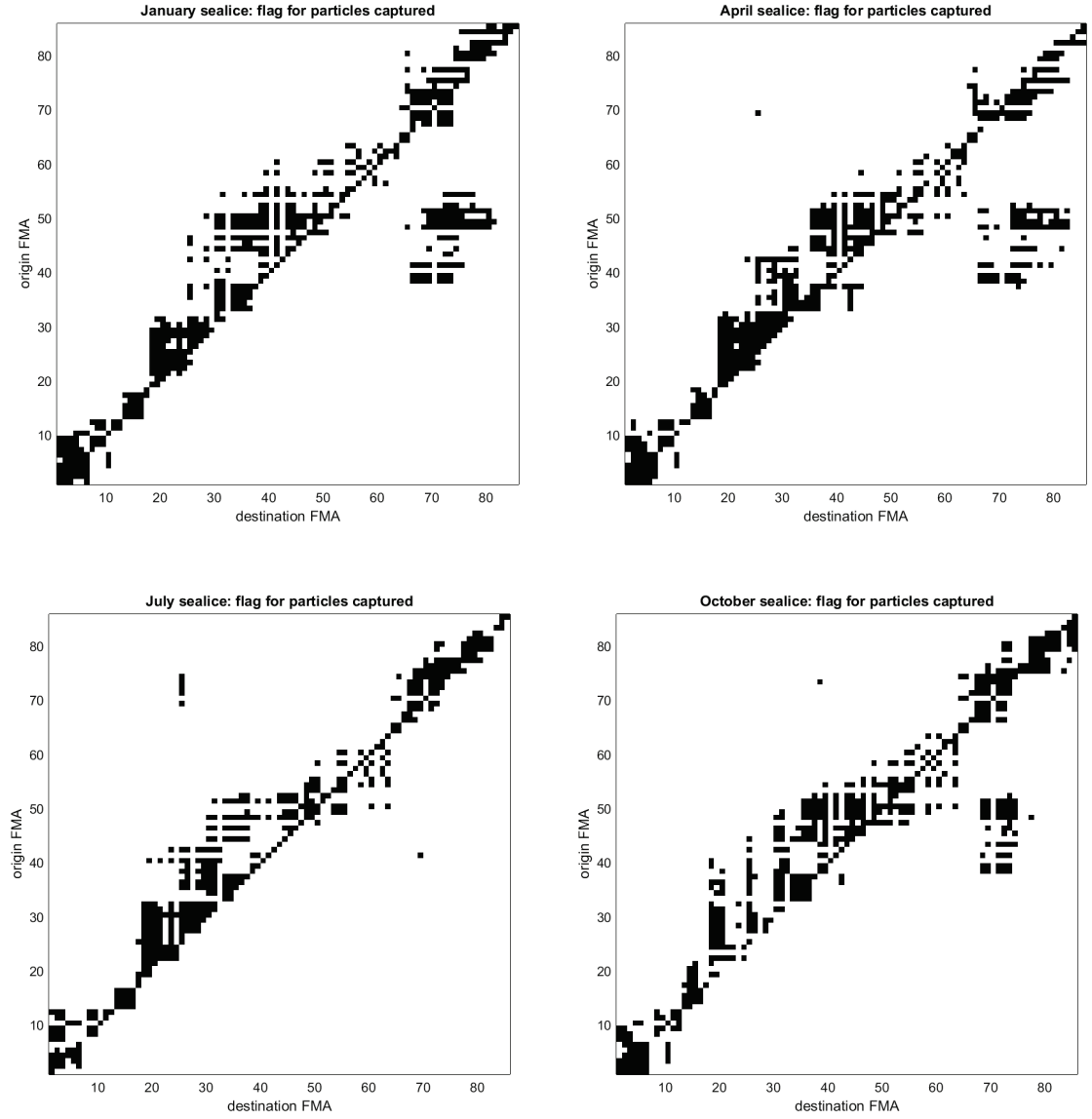


Figure 17: Connectivity flags for sea lice: top left – January; top right – April; bottom left – July; bottom right - October

○ Virus Connectivity

▪ ISA Virus

The following figures show results for the 1st 3 days of the virus-tracking period, representing the viable infective period of the ISA virus. This is a very short duration virus so less connectivity between adjacent areas is seen.

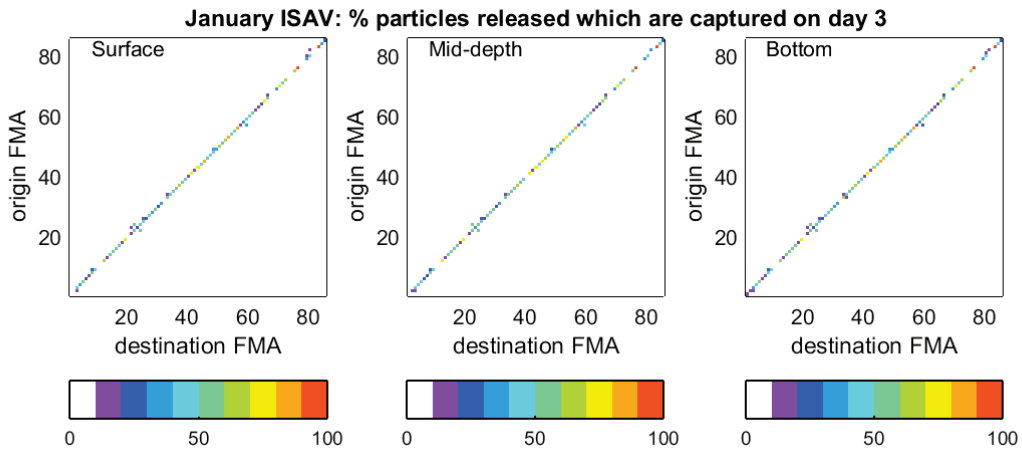


Figure 18: January ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

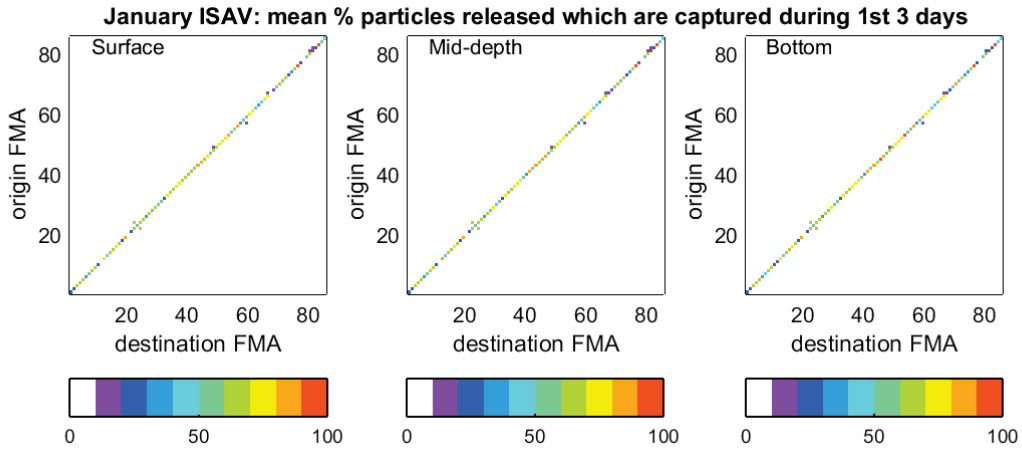


Figure 19: January ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

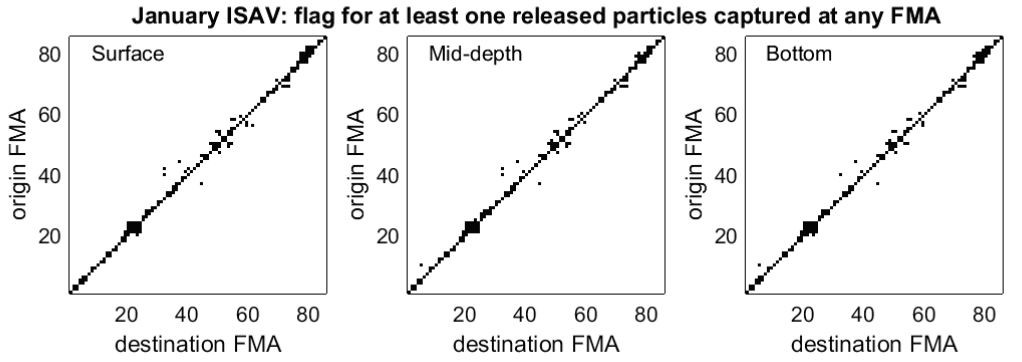


Figure 20: January ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

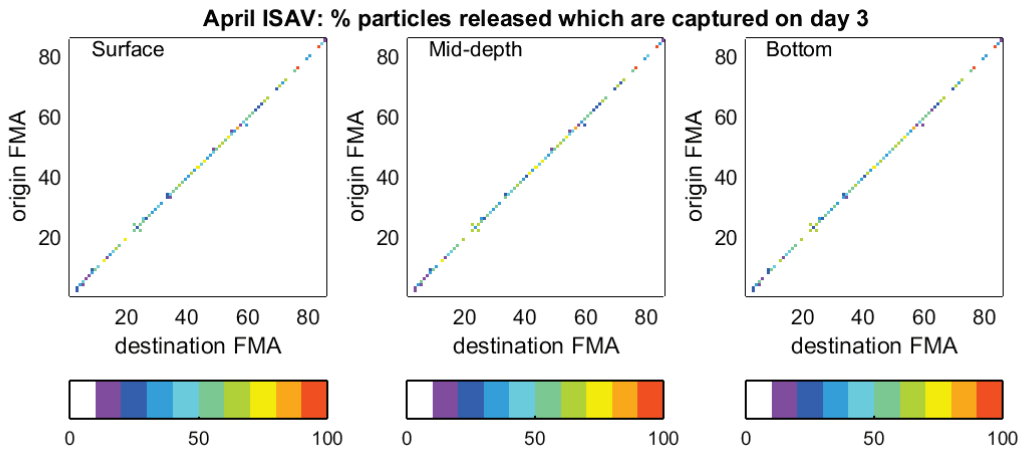


Figure 21: April ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

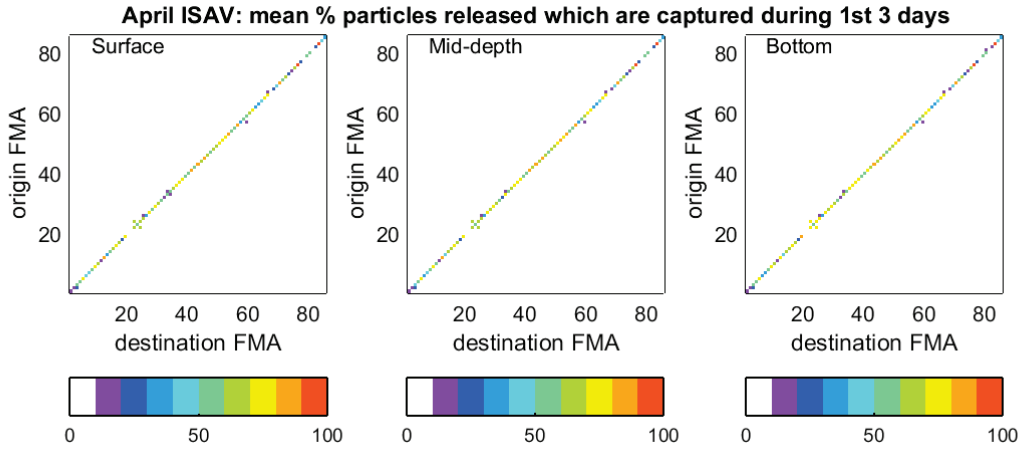


Figure 22: April ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

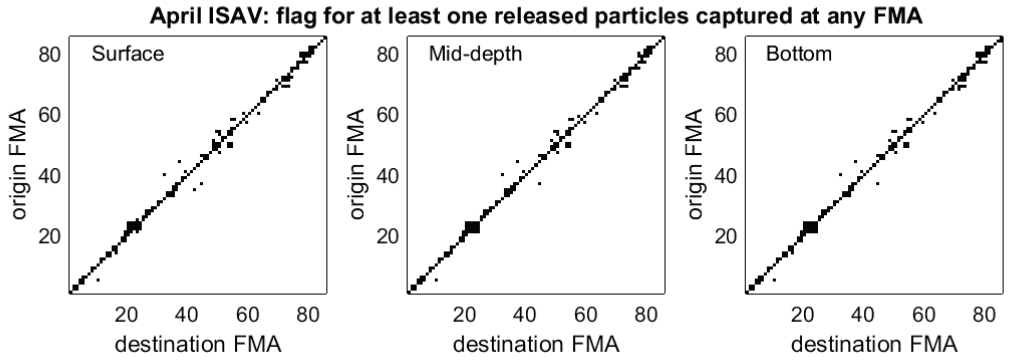


Figure 23: April ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

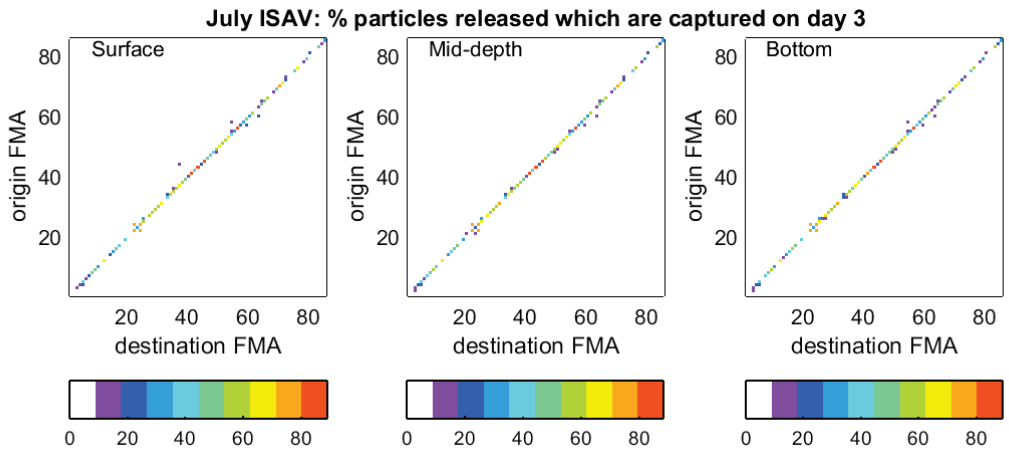


Figure 24: July ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

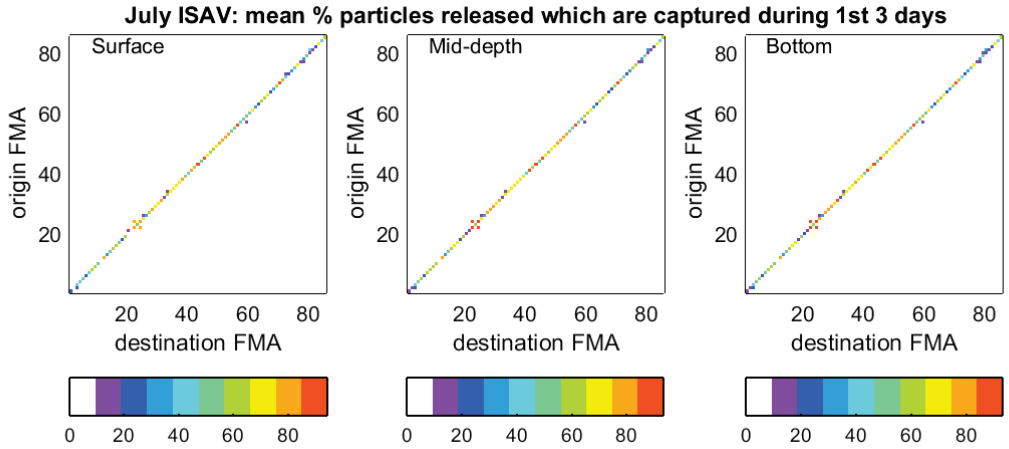


Figure 25: July ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

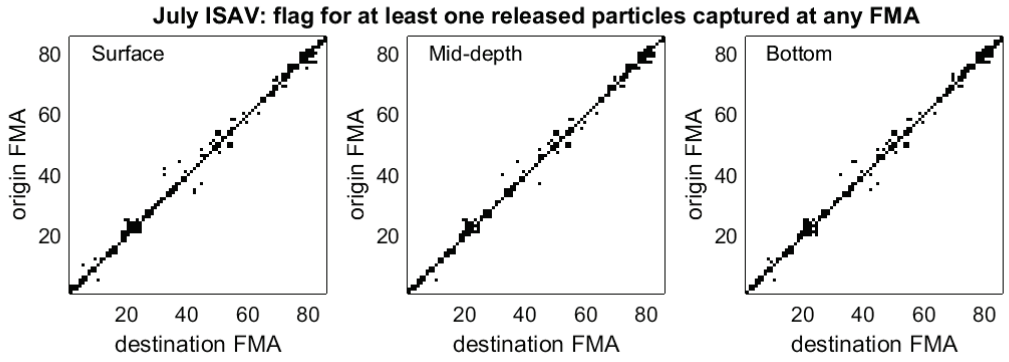


Figure 26: July ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

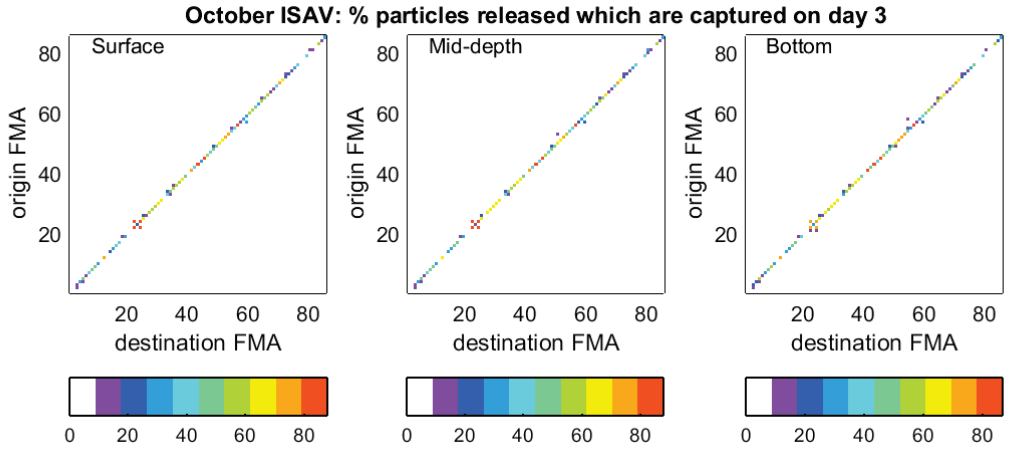


Figure 27: October ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

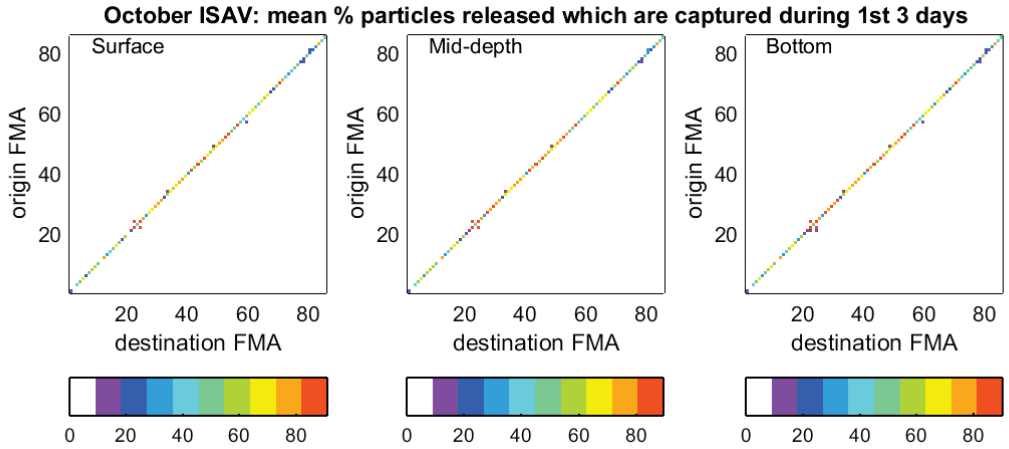


Figure 28: October ISAV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

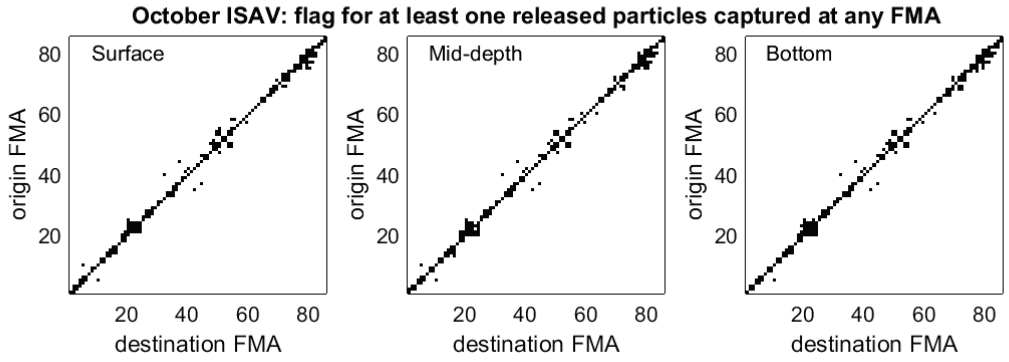


Figure 29: October ISAV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

- IPN Virus

The following figures show results for the whole of the virus-tracking period, representing the viable infective period of the IPN virus. Due to the longer duration there is more connectivity, similar to the sea lice tracks. It may be seen that there is little difference between particle releases at surface, mid-depth or bottom.

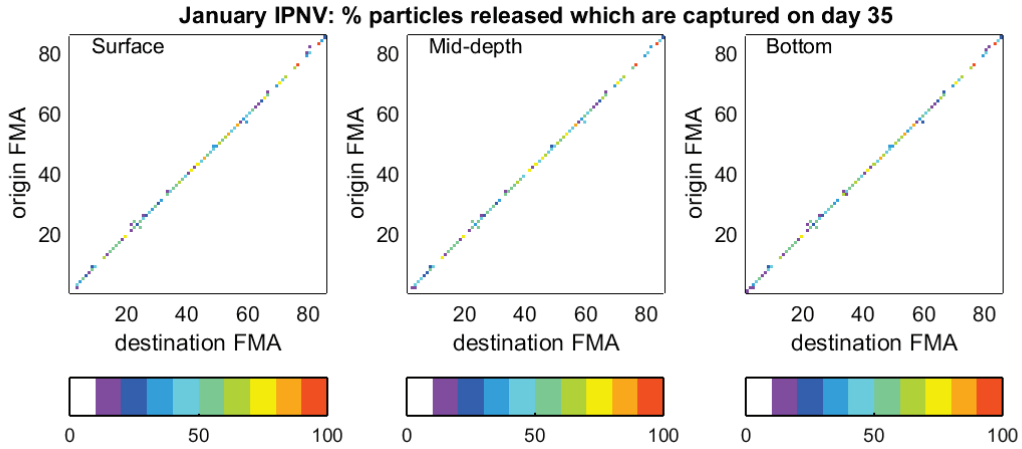


Figure 30: January IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

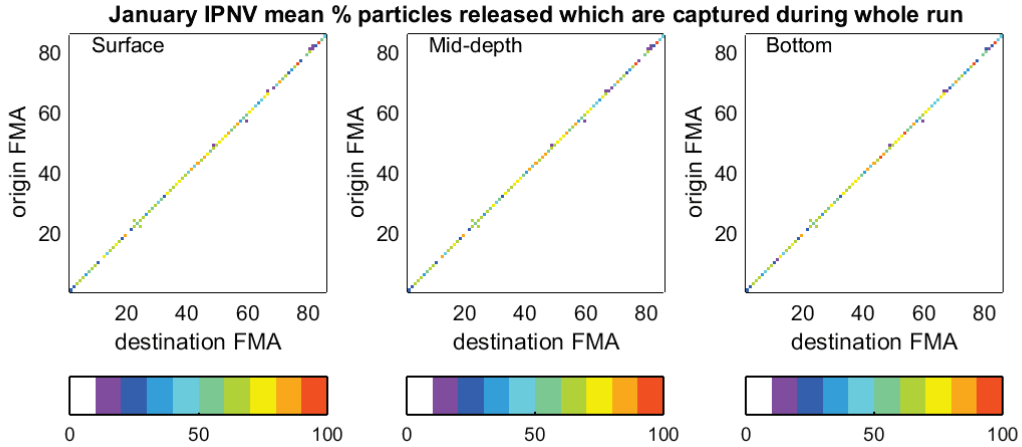


Figure 31: January IPNV connectivity indices: left panel – surface; centre - mid-depth; right – bottom

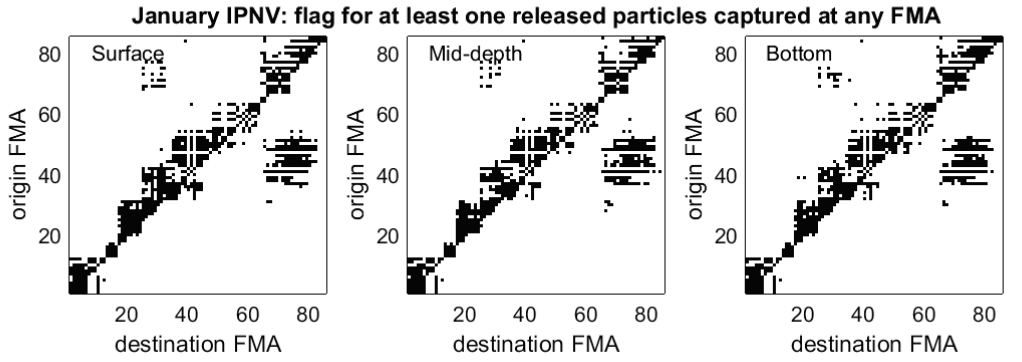


Figure 32: January IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

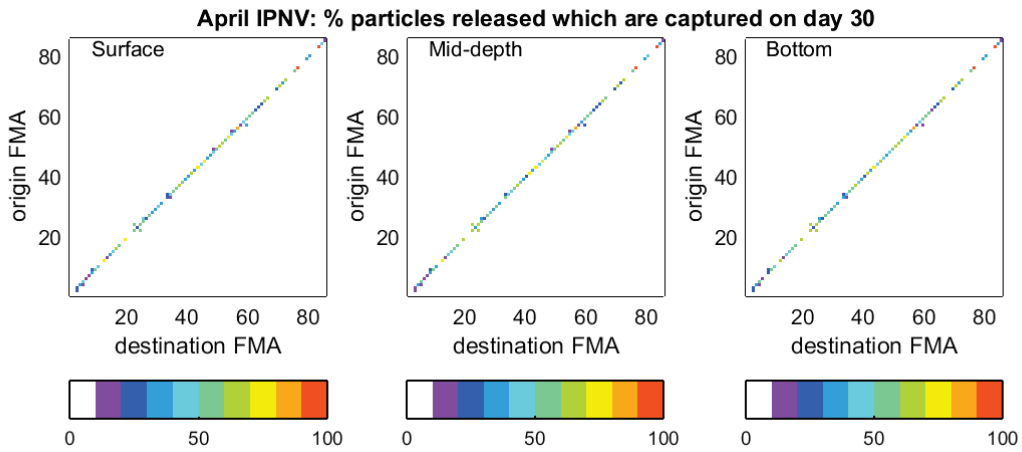


Figure 33: April IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

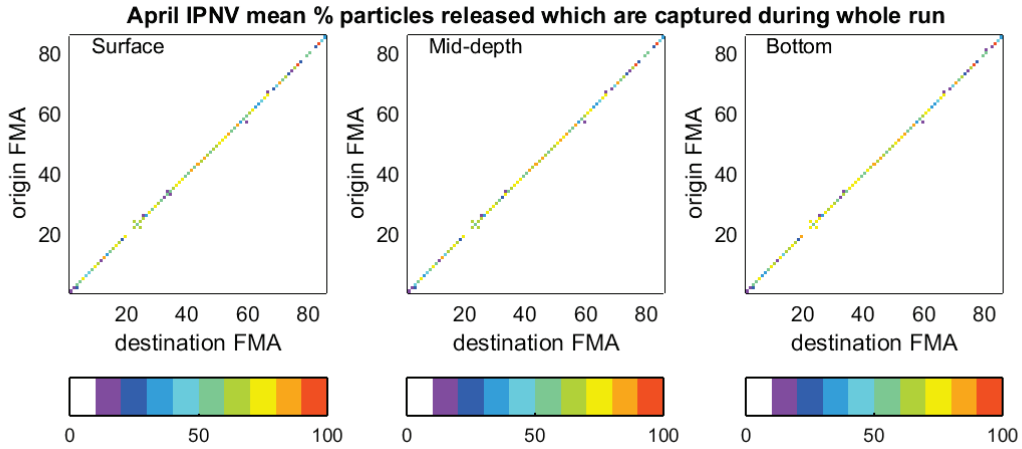


Figure 34: April IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

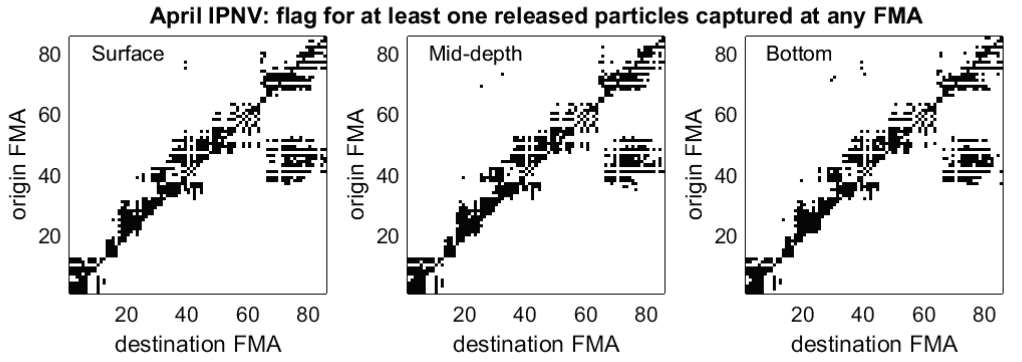


Figure 35: April IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

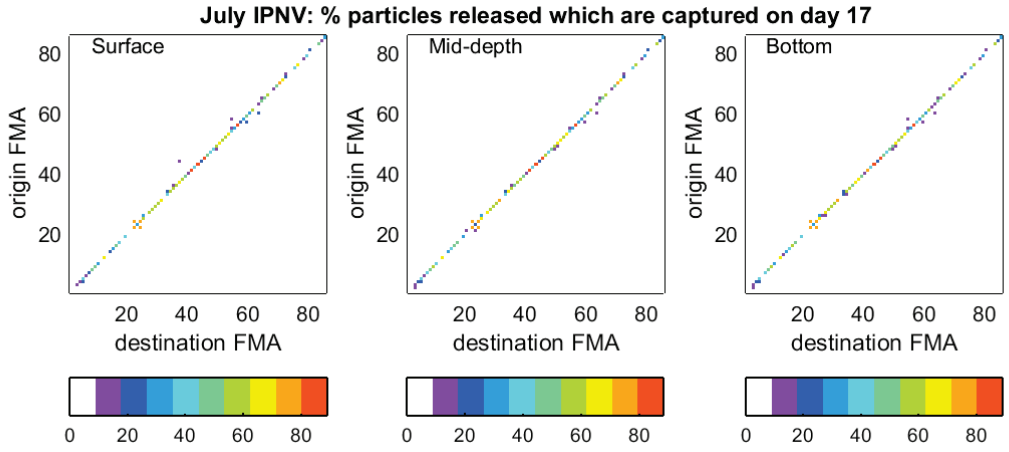


Figure 36: July IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

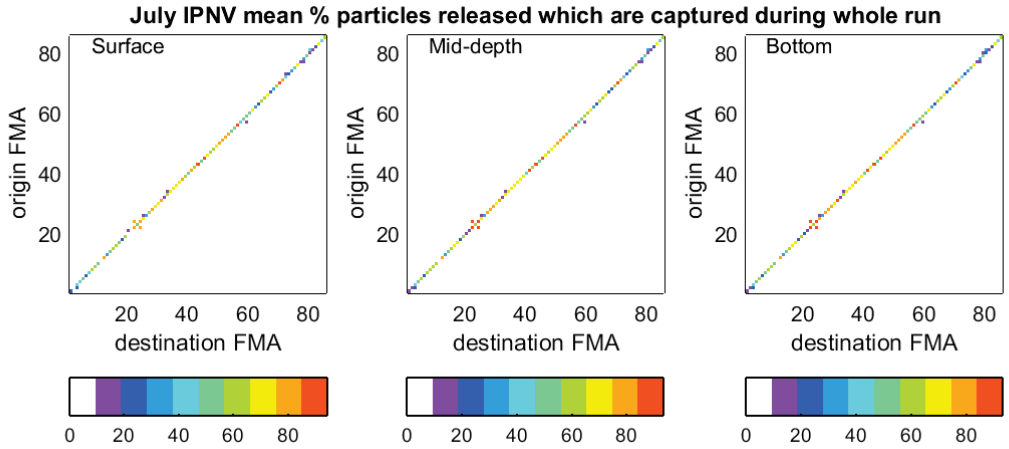


Figure 37: July IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

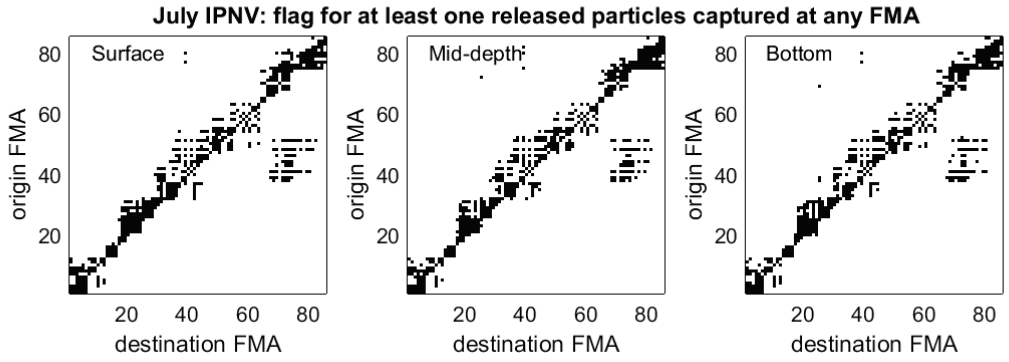


Figure 38: July IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

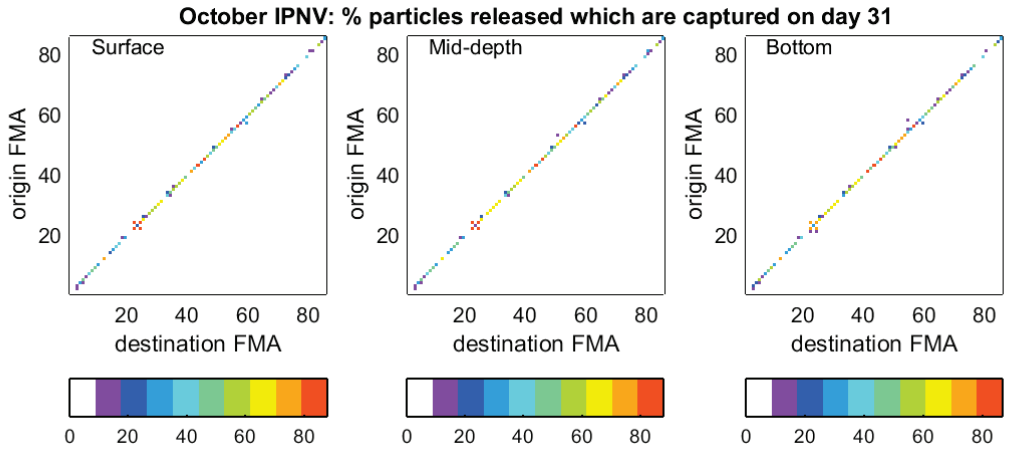


Figure 39: October IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

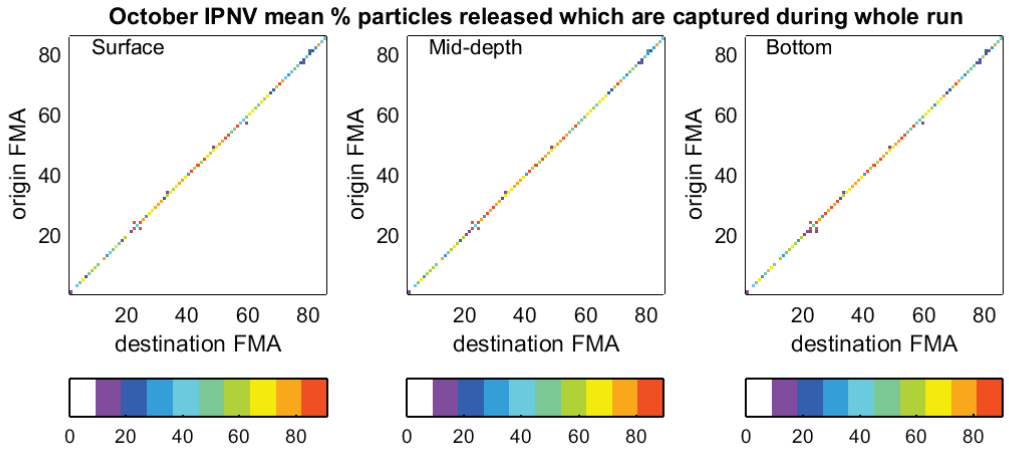


Figure 40: October IPNV connectivity indices: left panel – surface; centre - mid-depth; right - bottom

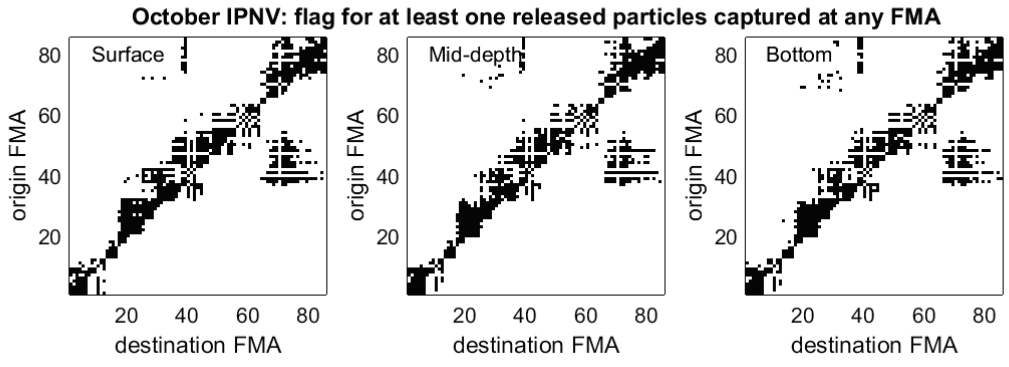


Figure 41: October IPNV connectivity flags: left panel – surface; centre - mid-depth; right - bottom

Summary

Particle tracking has been carried out for 4 seasons and different biological behaviour, representing 3 different organisms: sea lice, ISA virus and IPN virus. Multiple particles have been released at each of 86 FMAs and tracked for different durations, identifying when the particles remain in the original FMA or arrive at a new FMA. Connectivity indices have been calculated using different methods

- ## Recommendations for future work

There are some outstanding issues which could be discussed further but these are outside the scope of the present work:

6. How do wild salmon influence dispersion of sea lice?
7. What about the wall effect mentioned in several papers about particle dispersion e.g. Amundrud and Murray (2007; 2009)? Some rules may be applied when the particle comes close to land. There is no rule applied in the FVCOM offline particle tracking code.
8. The effect of winds will not be as strong as likely under certain wind events, as we are only including monthly mean wind stress in model climatology.

There are potential improvements to the particle tracking code which could be made relatively easily

1. Implement the option for lat/lon model output (Dmitry Aleynik has already produced code with this fix, which could be adopted).
2. Jim Clark (Plymouth Marine Laboratory) has provided a modified code in September 2015 – adding a local search for velocity elements to yield a substantial speed up in run times.
3. Another suggestion is to speed up the I/O by reading a whole daily file at once rather than hour by hour (this will have memory implications however).
4. Remove the hard-coded year number of *offlag.f90*.
5. Allow particle tracking to go beyond the year end and cross boundaries between April/May and October/November (latter is due to only 2 nested models being run for whole year so combined grid changes size).

References

Adams, T. P., Aleynik, D.L. and Burrows, M. T. (2014) Larval dispersal of intertidal organisms and the influence of coastline geography. Ecography 37: 001–013. dx.doi.org/10.1111/j.1600-0587.2013.00259.x

Adams, T. P., Miller, R.G., Aleynik, D.L. and Burrows, M. T. (2014) Offshore marine renewable energy devices as stepping stones across biogeographical boundaries. Journal of Applied Ecology, doi: 10.1111/1365-2664.12207.

Aldrin, M., Storvik, B., Kristoffersen, A. B. and Jansen, P. A. (2013) Space-Time Modelling of the Spread of Salmon Lice between and within Norwegian Marine Salmon Farms. PLoS ONE 8(5): e64039. doi:10.1371/journal.pone.0064039

Amundrud T.L. and Murray A.G. (2007) Validating particle tracking models of sea lice dispersion in Scottish Sea Lochs. ICES CM B05, 12.

Amundrud, T L and Murray, A G (2009) Modelling sea lice dispersion in a Scottish sea loch. Journal of Fish Diseases, 32, 27–44.

Brickman, D., and Smith, P. (2002) Lagrangian stochastic modeling in coastal oceanography. Journal of Atmospheric and Oceanic Technology, 19, 83 – 99.

Chen, C., Beardsley, Cowles, R.C.G., Qi, J., Lai, Z., Gao, G. Stuebe, D., Xu, Q., Xue, P. Ge, J., Hu, S., Ji, R., Tian, R., Huang, H., Wu, L., Lin, H., Sun, Y. and Zhao, L. (2013) FVCOM User Manual, SMAST/UMASSD-13-0701, 416pp.

Cowen, R.K. and Sponaugle, S. (2009) Larval Dispersal and Marine Population Connectivity, Annual Review of Marine Science, 1, 443–66.

Forward, R. B. and Tankersley, R. A. (2001) Selective tidal-stream transport of marine animals. In

Gallego, A., Gibb, F.M., Tulett, D. and Wright, P.J. (2013) Connectivity of Benthic Priority Marine Species within the Scottish MPA Network. Scottish Marine and Freshwater Science, 4, 02.

Gallego, A., North, E.W. and Petitgas, P. (2007) Introduction: status and future of modeling physical-biological interactions during the early life of fishes. Marine Ecology Progress Series, 347, 122–26.

Kingsford, M. J., Leis, J. M., Shanks, A., Lindeman, K. C., Morgan, S. G. and Pineda, J. (2002) Sensory environments, larval abilities and local selfrecruitment. Bulletin of Marine Science, 70(1, S):309–340.

McKibben, M.A. and Hay, D.W. (2004) Distributions of planktonic sea lice larvae Lepeophtheirus salmonis in the inter-tidal zone in Loch Torridon, Western Scotland in relation to salmon farm production cycles. Aquaculture Research, 35, 8, 742-750.

North, E.W., Gallego, A. and Petitgas, P. (eds) (2009) Manual of recommended practices for modelling physical−biological interactions during fish early life. ICES Coop Research Report 295

North, E.W., Schlag, Z., Hood, R.R., Li, M., Zhong, L., Gross, T., Kennedy, V.S. (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.

Murray, A.G. and Gillibrand, P.A. (2006) Modelling salmon lice dispersal in Loch Torridon, Scotland. Marine Pollution Bulletin, 53, 128–135.

Penston, M.J., McKibben, M.A., Hay, D.W. and Gillibrand, P.A. (2004) Observations on open-water densities of sea lice larvae in Loch Shieldaig, Western Scotland. Aquaculture Research, 35, 8, 793-805.

Phelps, J.J.C. (2015) Modelling Hydrodynamic Transport and Larval Dispersal in North-East Atlantic Shelf Seas. PhD thesis, Liverpool.

Phelps, J.J.C., Polton, J.A., Souza, A.J. and Robinson, L.R. (in press) Behaviour influences larval dispersal in shelf sea gyres: Nephrops norvegicus in the Irish Sea. Marine Ecology Progress Series.

Ross, O. N. and Sharples, J. (2004) Recipe for 1-D Lagrangian particle tracking models in space-varying diffusivity. Limnology and Oceanography: Methods, 2, 289-302.

Stashchuk, N., Vlasenko, V., Inall, M.E, and D. Aleynik (2014) Horizontal dispersion in shelf seas: high resolution modelling as an aid to sparse sampling. Progress in Oceanography, 128, 74–87, dx.doi.org/10.1016/j.pocean.2014.08.007

Treml, E., Roberts, J.J., Chao, Y., Halpin,P.N., Possingham, H.P. and Riginos, C. (2012) Reproductive Output and Duration of the Pelagic Larval Stage Determine Seascape-Wide Connectivity of Marine Populations. Integrative and Comparative Biology, 52, 4, 525–537, doi:10.1093/icb/ics101

Visser, A. W. (1997) Using random walk models to simulate the vertical distribution of particles in a turbulent water column. Marine Ecology Progress Series, 158, 275-281.

Appendix: Particle Tracking code

Program	PARTICLE_TRAJ	Module
Location	'root'/output/FVCOM_particle_tracking/source/	**OFFLAG.f90**
Description	This is the main program for offline particle tracking: • Read in control data • Read in model data • Read pre-calculated metrics if not first run • Calculate and save metrics if first run • Read initial particle locations • Update particle locations • Write output files	
Called from		
Subroutines and Functions called	DATA_RUN NCD_READ_GRID ALLOC_VARS NCD_READ_SHAPE NCD_READ_METRICS TRIANGLE_GRID_EDGE NCD_WRITE_METRICS SET_LAG LAG_UPDATE	DATA_RUN.f90 NCDIO.f90 ALLOC_VARS.f90 NCDIO.f90 NCDIO.f90 TRIANGLE_GRID_EDGE.f90 NCDIO.f90 OFFLAG.f90 OFFLAG.f90
User input files	'root'/output/FVCOM_particle_tracking/run/'basename'/'runname'_run.dat 'root'/output/FVCOM_particle_tracking/input/'basename'/'runname'_metrics.nc	
Model Input	'root'/output/FVCOM_particle_tracking/input/'basename'/'runname'_dddd.nc	
Output	'root'/output/FVCOM_particle_tracking/input/'basename'/'runname'_metrics.nc	

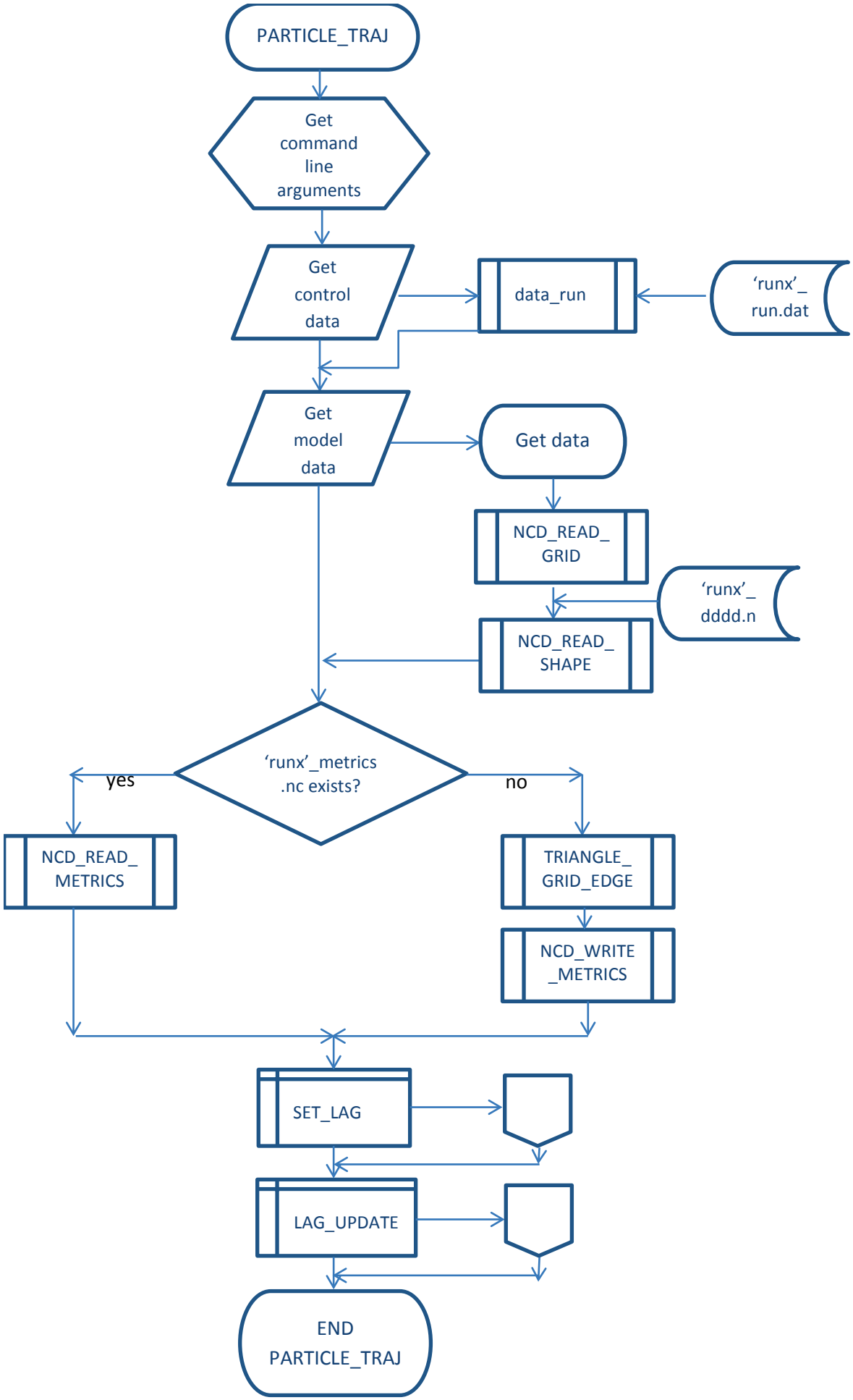
Subroutine	SET_LAG	Module
Location	'root'/output/FVCOM_particle_tracking/source/	**OFFLAG.f90**
Description	This subroutine reads initial particle positions and locates in model grid: • Reads in initial particle positions • Calculates particle locations in model grid • Writes first particle positions to output file	
Called from	PARTICLE_TRAJ	
Subroutines and Functions called	FHE_ROBUST NCD_READ INTERP_ELH NCD_WRITE	OFFLAG.f90 NCDIO.f90 OFFLAG.f90 NCDIO.f90
User input files	'root'/output/FVCOM_particle_tracking/input/'basename'/'runname'.dat	
Output	'root'/output/FVCOM_particle_tracking/output/'basename'/'dirname'/'runname'_LAG.nc	

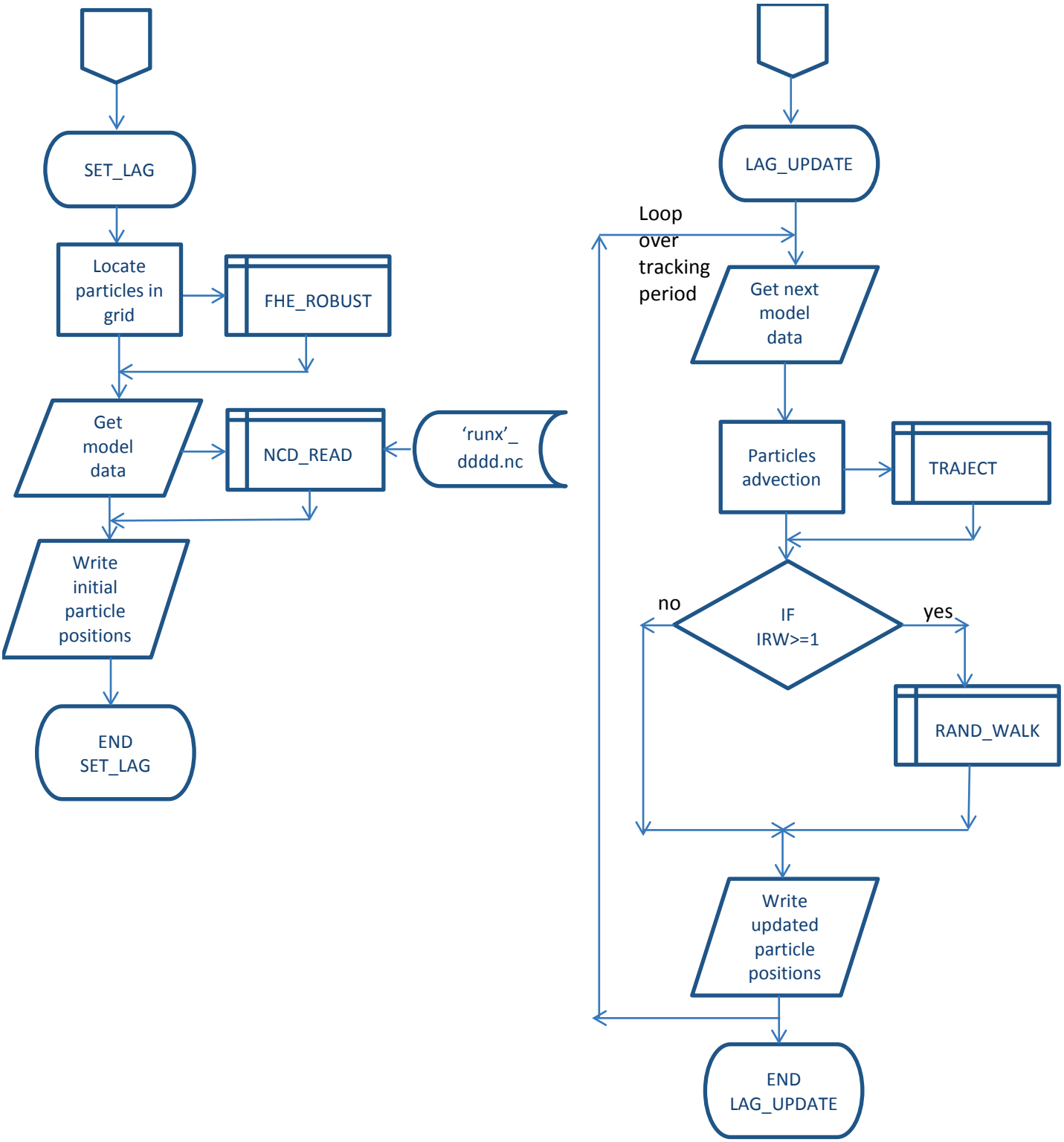
Subroutine	LAG_UPDATE	Module
Location	'root'/output/FVCOM_particle_tracking/source/	**OFFLAG.f90**
Description	This subroutine calculates new particle positions and locates in model grid: • Reads next model output • Calculates particle locations in model grid using advection and optional diffusion • Writes new particle positions to output file	
Called from	PARTICLE_TRAJ	
Subroutines and Functions called	NCD_READ TRAJECT RAND_WALK NCD_WRITE	NCDIO.f90 OFFLAG.f90 OFFLAG.f90 NCDIO.f90

Subroutine	LAG_UPDATE	Module
User input files	‘root’/output/FVCOM_particle_tracking/input/’basename’/‘runname’.dat	
Model Input	‘root’/output/FVCOM_particle_tracking/input/’basename’/’runname’_dddd.nc	
Output	‘root’/output/FVCOM_particle_tracking/output/’basename’/’dirname’/’runname’_LAG.nc	

Subroutine	TRAJECT	Module
Location	‘root’/output/FVCOM_particle_tracking/source/	**OFFLAG.f90**
Description	This subroutine calculates new particle positions and locates in model grid: • Calculates new particle positions using Runge-Kutta • Locates particles in model grid	
Called from	LAG_UPDATE	
Subroutines and Functions called	INTERP_V INTERP_ELH FHE_QUICK FHE_ROBUST	OFFLAG.f90 OFFLAG.f90 OFFLAG.f90 OFFLAG.f90
User input files	‘root’/output/FVCOM_particle_tracking/input/’basename’/‘runname’.dat	
Output	‘root’/output/FVCOM_particle_tracking/output/’basename’/’dirname’/’runname’_LAG.nc	

Subroutine	RAND_WALK	
Location	'root'/output/FVCOM_particle_tracking/source/	OFFLAG.f90
Description	This subroutine calculates horizontal and vertical random walk i.e. turbulent diffusion • Smooths vertical diffusivity KH (passed from model output) • Interpolates KH and its 2nd vertical derivative using CALL spline (see Ross and Sharples, 2004) • Calculates horizontal random walk • Calculates vertical random walk	
Called from	LAG_UPDATE	
Subroutines/ Functions called	Spline INTERP_ELH FHE_QUICK FHE_ROBUST	UTILS.f90 OFFLAG.f90 OFFLAG.f90 OFFLAG.f90
User input files	'root'/output/FVCOM_particle_tracking/input/'basename'/'runname'.dat	
Output	'root'/output/FVCOM_particle_tracking/output/'basename'/'dirname'/'runname'_LAG.nc	


PARTICLE_TRAJ
Get command line arguments
Get control data
data_run
'runx'_ run.dat
Get model data
Get data
NCD_READ_ GRID
'runx'_ dddd.n
NCD_READ_ SHAPE
'runx'_metrics .nc exists?
yes
no
NCD_READ_ METRICS
TRIANGLE_ GRID_EDGE
NCD_WRITE _METRICS
SET_LAG
LAG_UPDATE
END PARTICLE_TRAJ


SET_LAG
Locate particles in grid
FHE_ROBUST
Get model data
NCD_READ
'runx'_ dddd.nc
Write initial particle positions
END SET_LAG
LAG_UPDATE
Loop over tracking period
Get next model data
Particles advection
TRAJECT
no
IF IRW>=1
yes
RAND_WALK
Write updated particle positions
END LAG_UPDATE

© Crown copyright 2016

OGL

This publication is licensed under the terms of the Open Government Licence v3.0 except where otherwise stated. To view this licence, visit **nationalarchives.gov.uk/doc/open-government-licence/version/3** or write to the Information Policy Team, The National Archives, Kew, London TW9 4DU, or email: **psi@nationalarchives.gsi.gov.uk**.

Where we have identified any third party copyright information you will need to obtain permission from the copyright holders concerned.

This publication is available at **www.gov.scot**

Any enquiries regarding this publication should be sent to us at
The Scottish Government
St Andrew's House
Edinburgh
EH1 3DG

ISBN: 978-1-78652-009-8 (web only)

Published by The Scottish Government, February 2016

Produced for The Scottish Government by APS Group Scotland, 21 Tennant Street, Edinburgh EH6 5NA
PPDAS63356 (02/16)