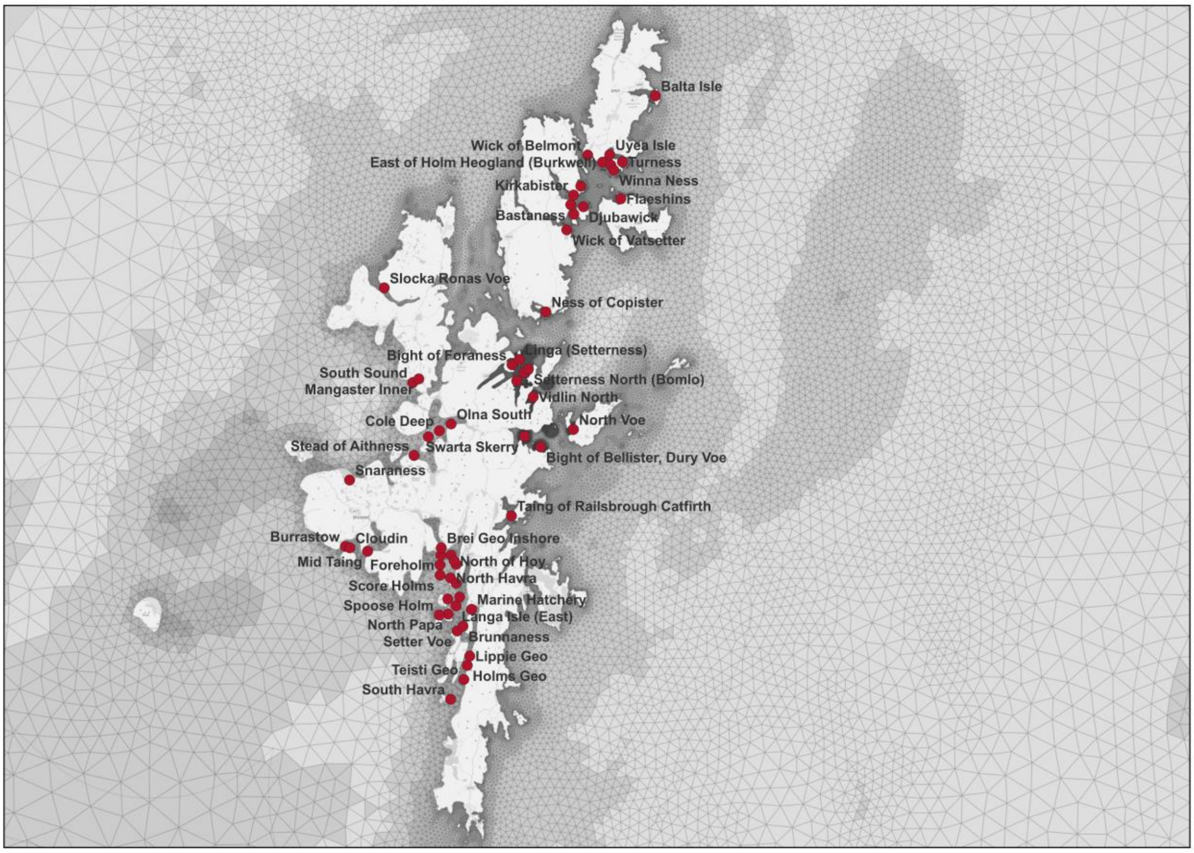
East of Shetland Aquaculture Modelling

Hydrodynamic Climatology and Hindcast Models

Model Setup Report



Scottish Sea Farms

Report

June 2023

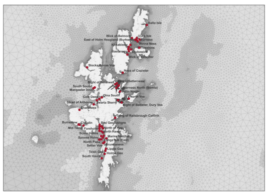
The expert in WATER ENVIRONMENTS

East of Shetland Aquaculture Modelling

Hydrodynamic Climatology and Hindcast Models

Model Setup Report

Prepared for Scottish Sea Farms Ltd.
Represented by [redacted] (Scottish Sea Farms Ltd.)



Area of interest and computational mesh of East of Shetland hydrodynamic model

[redacted]

Project number	26801744_WP003
Approval date	15th June 2023
Revision	Final 1.1 – 15th September 2023 : Minor typos/corrections from SSF Final 1.0 – 15th June 2023 : Final comments from SSF
Classification	**Restricted**

DHI WATER ENVIRONMENTS (UK) LTD • Ocean Village Innovation Centre • Ocean Way • SO14 3JZ
Southampton • United Kingdom
Telephone: +44 (0)2380 381961 • www.dhigroup.com
Company Reg. No.: 07890711

CONTENTS

FIGURES

TABLES

APPENDICES

NOMENCLATURE

Abbreviations	
CD	Chart Datum
DTM	Digital Terrain Model
ECMWF	European Centre for Medium-Range Weather Forecasts
EMODnet	European Marine Observation and Data Network
FM	Flexible Mesh
FVCOM	Finite-Volume Community Ocean Model
HD	Hydrodynamic
HWS	High water shoreline
IOS	Institute of Oceanographic Sciences
LAT	Lowest Astronomical Tide
MPFF	Marine Pen Fish Farm
MSL	Mean-Sea-Level
OGL	Open Government License
OS	Ordnance Survey
PSU	Practical Salinity Unit
RANS	Reynolds Averaged Navier-Stokes
SEPA	Scottish Environment Protection Agency
SSF	Scottish Sea Farms
SSM	Scottish Shelf Model
TKE	Turbulent Kinetic Energy
TS	Temperature and Salinity
UKHO	United Kingdom Hydrographic Office
UTM	Universal Transverse Mercator
WGS	World Geodetic System
2D	Two-dimensional

Definitions	
Time	Times are relative to UTC
Level	Levels are relative to MSL, CD, or LAT as specified
Co-ordinate system	Horizontal datum are established using World Geodetic System 1984 (WGS 84), UTM zone 30N (EPSG code: 32630)
Direction	Wind: °N coming from and positive clockwise
	Currents: °N going to and positive clockwise

Abbreviations – Quality Indices	
N	Number of data (synchronized)
MEAN	Mean (average) values
STD	Standard deviation
BIAS	Mean difference
AME	Absolute mean error
RMSE	Root mean square error
SI	Scatter index (unbiased)
EV	Explained variance
CC	Correlation coefficient
QQ	Quantile-Quantile (line slope and intercept)
PR	Peak ratio (of Number of peak highest events)

Tidal Levels	
HAT	Highest Astronomical Tide
LAT	Lowest Astronomical Tide
MHWS	Mean High Water Spring
MHWN	Mean High Water Neap
MLWN	Mean Low Water Neap
MLWS	Mean Low Water Spring
Z_0	Mean Water Level

ACKNOWLEDGEMENT

We wish to acknowledge the generous assistance provided by the Marine Scotland Science Oceanography group for providing access to the Scottish Shelf Climatology Model and respective meteorological forcing.

Executive Summary

Scottish Sea Farms (SSF) is a leading producer of farmed Atlantic salmon throughout the Scottish Mainland, Orkney and Shetland. To support ongoing operations, site developments and regulatory applications, SSF requires a detailed numerical hydrodynamic database covering the Shetland archipelago with a particular focus on three (3) areas within the East of Shetland, namely the areas of Setterness, Vidlin and Dury Voe, which contain aquaculture sites of immediate interest.

This report describes the development of two 3-dimensional (3D) hydrodynamic climatology/hindcast model databases for the East of Shetland.

The hydrodynamic model has been established using the MIKE 3 FM modelling suite (ver.2022) developed by DHI. This numerical engine simulates the water level variations and flows in response to a variety of forcing conditions. The HD model of East of Shetland is based on a variable resolution unstructured horizontal mesh with a resolution of <200m along the coastline of the East of Shetland islands complex and identified areas of interest. The climatological model is forced by offshore boundaries and climatologically averaged meteorological conditions from the SSM hydrodynamic database and is verified against the SSM at offshore locations. The hindcast version uses boundary and initial conditions from a 3D regional solution from the Copernicus service and the DTU10 global tidal solution for the tidal component. There is significant refinement of mesh discretisation as we proceed inshore to the islands complex with spatial resolution of around 40m in the area around existing marine pen fish farms.

A climatology is constructed as a representation of the 'mean' status of hydrodynamics over a period of years. This must be accounted for during any validation of a climatology forced model against an observational measurement campaign to determine model skill based on commonly used metrics. A hindcast version $HD_{ES\_hindcast}$ was thus constructed to inform on parameterisation of model settings and verification of model solution against the available observational record.

The hydrodynamic climatology model database and the hindcast version are provided alongside this report.

1 Introduction

This report has been prepared for **Scottish Sea Farms Ltd.** (SSF) by DHI in relation to hydrodynamic modelling services for aquaculture sites in the East of Shetland. The project will establish a dedicated three-dimensional (3D) hydrodynamic numerical model inclusive of the waters around Shetland:

- A one-year hydrodynamic climatology model
- A one-year hydrodynamic reanalysis model (summer-to-summer)

This document and its accompanying appendices constitute the **hydrodynamic database (climatology/reanalysis) model** report.

1.1 Background to the study

Shetland is an archipelago of over 100 islands located approximately 200km north of mainland Scotland. The islands mark the divide between the North Atlantic Ocean (to the west) and the North Sea (to the east). The rugged 2,700km coastline is characterised by numerous inlets (voes) and bays. Shetland has an oceanic climate and the Island's economy is closely linked to the sea; the main industries being offshore oil and gas, fishing, and aquaculture.

Aquaculture produces Scotland's most valuable food export and Shetland is among the country's primary aquaculture regions, with over 180 active finfish and shellfish sites. The area is responsible for producing around one third of the Scottish farmed salmon. Scottish Sea Farms is one of the main producers of farmed salmon in Shetland. The company currently operate around 25 active fish farms, situated throughout the islands.

Operational fish farms have the potential to affect the marine environment in several ways via the release of waste materials in the form of dissolved nutrients, medicines, and particulate organic matter. The management of the risks surrounding salmon lice are also of fundamental importance to producers. Consequently, the aquaculture sector is highly regulated by the Scottish Government. There is a requirement for fish farm operators to use modelling tools to demonstrate compliance with the environmental standards relating to the spatial extent and the intensity of impacts, both in the local area around fish pens and in the wider environment.

Increasingly, operators are required to use marine hydrodynamic modelling approaches to support license applications. Hydrodynamic modelling refers to a class of numerical models that simulate the flow of water within a specified geographic area in a physically realistic way. This includes flow due to a range of forcing conditions including tidal variations, density gradients, and meteorological factors (air pressure and wind). Hydrodynamic models provide the physical basis for many other types of numerical environmental modelling such as the transport, dispersion, and decay of dissolved or suspended substances.

1.2 Aims and objectives

The overall aim of the project is to develop a 3-dimensional hydrodynamic database to inform a risk-based approach to management and development of aquaculture sites in the waters around Shetland with specific focus to East of Shetland developments and activities.

To achieve this aim, the objectives of this hydrodynamic modelling report are to:

- develop a 3-dimensional hydrodynamic climatology model database that sufficiently represents the hydrodynamics as expressed by marine currents and water exchange around the East of Shetland and Yell/Unst sites with a specific focus on Setterness, Vidlin and Dury Voe areas.
- develop a dedicated, high-resolution, 3-dimensional hydrodynamic hindcast model of the East of Shetland area.

The model will provide a database for future modelling to support regulatory applications such as: assessing connectivity between fish farms sites within the East of Shetland area; site selection and site screening; dispersion modelling of waste solids and bath treatment medicines.

Climatology Model

The fundamental principle of a climatology model is the assumption that the conditions for a particular day (or month) and at a particular location do not change significantly from one year to the next; hence, the long-term average conditions on a certain day (or month) should be a good approximation to the expected conditions for that day (or month). This offers a simple technique for predicting the *mean status* of the atmospheric and oceanographic conditions within a region (i.e., to understand the seasonal variability, but not to the interannual variability).

The hydrodynamic climatology model thus provides a useful reference for how the expected flow patterns, temperature, and salinity vary over seasonal cycles that are driven by tide, the wind climate, and gradients in water density. However, the climatology model output does not reflect episodic weather events as for example winter storms which occur at relatively high frequency at these latitudes.

1.3 Layout of this report

The remaining sections of this report are organised as follows:

- Section 2 summarises information on the geographic and environmental setting of the Shetland.
- Section 3 provides an overview of the data basis for the modelling study, including coastline, bathymetry, boundary conditions, and meteorological forcing.
- Section 4 describes the setup of the 3D hydrodynamic model of East of Shetland. This includes the mesh and bathymetry development, initial and boundary conditions, model settings, and outputs.
- Section 5 presents the calibration/validation of the hindcast version.
- Section 6 presents the verification of the hydrodynamic climatology version.
- Section 7 provides a summary of the hydrodynamic model climatology/hindcast databases.

2 Geographic and environmental setting

2.1 Geographic setting

Shetland is an archipelago in the North Sea consisting of approximately 100 islands, of which approximately 16 are inhabited. The islands are located approximately 200km from north coast of mainland Scotland, 280km south-east of the Faroe Islands, and 350km west of Bergen, Norway (Figure 2.1).

Shetland itself covers almost 160km, from Fair Isle in the south to Muckle Flugga in the north and represents the northernmost extremity of the United Kingdom. The largest island is called "the Mainland" and is home to around 80% of Shetland's ~23,000 population. Settlements on the Mainland include Lerwick, the largest town and commercial centre, and the fishing port of Scalloway on the North Atlantic coast.

The coastline of Shetland is approximately 2,700km in length and is characterised by a rugged outer rocky shore and areas of high cliffs (particularly on the western facing shores). The inner part of the coastline comprised of many long open sea lochs ('voes'), former river and glacial valleys that are now flooded by the sea. The steeply sloping and indented character of these voes has generally hindered the formation of large, sandy beaches around Shetland [1].

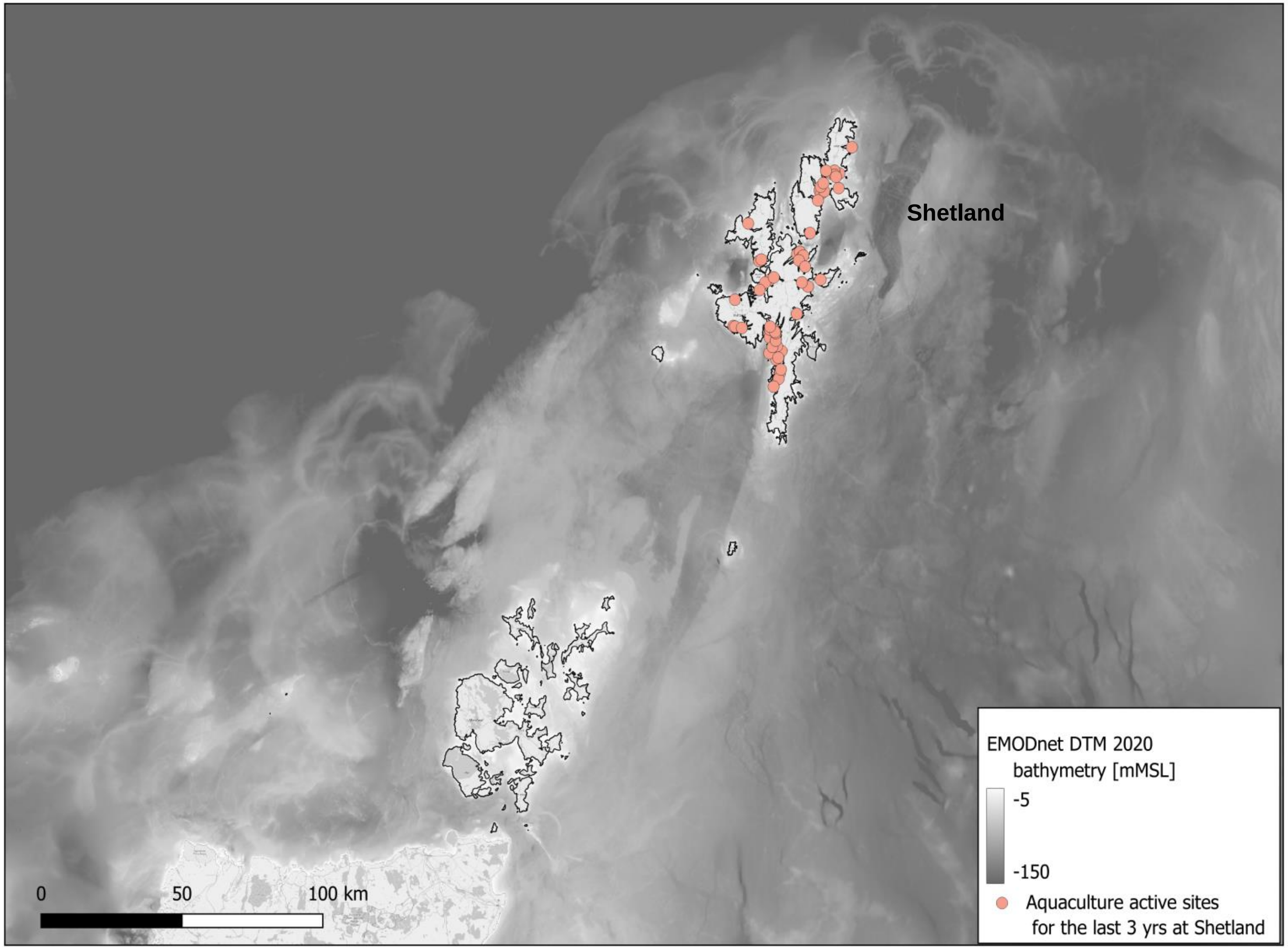


Figure 2.1 Map showing the geographic position of Shetland area of interest in relation to the UK mainland (left bottom corner) with chosen aquaculture farms sites displayed.

2.2 Climatic and oceanographic conditions

Currents

Considering its position at around 59°N of the equator, the climate of the Northern Isles is very mild compared to other parts of the world at a comparable latitude. This is explained by the role of the North Atlantic Current (Figure 2.2), a feature that is partly wind driven and partly driven by the density gradients between the warmer sub-tropical water (to the south) and the cooler sub-polar waters (to the north) [2]. The prevailing south-westerly winds pick up heat from the North Atlantic current, resulting in the relatively mild and wet maritime climate that characterises Scotland, and relatively stable sea temperatures typically ranging from approximately 8°C in March to a peak of 13°C in August [1]. In addition to the North Atlantic Current, a jet-like feature known as the Slope Current, flows along the edge of the continental slope from south-to-north roughly at the 400-500m depth contour (see Figure 2.2). The waters in the Slope Current originate from southern Europe (Iberia) and include North Atlantic Water that reaches the Bay of Biscay [2].

Winds

Although the prevailing wind direction is from the south-west, the passage of various low-pressure systems across the North Atlantic accounts for variability in the wind direction around northern and western parts of Scotland. This exposure to the North Atlantic means that Shetland is among the windiest parts of the United Kingdom, and the frequency and depth of these depressions is greatest in the winter months (December through to February). As Atlantic depressions pass the UK the wind typically starts to blow from the south-west, but often later comes from the west or north-west as the depression moves away [3]. The range of directions between south and north-west accounts for most occasions and the strongest winds nearly always blow from these directions (see Figure 2.3).

Tides

The tides all around Scotland are semi-diurnal characterised by a high and low water every ~12.5 hours. At Lerwick, the spring and neap tidal range are 1.58m and 0.74m, respectively (see Table 1 of [4]). This is set by the tides in the North Atlantic Ocean which propagate up the west coast of Scotland. Shetland acts as a natural blockage to the northwards sweep of the Atlantic tide, and the tidal wave swings eastwards to the north of the Islands and into the northern North Sea. The result is a difference in the timing of high and low water between the east and west coast, which sets up strong tidal currents where the flow is constrained around the headlands and in narrow channels that connect the North Atlantic and North Sea [5]. However, in the enclosed and deep water voes tidal currents are generally weak and the circulation is strongly influenced by wind and density-driven current conditions.

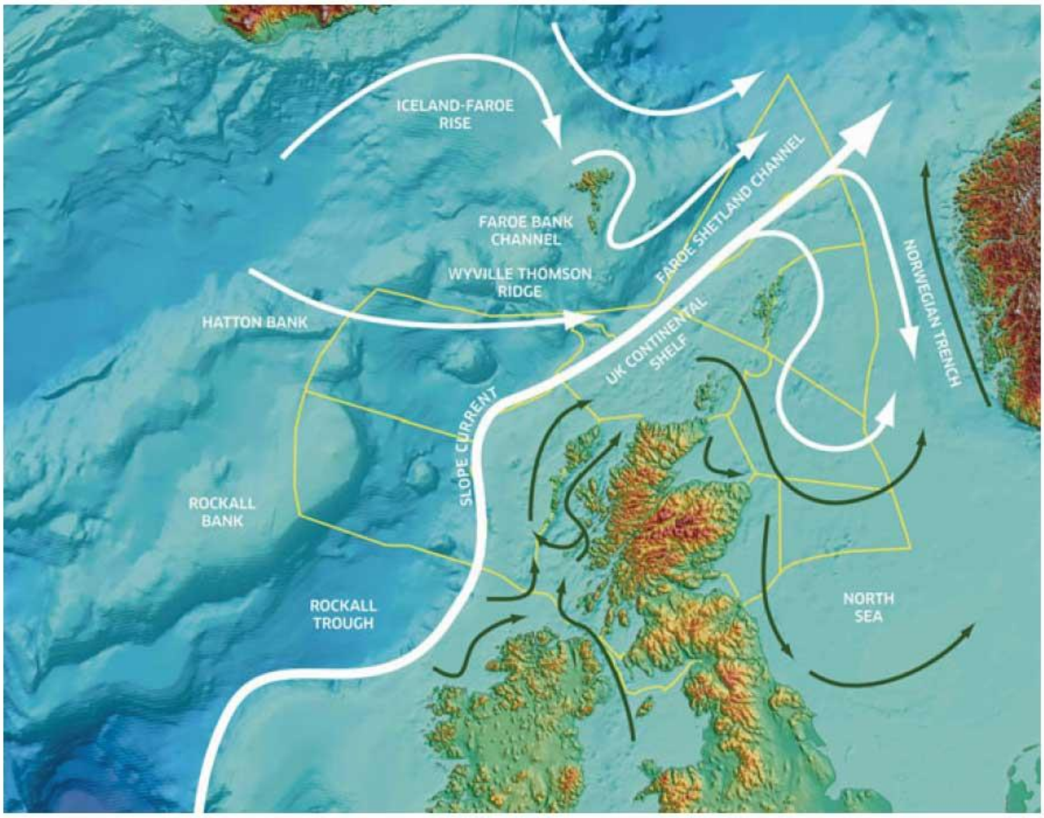


Figure 2.2 Map of the general circulation pattern within the North Atlantic and North Sea around Scotland (reproduced from [2]). The white arrows show the circulation of Atlantic water, while green arrows represent costal circulation.

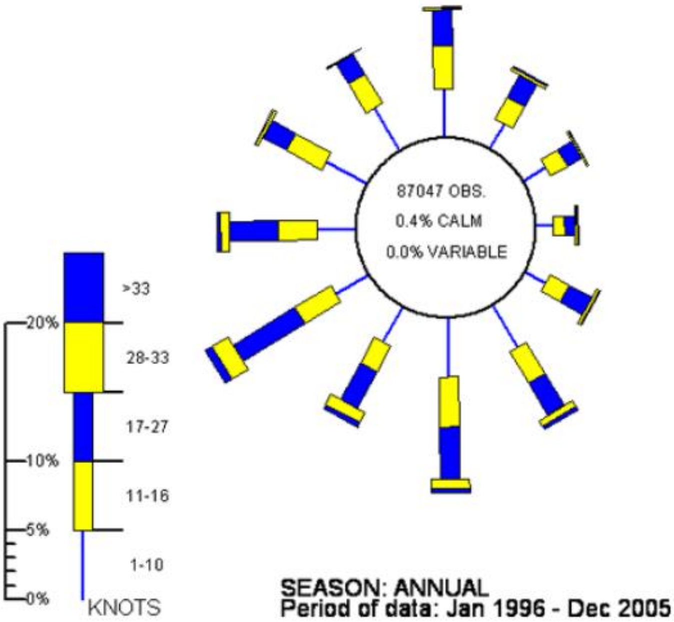


Figure 2.3 Annual (all-year) wind rose for Lerwick for the period 1996-2005 (Shetland), with a prevailing southwest wind direction through the year and frequent strong winds from southerly to north-westerly directional sectors (reproduced from [3])

2.3 Aquaculture in Shetland

Shetland is a key area for Scottish aquaculture, accounting for 26% of Scottish fin fish and 80% of shellfish production [1]. Production takes place within the voes and sounds around the coastline, with the highest concentration of sites on the west coast (see Figure 2.4).

Fin fish production is dominated by Atlantic salmon (*Salmo salar*). In the decade 2012-2021, the annual Salmon production in the waters around Shetland averaged around 40,000 Tonnes, representing a value of over £200 million. The sector directly employs about 200 full time staff [6], plus supports the wider economy of the islands via fish processing, marine engineering, and transportation [1].

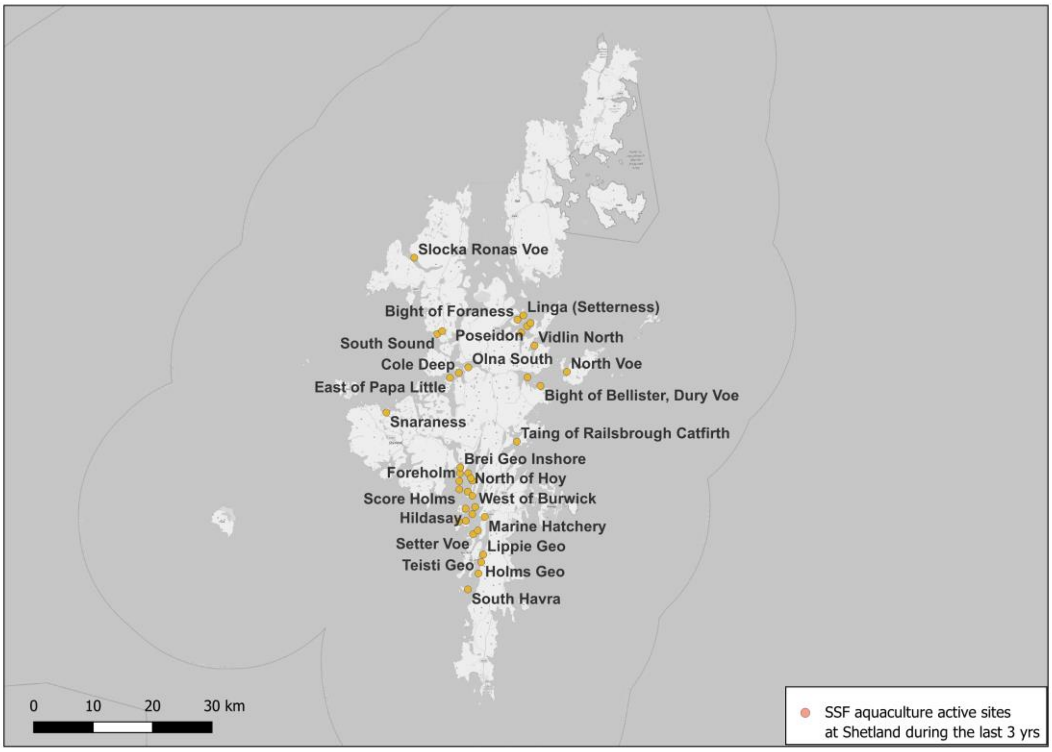


Figure 2.4 Map showing the locations of SSF's active production sites for the last 3 yrs at the Shetland islands.

3 Data Basis

In this section, the data sets that are used as input to the modelling study are described. This includes the coastline and bathymetry information (Section 3.1), the model boundary information for the hindcast and climatology versions (Section 4.3.4), and the meteorological forcing (Section 4.3.5).

3.1 Bathymetry and coastline

3.1.1 Coastline

Ordnance Survey highwater shoreline data (OS HWS) was applied as the governing indicator of the separation between land and water. These data were obtained via OS OpenData[1] licensed under Open Government License[2].

3.1.2 Bathymetry

The East of Shetland hydrodynamic model bathymetry was informed by a composite bathymetric database from open-source datasets[3] and proprietary surveys provided by SSF. These are summarised in Table 3.1 and briefly described below. The vertical reference datum of the baseline bathymetric dataset (EMODnet DTM) was Lowest Astronomical Tide[4] (LAT). All data were converted to a common reference vertical datum of mean-sea-level (MSL), see also section 4.1.1.

Local site bathymetry data

SSF provided several bathymetric soundings at the main areas of interest (see Figure 3.1) as part of the current data delivery to inform the development of the East of Shetland hydrodynamic database. The soundings derived bathymetric data are typically recorded using depth sounders installed on board fish farm vessels. Bathymetry information are provided relative to a vertical datum of CD, adjusted by the data provider for the depth of sounder below the surface and the predicted local tidal height. These spot depths were mainly used to cross-validate model bathymetry and inform of appropriateness of respective available sources.

UKHO Admiralty Data

High-resolution bathymetry data for the waters in the Shetland around the Isles were obtained from the United Kingdom Hydrographic Office (UKHO) Marine Data Portal[5]. The service provides access to the extensive UK bathymetry holdings held within the MEDIN accredited National Data Archive, allowing users to download bathymetry data under an Open Government Licence (OGL). The data are offered at a gridded resolution of <10m

---

[1] OpenData - Free GIS Data Download - Geospatial Data Sources for Mapping (ordnancesurvey.co.uk)

[2] Contains OS data © Crown copyright [and database right] (2021)

[3] While high-resolution bathymetry comprises a high percentage coverage of the Shetland in the areas of interest there still exist areas of lower resolution, especially straights and shallows, that could have a distinct impact of modelled hydrodynamics. EMODnet DTM in those areas is informed by the GEBCO 2020 DTM. The GEBCO global model is less accurate and detailed in coastal areas and should be used with caution when alternative datasets are not available. In those areas C-MAP data to a buffer zone of 2km from the coastline has been utilised.

[4] EMODnet uses a global tide surge model (GTSM, Deltares) for LAT to MSL vertical datum references, https://portal.emodnet-bathymetry.eu/

[5] Admiralty Marine Data Solution, Marine Data Portal (UKHO) accessed Jan 2022

vertically referenced to CD. Figure 3.2 shows the high-resolution datasets in and around areas of interest in Shetland.

EMODnet Digital Terrain Model (DTM)

For offshore areas that are not covered by the multibeam bathymetric datasets, bathymetric data from the Digital Terrain Model (DTM) data products have been adopted from the EMODnet Bathymetry portal (version 2020) (see Figure 3.3). This portal was initiated by the European Commission as part of developing the European Marine Observation and Data Network (EMODnet). The EMODnet digital terrain model has been produced from bathymetric survey data and aggregated bathymetry data sets collated from public and private organisations. The data are provided processed, and quality controlled at a grid resolution of 1/16 x 1/16 arc minutes (approximately 57m, zonal x 115m, meridional). Vertical datum is referenced to LAT derived from the Global Tide and Surge Model (GTSM) developed by Deltares[6]. Note that the baseline EMODnet 2020 bathymetric database incorporates already most of the available datasets from UKHO (even though the multibeam datasets are upscaled significantly at a final grid resolution of 60x117 m^2 from 4-8 m^2). Due to lack of available higher resolution bathymetric surveys, grey areas in the EMODnet composite product are filled in with non-gridded lower spatial resolution bathymetric datasets and the GEBCO 2021 global bathymetric model.

C-MAP

An alternative source of bathymetric data was obtained from the Global Electronic Sea Chart Database CM-93 provided by C-MAP. This provides digitised bathymetric chart data vertically referenced to CD. C-MAP data was used in the coastal areas and inlets where high-resolution bathymetric data or local soundings are not available (see also Figure 3.3).

Table 3.1 Summary of bathymetric databases used to inform HD_{NO} model bathymetry in order of highest to lowest priority.

Source	Resolution	Vertical Reference	Date
UKHO Admiralty Data	2m to 8m	Chart Datum [mCD]	Various
EMODnet DTM	57m x 115m grid resolution	Lowest Astronomical Tide [mLAT]	2020 version
C-MAP	Isobaths/spot depths	Lowest Astronomical Tide [mLAT]	Variable
Local soundings at fish farm sites	Spot depth soundings	Chart Datum [mCD]	2000 – 2020

[6] Which information layers? - Data products - EMODnet Bathymetry (emodnet-bathymetry.eu)

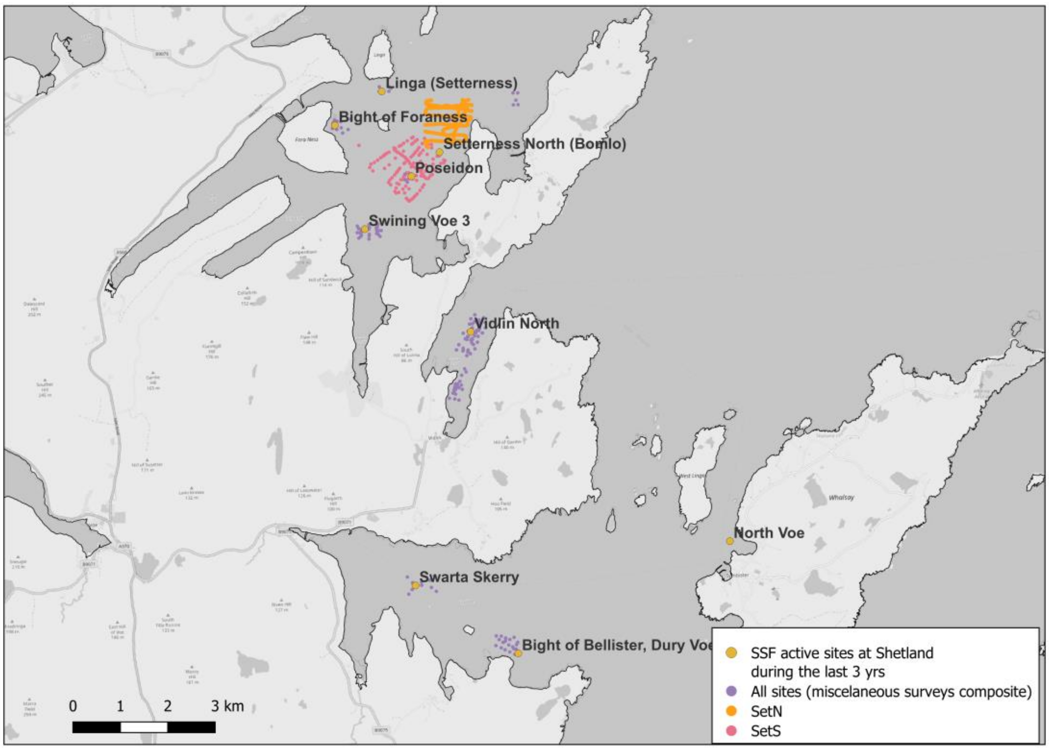


Figure 3.1 Map showing locations of a sample of the various bathymetry soundings-spot depths (purple, orange, pink markers) at MPFF sites (magenta markers) provided by SSF.

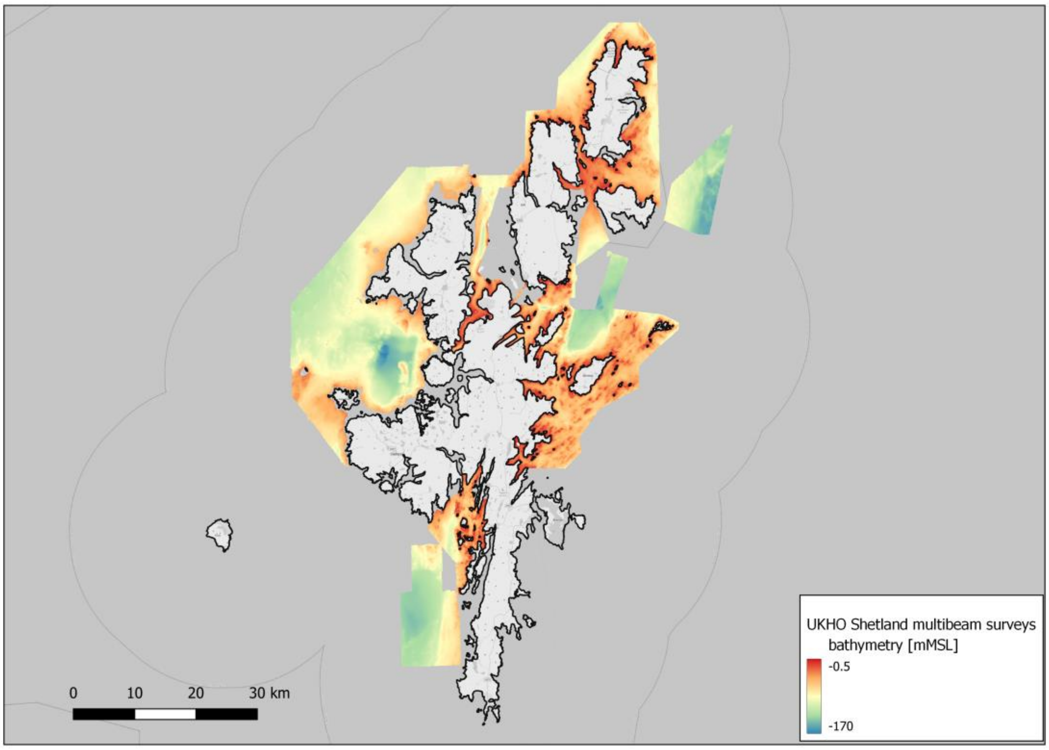


Figure 3.2 Map showing areas of high resolution multibeam gridded bathymetry bathymetric datasets (orange patched areas) around Shetland Isles used to inform model bathymetry herein (source UKHO Marine Data Portal).

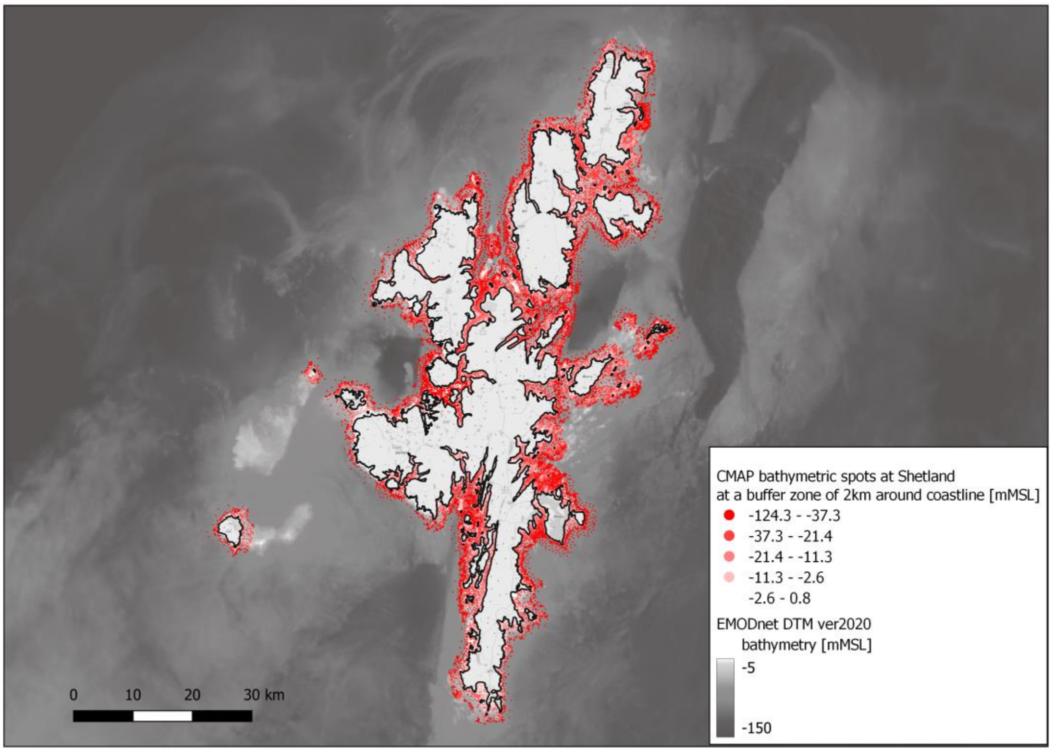


Figure 3.3 C-MAP bathymetric spots (red colour scale) within a buffer zone of 2km from the Shetland Isles coastline and EMODnet DTM ver2020 (grey scale) baseline bathymetry used to inform the bathymetry of the East of Shetland computational domain

3.2 Measurements

3.2.1 ADCP campaigns

Information on current speeds/directions, water levels and sea water temperature at instrument depth were provided by SSF during a series of Acoustic Doppler Current Profiler (ADCP) campaigns between 2007 and 2022, see also Table 3.2. Survey periods for each observational deployment provided by SSF are shown in Figure 3.4 and their respective geographic location in Figure 3.5.

The ADCP instruments were frame mounted on the seabed and use acoustic signals to record the current velocity vectors at various depths (bins) through the water column. The derived timeseries were examined to ensure that any anomalous or erroneous data were removed. This included data from the water surface, which are often contaminated by reflections from the surface (so-called side-lobe interference). Observed current speed and direction was depth averaged (current velocity vectors averaging) through the water column in order to be comparable to the depth averaging modelled currents. Current vectors comparisons throughout the water column were performed at respective, matching, vertical levels between the observational records and the modelled 3D currents (i.e., for each mid-depth of a sigma layer the closest matching observational bin depth and/or an average of observational bins within the respective sigma layer thickness).

The observational records included a total water depth record derived via a pressure sensor. Surface elevation for each site was determined by adding the frame height of the ADCP (sensor distance to seabed – included in the information shared by SSF) to the sensor depth record and then subtracting the MSL value for the ADCP deployment location from the data record.

The surface elevation and velocity vectors timeseries were further processed under the unified tidal analysis and prediction framework U-tide [7] in order to derive the tidal and residual components for records with sufficient duration (>30 days).

A temperature sensor affixed to the ADCP was also provided for certain deployments.

From the available datasets, several periods were identified for the calibration and validation periods of the hindcast model respectively, see also Figure 3.4:

- Cal Period (light green) covering records in years 2009 and 2018.
- Val Period (light blue) covering records in year 2021 and 2022.

Calibration runs were chosen on the basis to provide an overall good spatial coverage of the central model domain, see also Figure 3.5 with available deployments in the respective periods. The validation period was chosen to coincide with an extensive deployment record in the annual period covered while still closely related to the ongoing and prospect aquaculture activities of SSF.

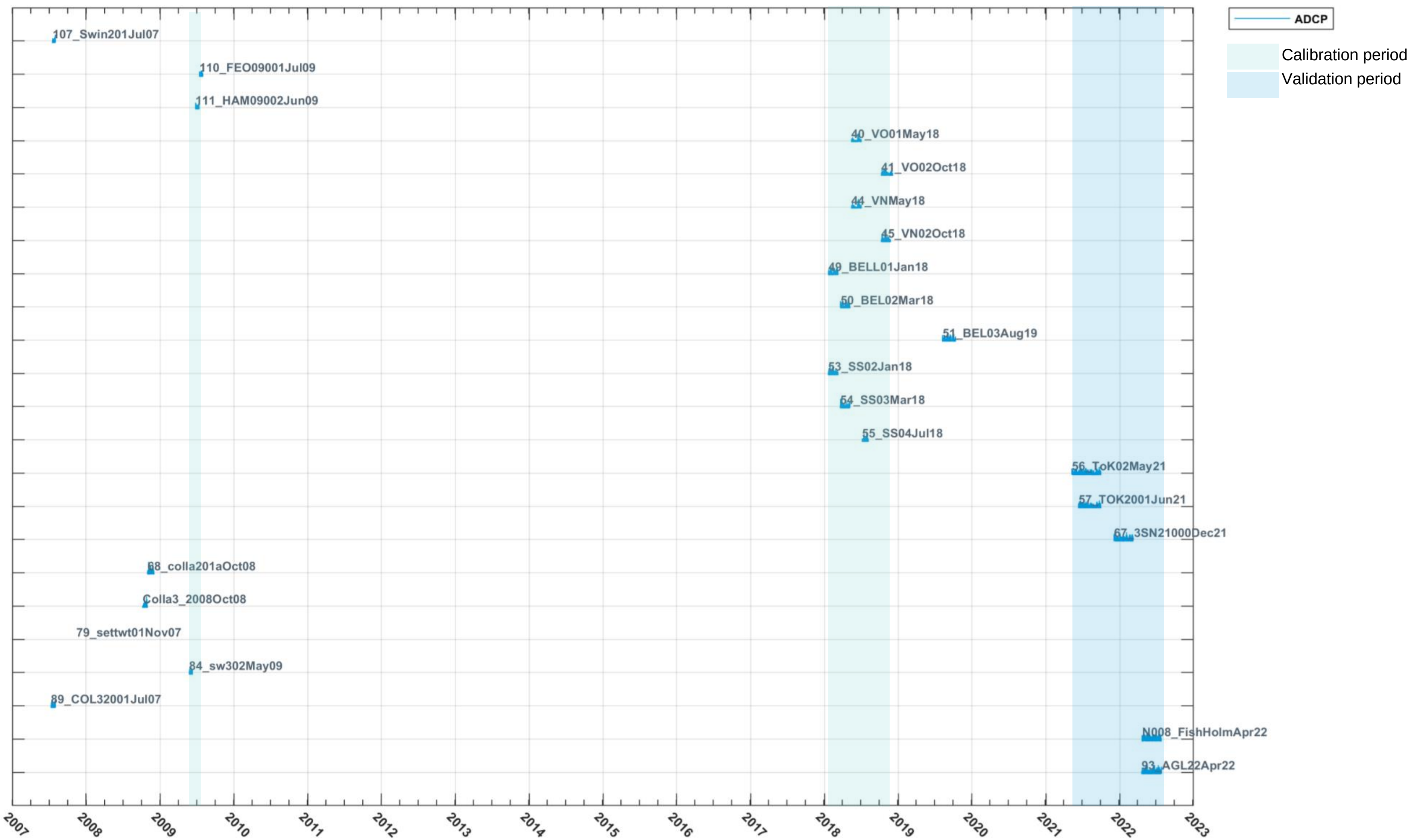


Figure 3.4 Survey periods of ADCP deployments provided by SSF at Shetland sites of interest for the period 2007-2022 that were considered during the hindcast model calibration and validation development stages (current speed ranges for each respective site also documented)

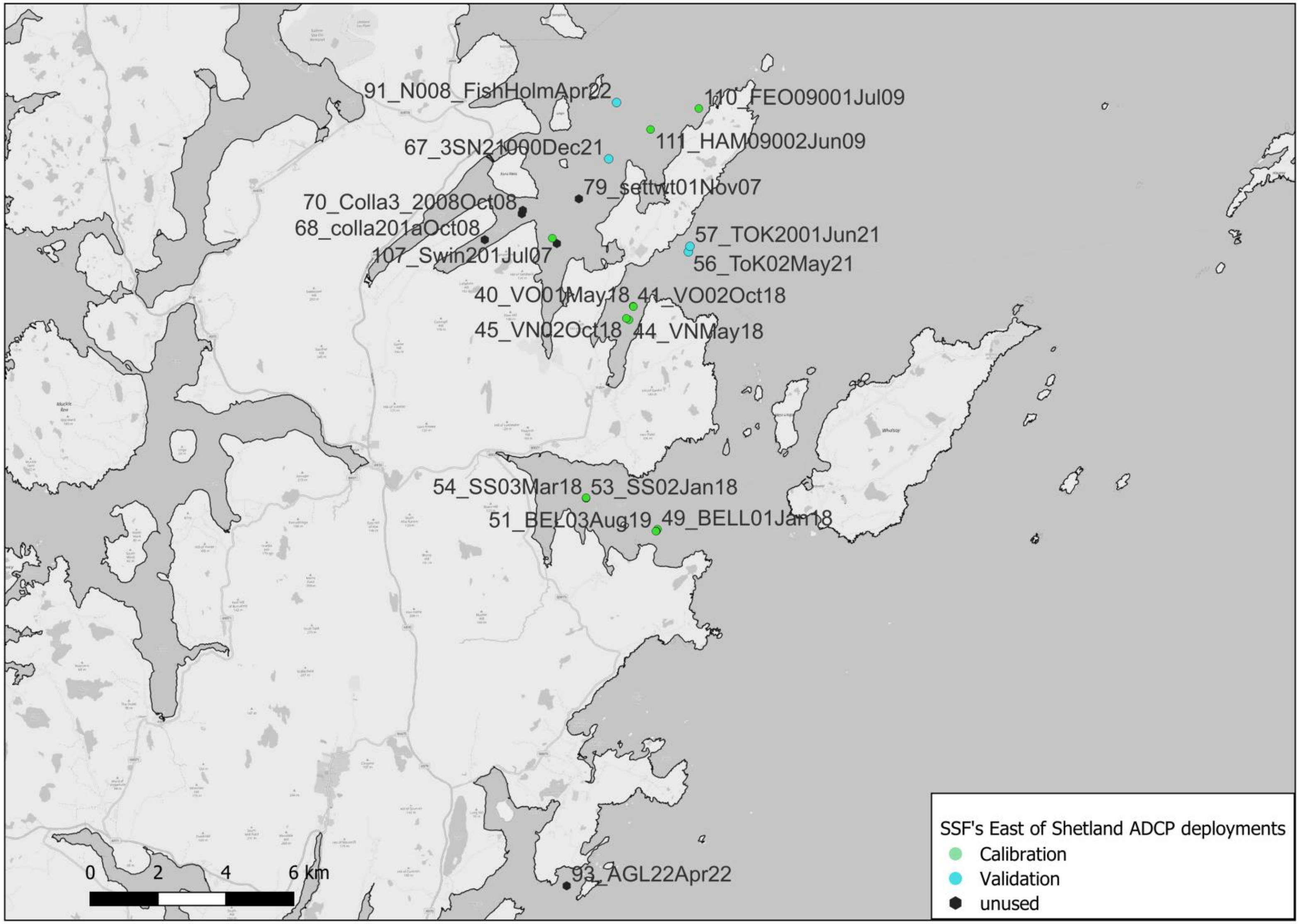


Figure 3.5 Geographic locations of ADCP deployments provided by SSF at East of Shetland sites of interest for the period 2007-2022 that were considered during the calibration and validation stages of the hindcast model development.

Table 3.2 Observational records database provided by SSF[7] to inform on hydrodynamic conditions in the area of interest and calibration stage of the HD model development.

Site	ID	Instrument	SurveyStart GMT	SurveyEnd GMT	Lat	Long	Deployment depth [m]	Declination (degrees)	Recording Interval [mins]
Vidlin Outer	40_VO01	TRDI Workhorse	14/05/2018	02/07/2018	60.390853	-1.117992	34.9	-2.160	20.0
Vidlin Outer	41_VO02	TRDI Workhorse	09/10/2018	04/12/2018	60.390730	-1.117850	35.0	-2.060	20.0
Vidlin North	44_VN	TRDI Sentinel V	14/05/2018	02/07/2018	60.387274	-1.120441	30.7	-2.150	20.0
Vidlin North	45_VN02	TRDI Sentinel V	09/10/2018	24/11/2018	60.387670	-1.121870	31.5	-2.060	20.0
Bellister	49_BELL01	TRDI Sentinel V	20/01/2018	09/03/2018	60.331658	-1.108401	40.9	-2.125	20.0
Bellister	50_BEL02	TRDI Workhorse	20/03/2018	07/05/2018	60.331184	-1.109061	38.2	-2.090	20.0
Bellister	51_BEL03	TRDI Sentinel V	07/08/2019	11/10/2019	60.331150	-1.109290	38.1	-1.522	20.0
Swarta Skerry	53_SS02	TRDI Workhorse	19/01/2018	09/03/2018	60.340400	-1.146050	37.0	-2.130	20.0
Swarta Skerry	54_SS03	TRDI Sentinel V	20/03/2018	07/05/2018	60.340441	-1.146093	36.8	-2.100	20.0
Swarta Skerry	55_SS04	TRDI Sentinel V	06/07/2018	06/08/2018	60.340550	-1.146050	36.7	-2.040	20.0
Taing of Kelswick	56_ToK02	TRDI Sentinel V	09/05/2021	29/09/2021	60.404800	-1.087633	-	-1.075	20.0
Taing of Kelswick	57_TOK2001	TRDI Workhorse 300kHz	10/06/2021	29/09/2021	60.406250	-1.086683	46.2	-1.064	20.0
Setterness North	67_3SN21000	TRDI Workhorse 600kHz	03/12/2021	08/03/2022	60.430000	-1.128840	54.7	-0.976	20.0
Collafirth Site 2 2008	68_colla201a	Aquadopp 600kHz ADP	30/10/2008	01/12/2008	60.409517	-1.196400	34.4	-4.190	20.0
Collafirth Site 3 2008	70_Colla3_2008	[unknown]	06/10/2008	30/10/2008	60.416111	-1.176163	49.7	-4.230	20.0
Swining Site 3	84_sw302	Aquadopp 600kHz ADP	25/05/2009	10/06/2009	60.409433	-1.160217	48.4	-4.040	20.0
Collafirth Site 3 2007	89_COL32001	Nortek NDP	11/07/2007	02/08/2007	60.417017	-1.175600	50.6	-4.460	15.0
Fish Holm 2022	91_N008_FishHolm	Nortek Signature 500kHz	21/04/2022	25/07/2022	60.444833	-1.123783	66.9	-0.883	20.0
Gletness	93_AGL22	TRDI Workhorse 600kHz	19/04/2022	26/07/2022	60.238033	-1.162183	26.5	-0.875	20.0
Swining Site 3 2007	107_Swin201	Nortek 400kHz Aquadopp Profiler	18/07/2007	02/08/2007	60.407983	-1.157883	46.4	-4.460	15.0
Feowick 2009	110_FEO09001	Nortek NDP	14/07/2009	31/07/2009	60.442633	-1.079797	19.7	-4.180	20.0
Hamnavoe 2009 (Deployment 2)	111_HAM09002	Nortek NDP	25/06/2009	13/07/2009	60.437450	-1.105983	30.3	-4.170	20.0

[7] Following DHI's quality assessment and SSF's commentary on sensor errors and/or instrument drift during survey campaigns

4 Model Development

This section describes the development of the three-dimensional East of Shetland hydrodynamic models (hindcast and climatology) within the scope of the project.

4.1 Model selection

4.1.1 Three-dimensional model

Many of the aquaculture sites in the waters around Shetland are located within the relatively long and deep voes. These areas have the potential to exhibit vertical stratification due to density gradients (due to difference in water temperature and salinity), which may have important implications for vertical mixing and flow velocities. In such environments, a three-dimensional (3D) model may be necessary to capture the important processes [8]. Temperature and salinity are also important factors in biological modelling (e.g., for sea-lice development). Finally, wind forcing will also play an important role in driving local flow patterns, which is important for surface dispersion (e.g., for modelling bath-treatment) so this must also be included in the model setup.

As such, a modelling package which computes conditions throughout the water column was used to represent the hydrodynamic conditions in and around Shetland. The MIKE 3 FM modelling system was chosen as these allowed changes throughout the water column to be considered (see Section 4.1.2).

4.1.2 MIKE 3 hydrodynamic model

The Shetland hydrodynamic modelling has been performed using the MIKE 3 modelling package developed by DHI. MIKE 3 includes the simulation tools to model 3D free surface flows and associated sediment or water quality processes. The following modules available within MIKE 3 were used during this study:

- HD – Hydrodynamics: This module simulates the water level variations and flows in response to a variety of forcing functions. It includes a wide range of hydraulic phenomena in the simulations, and it can be used for any 3D free surface flow. The Flexible Mesh version, which uses a depth and surface adaptive vertical grid, is particularly suitable in areas with a high tidal range.

The MIKE 3 Model used for the present study was version 2022 [9].

The Hydrodynamic Module is the basic computational component of the entire MIKE 3 Flow Model FM, and has been developed for applications within oceanographic, coastal, and estuarine environments [9]. The hydrodynamic module provides the basis for the other modules such as sand transport, mud transport, particle tracking, and ECO Lab.

The computational mesh is based on the unstructured grid in the horizontal direction, an approach which gives maximum degree of flexibility when handling problems in complex domains (such as in the voes and narrow straits around Shetland). In the vertical direction a sigma (σ) discretisation is used meaning that model elements are represented as 3-sided prisms (Figure 4.1)

The MIKE3 modelling system is based on the numerical solution of the three-dimensional incompressible Reynolds Averaged Navier-Stokes (RANS) equations, invoking the assumptions of Boussinesq, and of hydrostatic pressure. Thus, the MIKE 3 flow model consists of continuity, momentum, temperature, salinity, and density equations and is closed by a turbulent closure scheme. In the horizontal domain both Cartesian and spherical coordinates can be used. The free surface is considered using a sigma-coordinate transformation approach.

The spatial discretisation of the primitive equations is performed using a cell-centred finite volume method. The spatial domain is discretised by subdivision of the continuum into non-overlapping element/cells. In the horizontal plane an unstructured grid is used while in the vertical domain a structured discretisation is used. The elements can be prisms or bricks whose horizontal faces are triangles and quadrilateral elements, respectively. An approximative Riemann solver is used for computation of the convective fluxes, which makes it possible to handle discontinuous solutions.

For the time integration a semi-implicit approach is used where the horizontal terms are treated explicitly, and the vertical terms are treated implicitly.

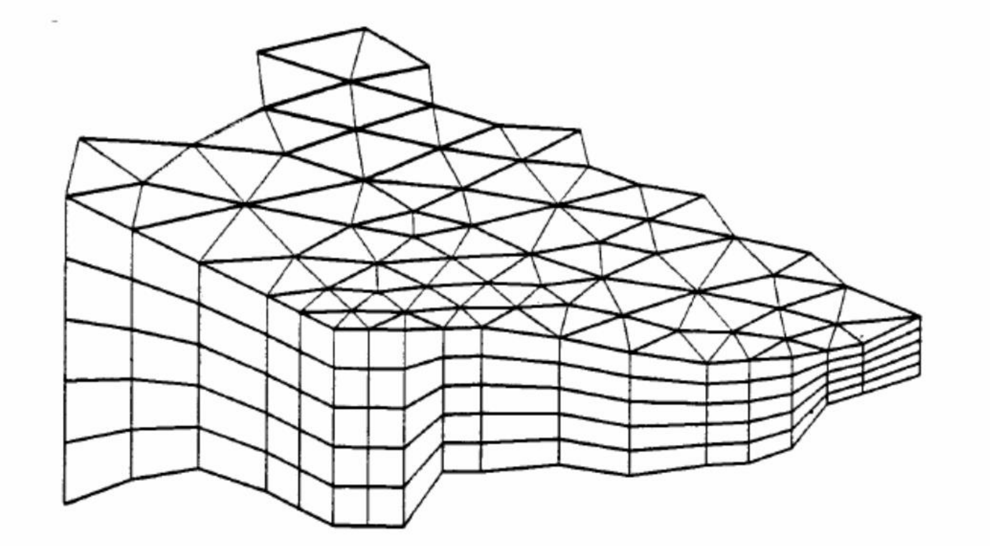


Figure 4.1 Example of an unstructured mesh in MIKE3 with 5 sigma (σ) layers.

4.2 Datums

Unless explicitly stated otherwise, the following reference datums were adopted for the models developed during this project.

- Horizontal datum is established using World Geodetic System 1984 (WGS 84), UTM zone 30N.
- Vertical datum is referenced to mean-sea-level (MSL). Conversion from LAT to MSL is performed using EMODnet LAT to MSL gridded product[8].

[8] EMODnet uses a global tide surge model (GTSM, Deltares) for LAT to MSL vertical datum references, https://portal.emodnet-bathymetry.eu/

4.3 East of Shetland hydrodynamic hindcast and climatology models

The regional 3D hydrodynamic model of East of Shetland was established both as a hindcast and climatology version. The HD_{ES_clima} model is a dynamically downscaled version of the SSM (see Section 4.3.1). Thus, HD_{ES_clima} is a high-resolution regional model that dynamically extrapolates the effects of the large-scale processes of the SSM to regional scales of interest around the waters of the Shetland archipelago.

A climatology is constructed as a representation of the 'mean' status of hydrodynamics over a period of years. On that basis, it is difficult to justify a calibration/validation of a climatology forced model with an observational record as a measure of model skill. Therefore, a hindcast version $HD_{ES\_hindcast}$ was constructed which was calibrated and then validated against the available observational records through the measurement campaigns provided by SSF, see also section 3.2, to justify parameterisations and calibration settings considered applicable then for the climatology version of the model.

The following sections describe the establishment of the $HD_{ES\_hindcast}$ and subsequently HD_{ES_clima} model, including the model mesh and bathymetry, the specification, and model outputs.

4.3.1 The Scottish Shelf Climatology Model

The Scottish Shelf Model (SSM) is a suite of hydrodynamic numerical models of Scottish continental shelf waters, developed for and maintained by Marine Scotland Science, to describe the circulation of the Scottish continental shelf waters [10]. The SSM has been designed to support a varied range of marine science and policy applications, including for rapidly developing marine renewable energy and aquaculture sectors.

The wider domain SSM encompasses most of UK waters and the entire Scottish Continental shelf area (Figure 4.2). The horizontal resolution varies from approximately 10km in the outer domain to around 1km around the Scottish Coast (Figure 4.3). For the vertical discretization a σ coordinate system (terrain following coordinates) based on 20 uniform layers is used. The SSM suite of models also includes several smaller domain sub-models, with higher resolution, covering specific areas of interest including the Firth of Clyde, Pentland Firth and Orkney Waters, Loch Linnhe, St Magnus Bay and the east Coast of Lewis and Harris (see [10]). In this report we shall only be using the wider domain Scottish Shelf Model (version 2.01) as this provides the most suitable climatology-based boundary forcing for Shetland and shall henceforth use the abbreviation SSM when referring to this model.

Full details of the SSM climatology are provided in [11, 12], and a brief summary of the model setup is provided below.

The SSM is a one-year climatology model that represents average conditions with a 1993 tidal component. The model was implemented using an unstructured grid coastal ocean model, FVCOM (Finite-Volume Community Ocean Model) [13]. The model forcing includes:

- Offshore boundary conditions (temperature, salinity, currents, and sea-surface elevation) from monthly mean over the 25-year period (1990-2014) provided by the Atlantic Margin Model 7km (AMM7) [14, 15]
- Climatology atmospheric forcing is also included based on monthly 1990–2014 data set derived from ERA-Interim data [16] (further discussed in Section 4.3.1.1)

- Freshwater inputs from river runoff volume flux climatology were obtained from the Centre for Ecology and Hydrology (CEH) Grid-to-Grid (G2G) model [17, 18], covering the period from 1962 to 2011 and including 577 rivers in Scottish Waters.

As the conditions of the SSM encompass an averaging period of 25-years (1990-2014), the climatology seeks to smooth the natural variability of the climate and achieve an approximately stationary characterisation that averages out the interannual variability.

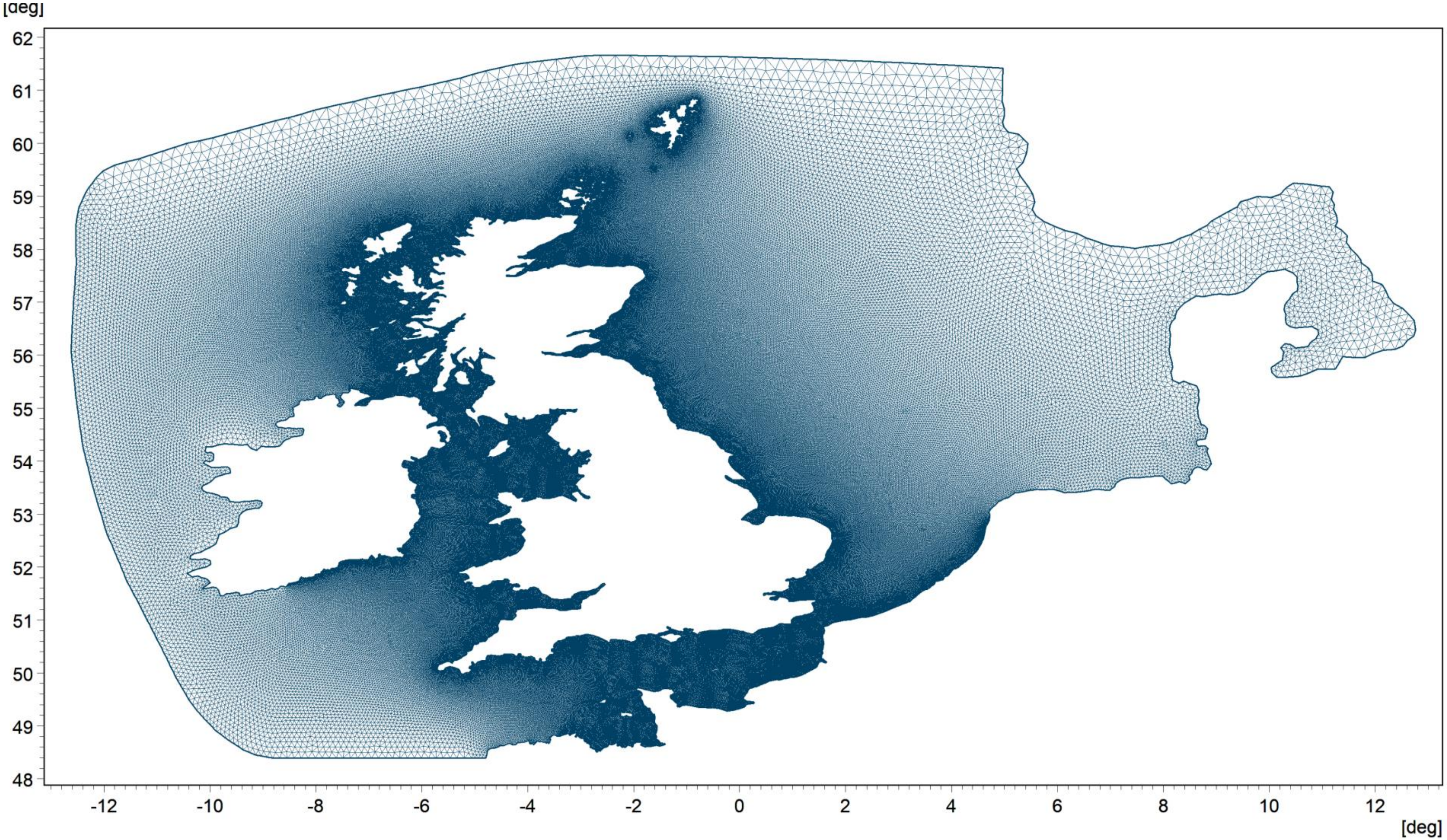


Figure 4.2 Scottish Shelf Model (SSM) numerical mesh showing the entire model domain.

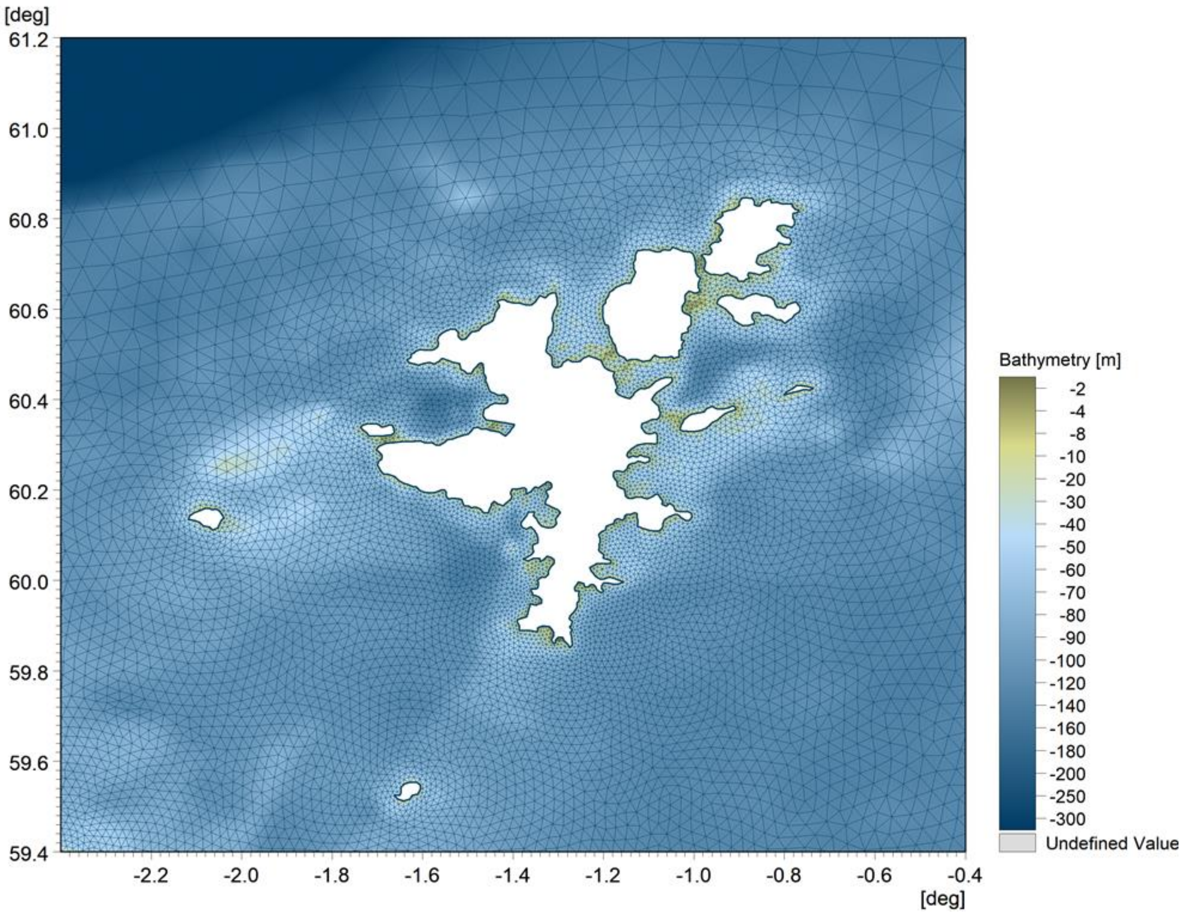


Figure 4.3 Scottish Shelf Model (SSM) computational mesh at the Shetland islands complex. See also Figure 4.6 (right panel) for a comparison in spatial discretisation improvement for the area of interest.

4.3.1.1 Meteorological conditions

Climatologically averaged meteorological conditions used to force the SSM are derived from the ERA-40 and ERA-Interim re-analysis products produced by the European Centre for Medium-Range Weather Forecasts (ECMWF) [16]. A monthly mean wind climatology was derived from these data. The met forcing was derived as monthly means, which were then linearly interpolated to 6-hourly smoothed forcing data for each grid-point, i.e. mean February data were applied at the middle of February; then mean March data were applied mid-March etc., with time-interpolation between (see Section 5.3 of [11]).

The atmospheric conditions include wind conditions (wind speed and direction), atmospheric pressure, surface heat flux, precipitation, evaporation, relative humidity, air temperature, thermal/solar radiation. For wind, the 6-hourly data were used to construct a monthly mean wind stress, which was then converted back into an equivalent wind field [12]. It should be noted that the AMM7 model, that was used to derive the offshore boundary conditions for the SSM climatology, were also forced by ERA-Interim reanalysis; hence, providing some consistency in the boundary forcing of the SSM.

Figure 4.4 shows a time-series plot of the climatologically averaged meteorology for selected parameters for a location at the south-east corner of the $HD_{ES\_hindcast/clima}$ computation domain. As expected for a climatology model there is a low temporal variability at shorter temporal scales (hours and days), but the seasonal pattern is quite clear. For example, the largest wind speeds occur during the winter months (December to February) with lowest wind speeds in the summer (June to August). Conversely, air temperatures are lowest in the winter and largest during the summer.

The time-series of wind direction (second panel in Figure 4.4) shows only very slight variation throughout the year. This can also be observed in Figure 4.5, which shows a rose plot of the distribution of wind speed and wind direction (coming from) extracted the climatologically averaged meteorology for the same offshore location. The wind direction is dominated by south-westerly conditions; directional sectors from 210°N to 240°N accounting for approximately 80% of the total. This is consistent with the prevailing wind direction for the Northern Isles. However, this does not reflect the full range of wind directions that may occur on these latitudes during the passage of low-pressure systems (as mentioned in Section 2.2), which are averaged out in the model climatology.

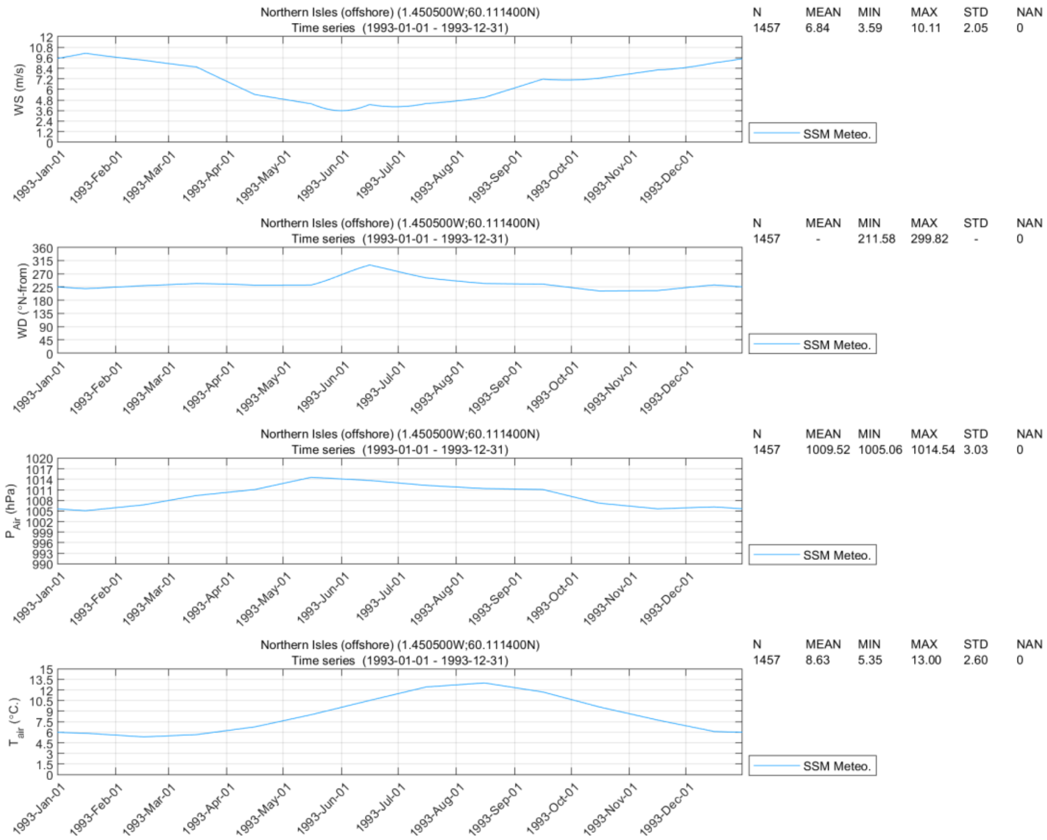


Figure 4.4 Time-series and annual statistics of climatologically averaged meteorological conditions for a location at the centre of the $HD_{ES\_hindcast/clima}$ computational domain. From top to bottom: wind speed, wind direction, atmospheric pressure, and air temperature.

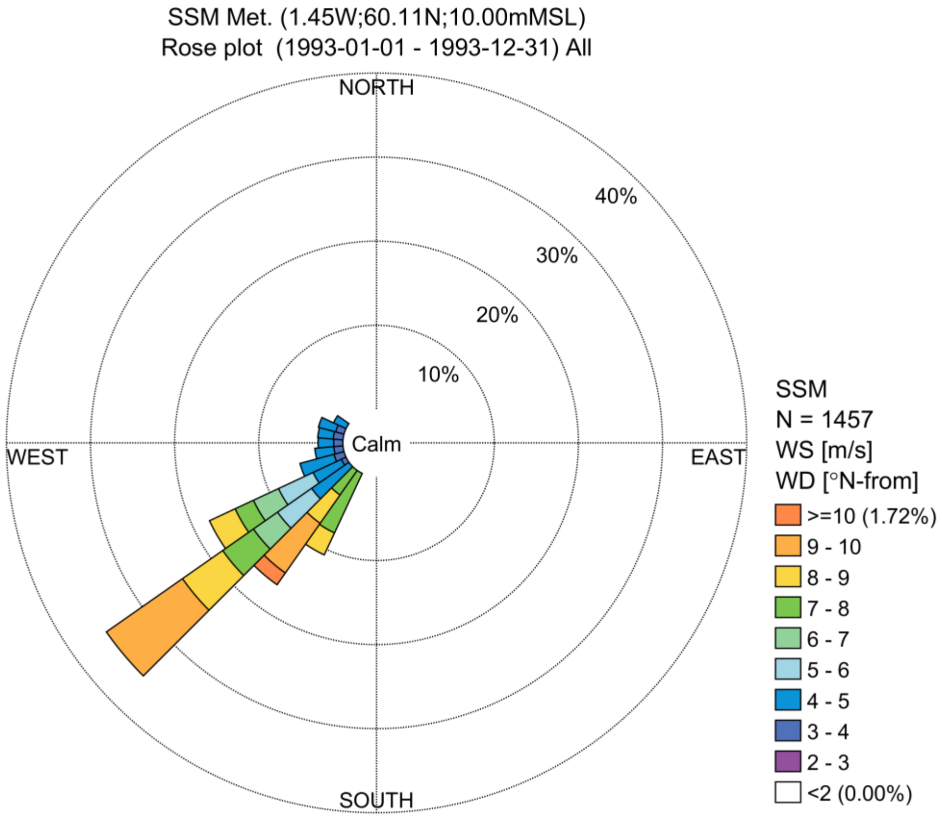


Figure 4.5 Annual wind rose for a location at the south-east corner of the $HD_{ES\_hindcast/clima}$ computational domain from the climatology atmospheric forcing used as input to the SSM.

4.3.2 Model domain

The computational domain of the regional model encompasses the entire area of the Shetland islands, see Figure 4.6. The model has six open (sea) boundaries to the North Atlantic Ocean and North Sea, and land boundaries defined according to OS HWS (see Section 3.1.1). In total the model area encloses an area of slightly over 48,322 km^2.

4.3.3 Mesh and bathymetry

The computational mesh is based on a variable resolution unstructured grid in the horizontal direction. The mesh resolution was chosen to capture the important hydrodynamic processes within the scope of this hydrodynamic database construction, while maintaining practical computational run times. This was also informed by similar regional scale models (such as the SSM sub-domain for the East coast of Lewis and Harris “ECLH” model) and following discussions with SSF on model scoping.

The computational mesh of the hydrodynamic model is shown in Figure 4.6. In the outer domain, close to the model boundaries, the horizontal mesh element length is set at around 3.5km (see also Figure 4.7). The mesh element length gradually reduces to between 400m and 150m in the coastal areas within the Shetland archipelago (right panel, Figure 4.6 and Figure 4.7). The highest resolution is specified in the focus areas of Setterness, Vidlin and Dury Voe (element side length ~40m) and subsequently near the shoreline, designated PMF areas, narrow straits between islands and within inlets. In these areas, the mesh element length is <150m. In total the horizontal mesh consists of 40,346 nodes defining 73,393 mesh elements. In the vertical dimension the discretisation is based on ten (10) non-equidistant sigma (terrain following) layers with increasing resolution (decreasing layer thickness) towards the surface (see also 4.3.6).

Thus, the down-scaled regional climatology model HD_{ES_Clima} offers significant improvement in the resolution around the coastline and includes details of features (e.g., smaller islands and inlets) that are absent in the shelf-sea scale SSM model, see also Figure 4.6 and Figure 4.7 - right panels.

The bathymetry datasets described in Section 3.1.2 were interpolated to the computational mesh as shown in Figure 4.6. Careful attention was given to smoothing of bathymetry to alleviate large bathymetric gradients between adjacent computational cells.

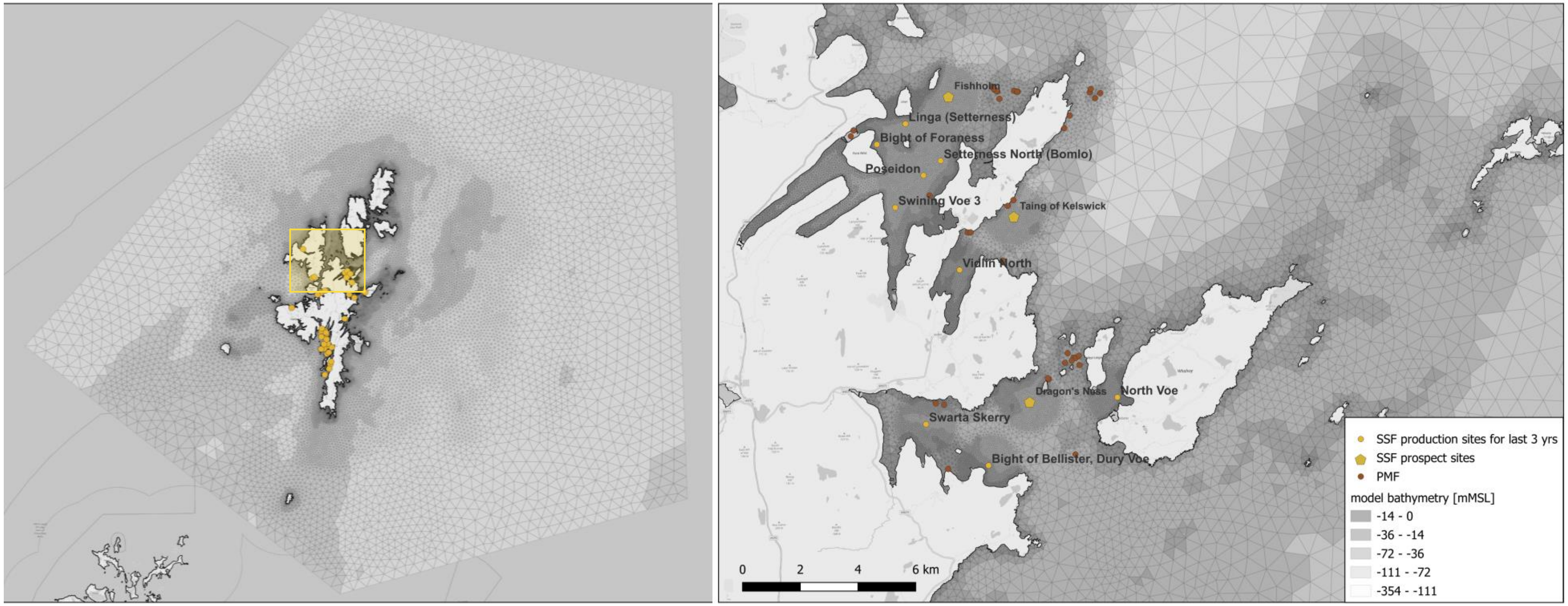


Figure 4.6 Computational domain of the regional East of Shetland hydrodynamic model (left) and zoomed in perspective of the main areas of interest (right). Mesh resolution is significantly improved in the area of interest versus SSM, as seen in Figure 4.3, allowing for a better representation of coastal and bathymetric features.

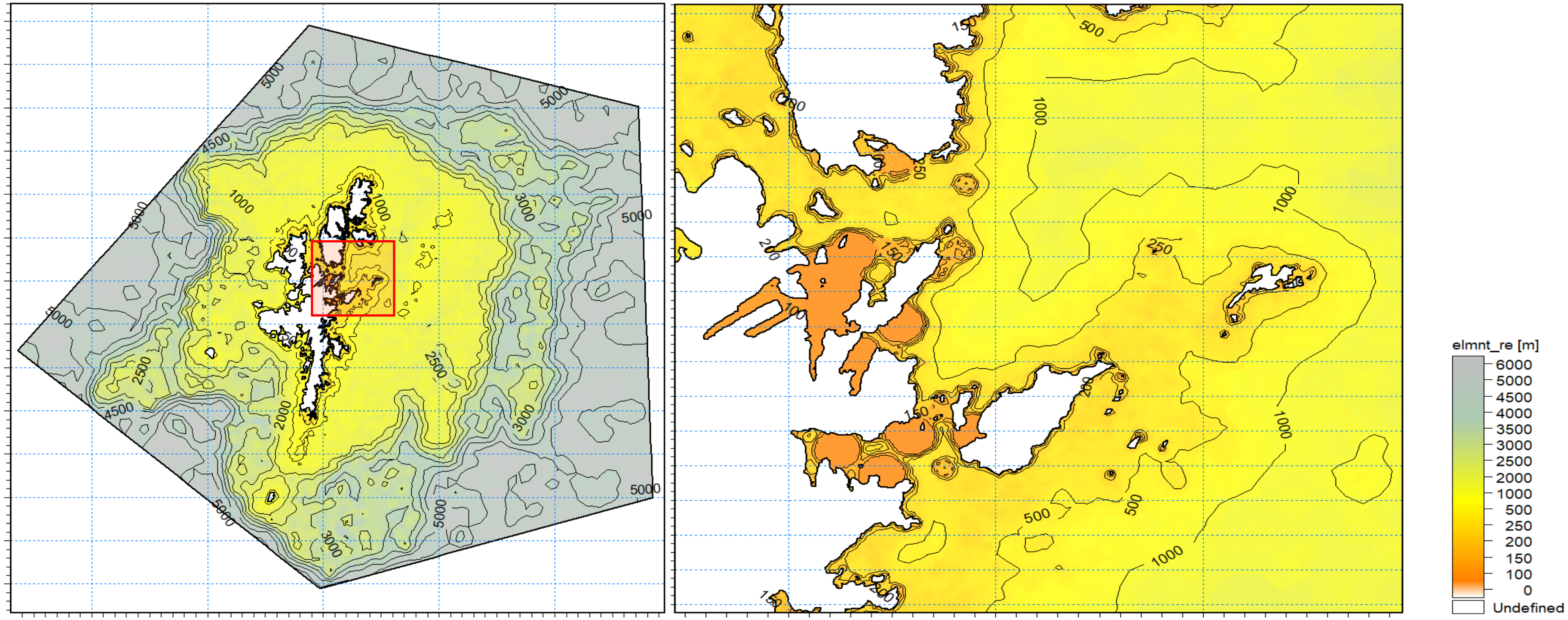


Figure 4.7 Mesh resolution [m] across the $HD_{ES\_Hindcast/Clima}$ computational domain (left panel) and zoomed in perspective in the main areas of interest of SSF (right panel)

4.3.4 Initial and boundary conditions

4.3.4.1 Hindcast

The barotropic component comes from a global tidal model produced by *Denmark's Technical University* at DTU Space in 2010 (DTU10)[9] using a response method of residual analysis of multi mission altimeter data. The model has a resolution of 0.125 x 0.125 degrees and includes the 12 major tidal constituents. The model is an empirical ocean tide model which means that it does not include tidal currents [19].

Hydrodynamic boundaries (water levels and 3D current velocities) were specified as Flather boundary conditions [20]. This is an efficient open boundary condition method for downscaling coarse model simulations to local areas. When also imposing stratified density at water level boundaries this approach can generally help to avoid model instabilities.

The baroclinic component of current velocities as also the temperature and salinity physical parameters derived from the Copernicus Global Ocean Physics Analysis and Forecast[10] product (CMEMS). The baroclinic velocity component is combined with the barotropic tidal signal to inform boundary forcing of current velocities throughout the water column.

4.3.4.2 Climatology

Initial and boundary conditions were derived from the SSM one-year climatology (see Section 4.3.1). This included temporally and spatially varying water surface elevation (1D, horizontal), and current velocities (2D, vertical).

Hydrodynamic boundaries (water levels and current velocities) were specified as Flather boundary conditions [20]. This is an efficient open boundary condition method for downscaling coarse model simulations to local areas. When also imposing stratified density at water level boundaries this approach can generally help to avoid model instabilities.

Initial conditions were set for the spatially varying distribution of water levels (2D) and temperature and salinity (3D) throughout the computational domain at the beginning of the simulation. These were derived from the SSM initial conditions (interpolated onto the HD_{ES_Clima} computational mesh). Similarly, boundary conditions are based on the SSM one-year climatology for both surface elevation (1D, horizontal) and current velocities (2D, vertical) as also for temperature and salinities (2D, vertical). Temperature and salinity physical parameters from the SSM climatology are also nudged to the solution (3D, volume) working in essence as internal boundaries for the HD_{ES_Clima}.

4.3.5 Atmospheric forcing

4.3.5.1 Hindcast

Atmospheric forcing applied in $HD_{ES\_Hindcast}$ model comes from the ERA5 (ECMWF meteorological reanalysis 5). The ERA5 dataset is a reanalysis of hourly meteorological conditions from 1979 to present, established by the European Centre for Medium Range Weather Forecasting (ECMWF) and provided by Copernicus, the European Union's Earth Observation Programme. The dataset was extracted from the meteorological ERA5

[9] https://www.space.dtu.dk/English/Research/Scientific_data_and_models/Global_Ocean_Tide_Model.aspx

[10] https://data.marine.copernicus.eu/product/GLOBAL_ANALYSISFORECAST_PHY_001_024/description

database and combines a meteorological model with observational data from satellites and ground sensors to build a consistent long-term record of the climate [21].

ERA5 offers a resolution of ~30 km in space and assimilates more observational datasets than previous ECMWF's re-analyses. It contains estimates of atmospheric variables such as air temperature, pressure and wind at different altitudes, as well as surface variables such as rainfall, soil moisture content and ocean wave height.

The ERA5 parameters applied in this study are summarised in Table 4.1. Based on experience, DHI approximate the temporal scale of the ERA5 wind datasets to be equivalent of a 2-hour averaging period.

No other meteorological inputs (such as those related to the heat exchange between the sea and the atmosphere) were included for the hindcast version. The assumption is that the hindcast annual simulation is a realisation of conditions for an actual calendar year, and as such any high frequency variability of heat exchange related parameters (as for example short/long wave downward radiation), would be subdued to lower frequency intraseasonal variability imprinted on the temperature salinity field used to inform the density driven circulation[11]. The temperature variations are used in the MIKE3 temperature/salinity (TS) module which sets up additional transport equations in the model. The calculated temperature and salinity are fed-back to the hydrodynamic equations through buoyancy forcing induced by density gradients. The inputs to the heat exchange include air temperature, short-wave radiation, and long-wave radiation.

Table 4.1 Specification of ERA5 atmospheric model.

Abbreviation	Unit	Description
U_{10}	m/s	Wind speed at 10m above MSL
D_{10}	˚N (coming from)	Wind direction at 10m above MSL

4.3.5.2 Climatology

Atmospheric forcing applied in HD_{ES_Clima} model include the wind speed and wind direction at 10m MSL, atmospheric pressure at mean-sea-level, total precipitation, and evaporation. This forcing was adopted climatologically averaged meteorological conditions derived from the ERA-40 and ERA-Interim re-analysis product (see Section 4.3.1.1). This is the same meteorological forcing as used in the wider domain SSM model; hence, achieving consistency with the model boundary forcing.

Other meteorological inputs specified in HD_{ES_Clima} include items related to heat exchange between the sea and the atmosphere. The temperature variations are used in the MIKE3 temperature/salinity (TS) module which sets up additional transport equations in the model. The calculated temperature and salinity are fed-back to the hydrodynamic equations through buoyancy forcing induced by density gradients. The inputs to the heat exchange include air temperature, short-wave radiation, and long-wave radiation. Once again, these data were adopted climatologically averaged meteorological conditions used in the SSM (see Section 4.3.1.1).

[11] The same is not the case when referring to the climatological model version as any heat exchange parameters are representative of longer trends and intraseasonal signals.

4.3.6 Model configuration

The configuration of the $HD_{ES\_Hindcast/Clima}$ model is summarised in Table 4.2. For more information on the scientific background of the model settings or the governing equations of the model, please refer to [22, 23].

Table 4.2 Summary of $HD_{ES\_Hindcast/Clima}$ model settings.

Setting	Description/Value
Basic equations	Shallow water equations
Numerical scheme	Higher order scheme (time integration and space discretisation)
Horizontal mesh	Variable resolution unstructured grid (see Section 4.3.3)
Simulation period	Hindcast: A one-year hindcast run representing actual conditions in the period June 2017- June 2018 Climatology: A one-year climatological run, which represents average conditions for the period 1990-2014 with a 1993 tidal component.
Model time step (adaptive)	0.01 to 30 seconds
Flooding and drying	Drying depth 0.005m, wetting depth 0.1m
Density	Function of temperature and salinity
Horizontal Eddy viscosity	Smagorinsky formulation with constant = 0.28
Vertical Eddy viscosity	K-epsilon formulation with eddy viscosity values min:1.8e-06/max:0.4 [m^2/s]
Bed resistance	Roughness height (based on material zones) 0.05 to 0.1 (for coastal zones)
Coriolis Forcing	Varying in domain
Wind forcing	Hindcast: Varying in time and domain specified from ERA5 reanalysis Climatology: Varying in time and domain climatologically averaged meteorological conditions derived from the ERA-40 and ERA-Interim re-analysis products used in the SSM climatology forcing
Wind friction	Varying with wind speed (Linear variation Speed): • 7 [m/s] Friction: 0.001255 • 25 [m/s], Friction: 0.002425
Tidal potential	Not included
Precipitation/Evaporation	Hindcast: Not included Climatology: Varying in time and domain climatologically averaged meteorological conditions derived from the ERA-40 and ERA-Interim re-analysis products used in the SSM climatology forcing
Initial conditions	Hindcast: Spatially varying surface elevation (2D) derived from DTU10 global tide model, temperature and salinity (3D) derived from Copernicus Global Ocean Physics Analysis and Forecast[12] product (interpolated to the $HD_{ES\_Hindcast}$ mesh) Climatology: Spatially varying surface elevation (2D) derived from SSM and temperature and salinity (3D) from the SSM climatology (interpolated to the HD_{ES_Clima} mesh)

[12] https://data.marine.copernicus.eu/product/GLOBAL_ANALYSISFORECAST_PHY_001_024/description

Setting	Description/Value
Boundary conditions	Hindcast: Flather boundary conditions, temporally and spatially water levels derived from DTU10 global tide model (1D, horizontal), combined currents from DTU10 and CMEMS (2D, vertical) Climatology: Flather boundary conditions, temporally and spatially water levels and 3D current velocities from SSM climatology
Temperature and salinity module	Hindcast: Temporally and spatially boundaries from CMEMS Climatology: Temporally and spatially boundaries from the SSM plus nudging of the temperature and salinity fields.

4.4 Model outputs

The outputs from the hydrodynamic hindcast and climatology models are summarised in Table 4.3 and Table 4.4. All parameters were saved in all model mesh elements (grid cells) at 0.5-hourly time intervals.

Table 4.3 2D model outputs from $HD_{ES\_Hindcast/Clima}$.

Parameter	Unit	Description
Surface elevation	m	Still water level relative to MSL
Total water depth	m	Total water depth
u-velocity component	ms^{-1}	Depth-averaged velocity speed in the west-to-east direction
v-velocity component	ms^{-1}	Depth-averaged velocity in the south-to-north direction
P Flux	$m^3s^{-1}m^{-1}$	Flow flux per metre in west-to-east direction
Q Flux	$m^3s^{-1}m^{-1}$	Flow flux per metre in south-to-north direction

Table 4.4 3D model outputs from $HD_{ES\_Hindcast/Clima}$

Parameter	Unit	Description
u-velocity component	ms^{-1}	Current velocity in the west-to-east direction
v-velocity component	ms^{-1}	Current velocity in the south-to-north direction
w-velocity component	ms^{-1}	Current velocity in the vertical direction
Density	kgm^{-3}	-
Temperature	°C	-
Salinity	PSU	Practical Salinity Unit
TKE	m^2s^{-2}	Turbulent Kinetic Energy
ε	m^2s^{-3}	Dissipation of turbulent kinetic energy

Also provided are the decoupled files comprising of setup files, area output (Total water depth, U, V - velocity components) and fluxes which can be utilised to run both future AD simulations and particle tracking results. Still water depth and element size of the computational mesh (common for both model realisations) are provided as a separate time-invariant output.

4.5 Model files

The hydrodynamic climatology and hindcast models are supplied to SSF as part of the project deliverables. The data are provided in DHI MIKE format and can be used to generate boundary conditions for local climatology/hindcast modelling or as input for scenario modelling.

Appendix A includes a description of the model files that are provided alongside this report.

5 Hydrodynamic hindcast model calibration and validation

In this section, the calibration and validation of the hydrodynamic hindcast models are presented.

In general, all stations examined had a good representation of the water level signal and thus the model was well replicating the tidal signal propagation. The model was also well capturing sites with current speeds < 0.3m/s (as for example Swarta Skerry and Vidlin North/Outer) but was failing to fully capture conditions at more energetic sites such as Bellister, especially the highest range of observed velocities. This discrepancy guided final calibration efforts towards adjusting the velocity field that was being used as boundary forcing. The adjustment was based on the bias of the tidal current speed signal used as forcing versus the inferred one following tidal analysis of the observational records at the stations in question.

5.1 Model Calibration

The East of Shetland hydrodynamic hindcast model was calibrated against observed hydrographic data (water levels and currents) provided by SSF as part of their measurement campaigns in respective sites of interest at the East of Shetland general area, see also Section 3.2.

The model calibration/validation periods were selected based on the temporal and spatial coverage of the available data as described in Section 3.2. These are detailed in Table 5.1 (see also Table 3.2 for specific deployment details) and shown in Figure 5.1.

Table 5.1 East of Shetland hydrodynamic hindcast model calibration/validation deployment campaigns.

Site	ID	Survey Start (yyyymmdd)	Survey End (yyyymmdd)	Deployment depth (mMSL)	Lat (degrees)	Long (degrees)
Calibration stations						
Swarta Skerry	53_SS02Jan18	20180119	20180309	37.0	60.340400	-1.146049
Bellister	49_BELL01Jan18	20180120	20180309	40.9	60.331658	-1.108400
Swarta Skerry	54_SS03Mar18	20180320	20180507	36.8	60.340441	-1.146092
Bellister	50_BEL02Mar18	20180320	20180507	38.2	60.331184	-1.109060
Vidlin Outer	40_VO01May18	20180514	20180702	34.9	60.390853	-1.117991
Vidlin North	44_VNMay18	20180514	20180702	30.7	60.387273	-1.120441
Swarta Skerry	55_SS04Jul18	20180706	20180806	36.7	60.340550	-1.146050
Vidlin North	45_VN02Oct18	20181009	20181123	31.5	60.387670	-1.121870
Vidlin Outer	41_VO02Oct18	20181009	20181204	35.0	60.390730	-1.117850
Validation stations						
Taing of Kelswick	56_ToK02May21	20210509	20210929	52.2	60.4048	-1.087633
Taing of Kelswick	57_TOK2001Jun21	20210610	20210929	46.2	60.40625	-1.086683
Setterness North	67_3SN21000Dec21	20211203	20220308	54.7	60.43	-1.12884
Fish Holm	91_N008_FishHolm	20220421	20220725	66.9	60.44483	-1.123783

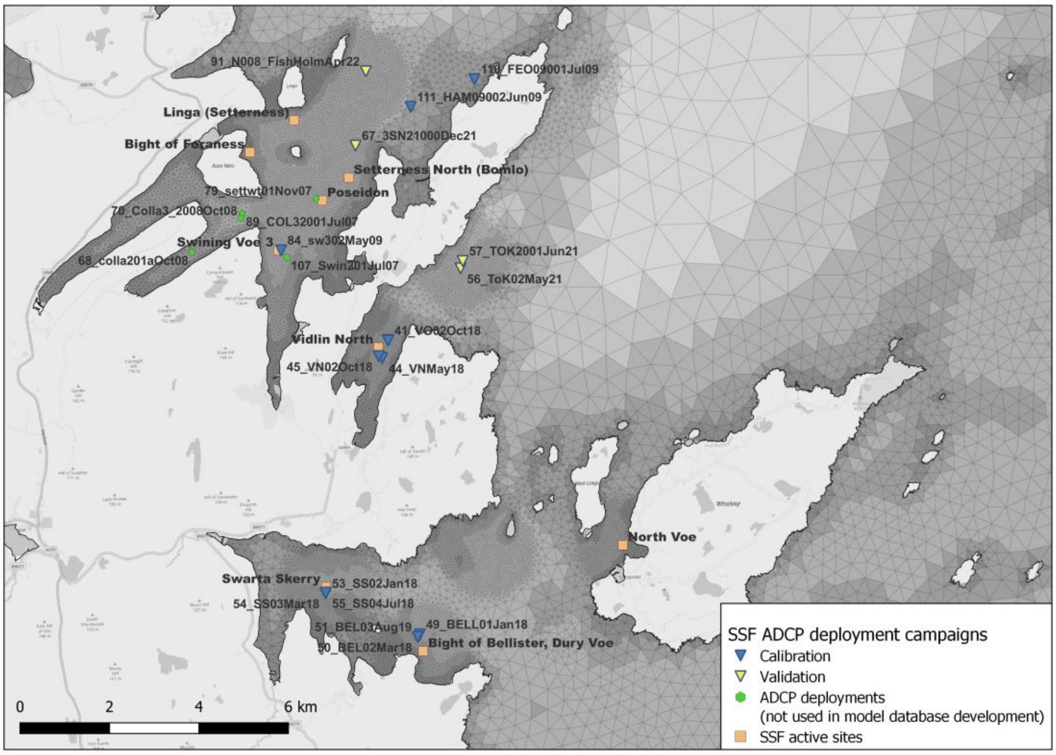


Figure 5.1 East of Shetland hydrodynamic hindcast model calibration and validation sites

Section 5.3 details the results from these calibration periods and sites. A brief mention at each calibration site is detailed below.

Several iterations in the context of sensitivity runs, involving parameter adjustments (for example spatial varying bed friction and/or bathymetric adjustments), were initially assessed to define calibration limits. Choice of final setup was based on achieving good model skill (in terms of performance metrics against the observational record with special focus on the velocity field i.e., current speeds and directions) collectively in the whole East of Shetland area. Validation was focused on the Taing of Kelswick and Fish Holm measurement campaigns. Table 5.2 provides a brief account of the second phase[13] of calibration aiming to improve model skill on observational record 3D current speed representation.

Table 5.2 Main setups for second phase of calibration on improving model skill on current speeds.

Calibration setup name	period	Forcing		
		Tidal (boundaries)	Baroclinic (boundaries)	Wind (domain)
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018 (p2)	2018	See Table 4.2	See Table 4.2	See Table 4.2
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018 (p2)	2018	Adjusted tidal velocities upwards by a factor of 2	See Table 4.2	See Table 4.2

[13] The first phase, not presented herein, was focused on assessment of propagation of tidal signals across the computational domain and relevant parameterisations as bed friction etc.

5.1.1 Initial calibration and velocity adjustment

Surface elevation (water level), both total and tidal components, was well represented at most of the calibration sites, Figure 5.2. Thus, the tidal water level signal was correctly propagated throughout the computational domain. The magnitude of the 3D velocity field represented that observed in most locations quite well. However, current speeds in the Bellister area were underestimated significantly in comparison to the observational records at the same location, Figure 5.3. It was therefore decided to adjust the tidal velocities[14] at the boundaries. While this improved representation of the velocity field throughout the calibration stations it resulted in a phase shift in water levels, meaning a less favourable comparison with the observational records. Below an account on model performance about water levels at the Bellister, Vidlin North and Swarta Skerry measurement stations is provided prior to the velocity field adjustment and after.

[14] The adjustment of the velocity field was focused on the tidal component based on the statistics of the modelled tidal currents vs those reconstructed from the observational deployment at Bellister stations supported with anecdotal evidence from SSF on intensity of tidal currents during operations at the Bellister site. Velocities (tidal component) were scaled by a factor of 2 at all boundaries (see text below).

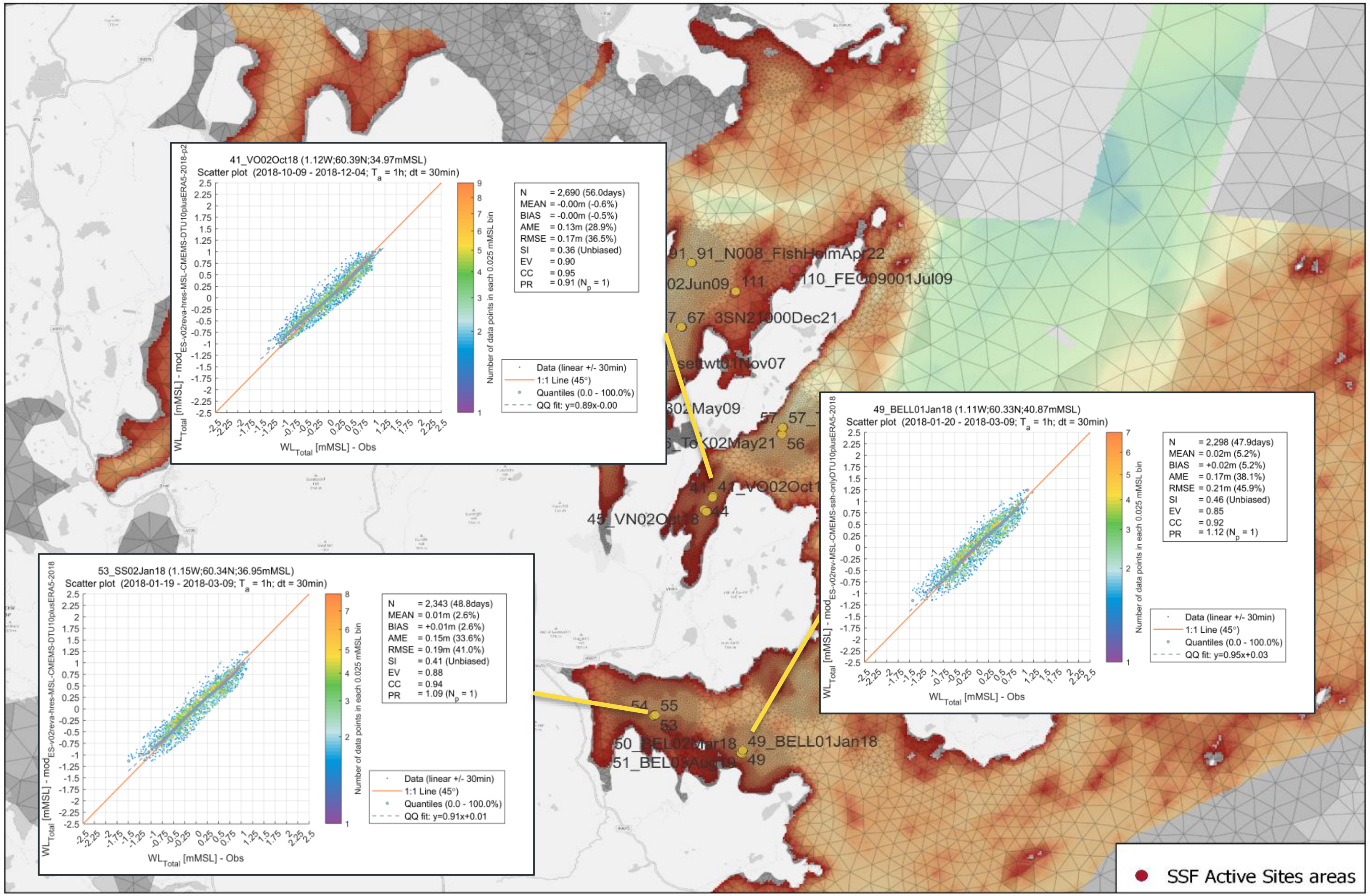


Figure 5.2 Selected locations depicting water level comparisons to observational record BEFORE adjustment of the velocity field.

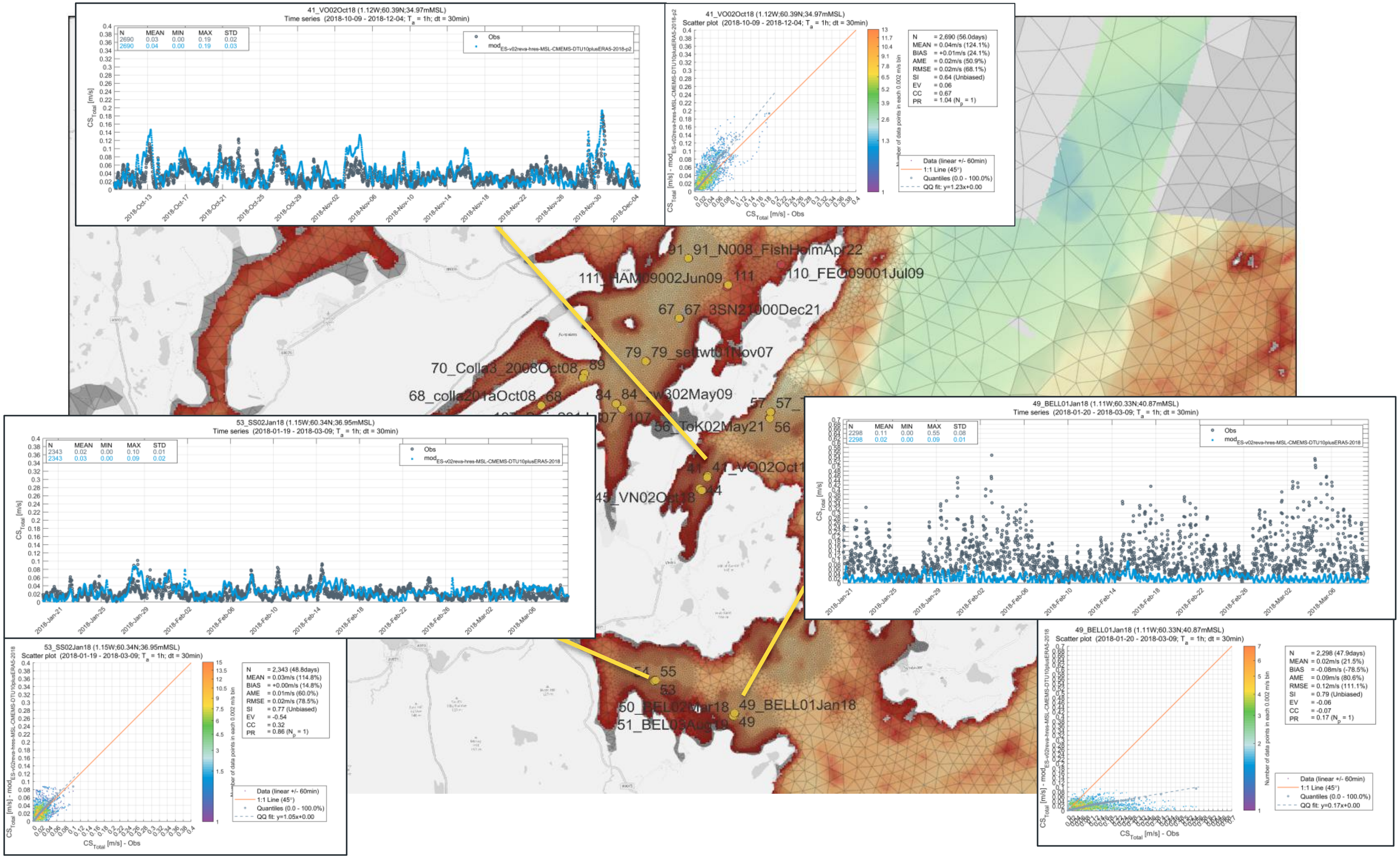


Figure 5.3 Selected locations depicting timeseries and scatterplots comparisons of modelled depth averaged currents' magnitude versus the observational record BEFORE adjustment of the velocity field. Statistical metrics are provided in detail in section 5.3.

5.1.2 Water levels

Scatterplots comparisons of observed versus modelled water levels for selected calibration sites prior to the velocity field adjustment are presented in Figure 5.4 (left column). Inspection of the calibration plots show that for total (and tidal) water level - not shown herein - there is a good overall fit between the observations and the model output especially with respect to the timing of high and low water. Discrepancies could be attributed to the observational record itself and/or misrepresentation of local bathymetric features rather than episodic events not within the variability resolution capacity of the modelled hydrodynamics. The latter is less probable though given the model mesh bathymetry is informed by high resolution multibeam surveys (see also 4.3.3).

Also, in Figure 5.4 (right panel) are shown comparisons of observed versus modelled water levels following the revision of velocity field forcing at the model boundaries. Adjustment of the tidal component of the velocity field results in the introduction of a phase error ‘globally’ at all calibration stations examined; the overall Q-Q fit though is remains good, approximately 1:1, with the same range of water level as before (no changes on actual surface elevation forcing was performed).

Additional steps to alleviate the phase error during the calibration phase were focused on bed friction changes and shifting actual timing of water level signal forcing at the boundaries. There was none to minimal observed changes in model skill in relation to water level comparisons versus the observational record in all these efforts. Given the focus was mainly on the robust representation of the 3D velocity field throughout the computational domain it was, thus, decided to proceed with the adjustment of the velocity forcing regardless of the introduced phase error in the water levels.

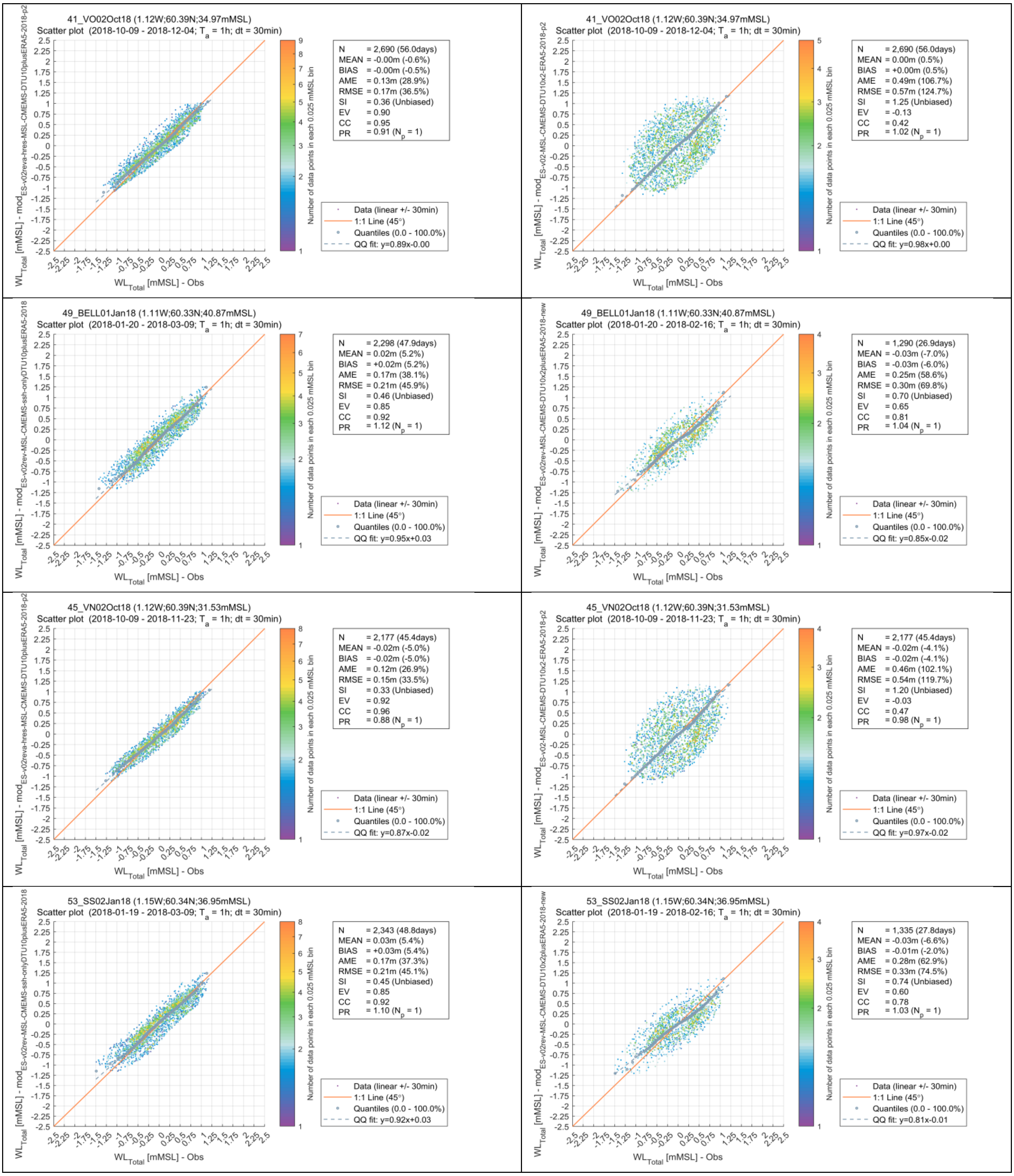


Figure 5.4 Scatterplot comparisons of observed versus modelled water levels at selected calibration sites as in Table 5.1 (left column) prior to final adjustment of the velocity field forcing at the model boundaries and (right column) following the final adjustment of the velocity field forcing at the model boundaries.

5.1.3 Currents

The model skill on current speed and directions representation, following the velocity field adjustment, throughout the computational domain within the East of Shetlands area is considered good on basic qualitative judgement. Current speeds satisfy criteria as set out in [8] in the majority of the sites of interest. Mean directions are well represented in general, but with low conformity to criteria as in [8].

In Figure 5.5, depth-averaged current speeds and directions are depicted for selected locations as in Table 5.1. At Bellister area (station 49_BELL01) there is measurable improvement in current speed representation versus initial assessment. At calibration stations at the respective sites of Vidlin North and Outer the model skill is also good. At Swarta Skerry site, 53_SS02Jan18 station is well represented in terms of magnitude of depth-averaged currents but current directions when averaged over the whole water column are not depicted accurately. On the contrary, at station 67_3SN21000 at Setterness North site while depth averaged directions are represented well the depth-averaged current speed maxima are underestimated even following the velocity field adjustment.

When examining the 3D velocity representations, at all calibration stations there is consistently good representation of current speeds at near surface, cage bottom and near bed levels. **Bellister** site is well replicated in the model with a better depiction of cage bottom directional distributions of current speed. **Vidlin North** and **Outer** have also well replicated current speeds at all levels but directions for both locations are better represented for the deeper levels rather than the near surface ones. For **Swarta Skerry** site the near surface directional distribution of current speed is better depicted versus that at the lower water column levels. The discrepancies can potentially be associated to the resolution of surface wind forcing given the grid resolution of the ERA5 dataset, used herein in for the atmospheric forcing of the modelled hydrodynamics, is far coarser than the spatial dimensions of Vidlin Voe and similarly sheltered locations.

Timeseries, scatter and dual rose plots comparisons of observed versus modelled currents are shown in Figure 5.6-Figure 5.9 for the near surface, cage bottom[15] and near bed levels for the Bellister, Vidlin Voe and Swarta Skerry locations.

[15] Cage bottom is here selected as the model sigma layer mid-depth which is in the range between 15-20m from water surface.

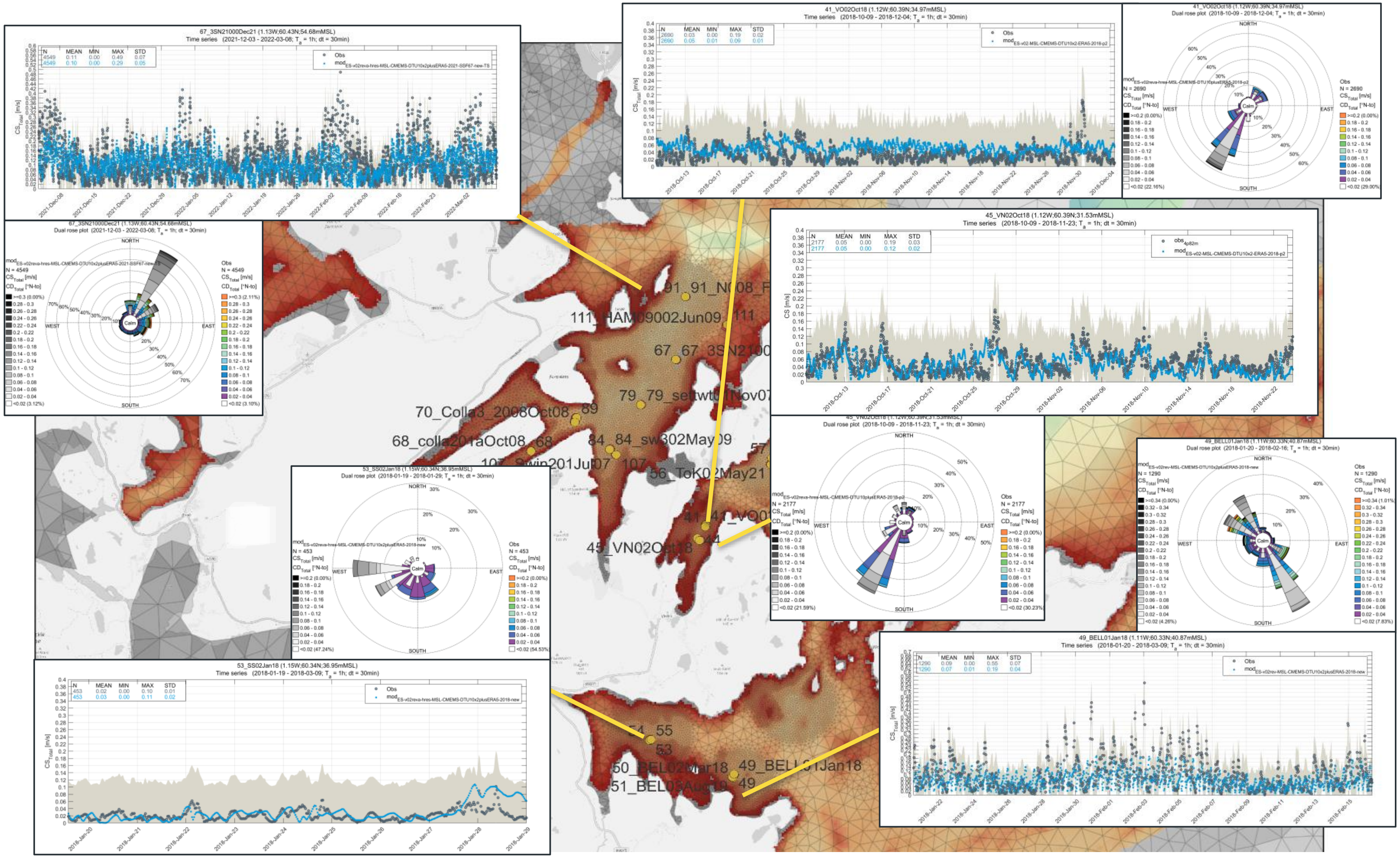


Figure 5.5 Dual rose plots and timeseries of current speed and directions of observational records vs model output for selected calibration sites. SEPA's regulatory criteria for current speeds [8] shown as shaded area. Statistical metrics are provided in detail in section 5.3.

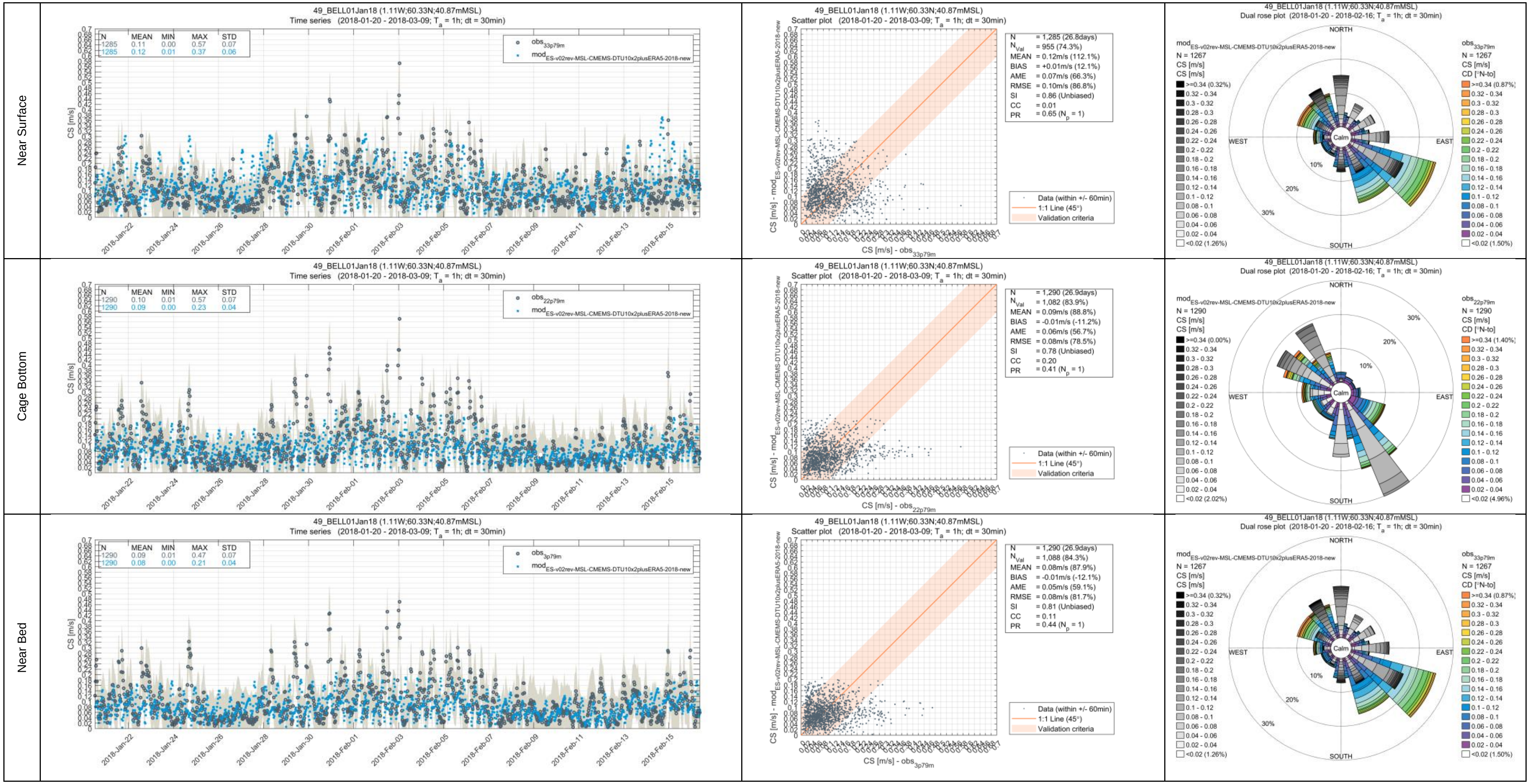


Figure 5.6 Station **49_BELL01Jan18**. Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons for near surface (top row), cage bottom (middle row) and near bed (bottom row) current speed and directions, see Table 5.1. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

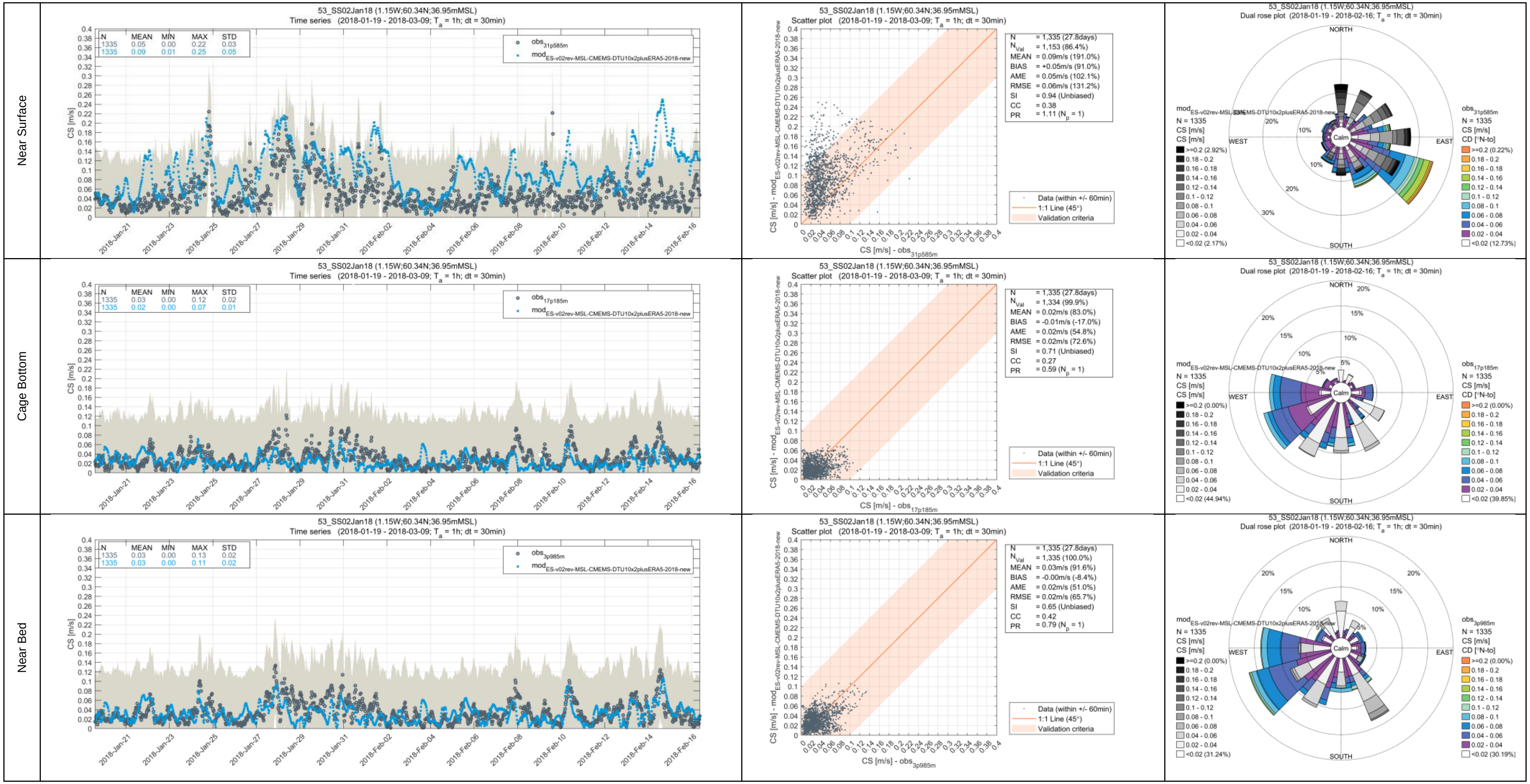


Figure 5.7 Station **53_SS02Jan18.** Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons for near surface (top row), cage bottom (middle row) and near bed (bottom row) current speed and directions, see Table 5.1. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

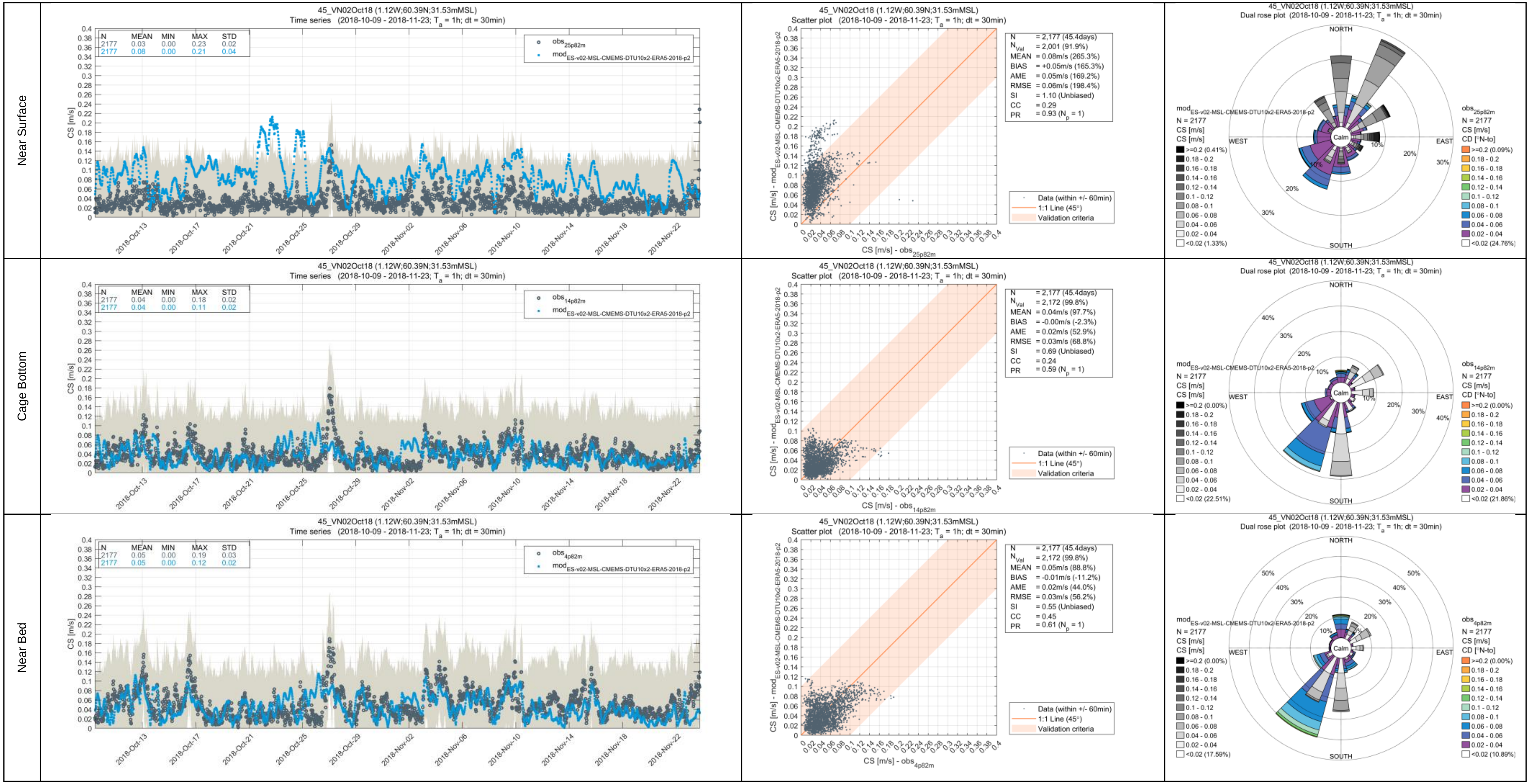


Figure 5.8 Station **45_VN02Oct18**. Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons for near surface (top row), cage bottom (middle row) and near bed (bottom row) current speed and directions, see Table 5.1. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

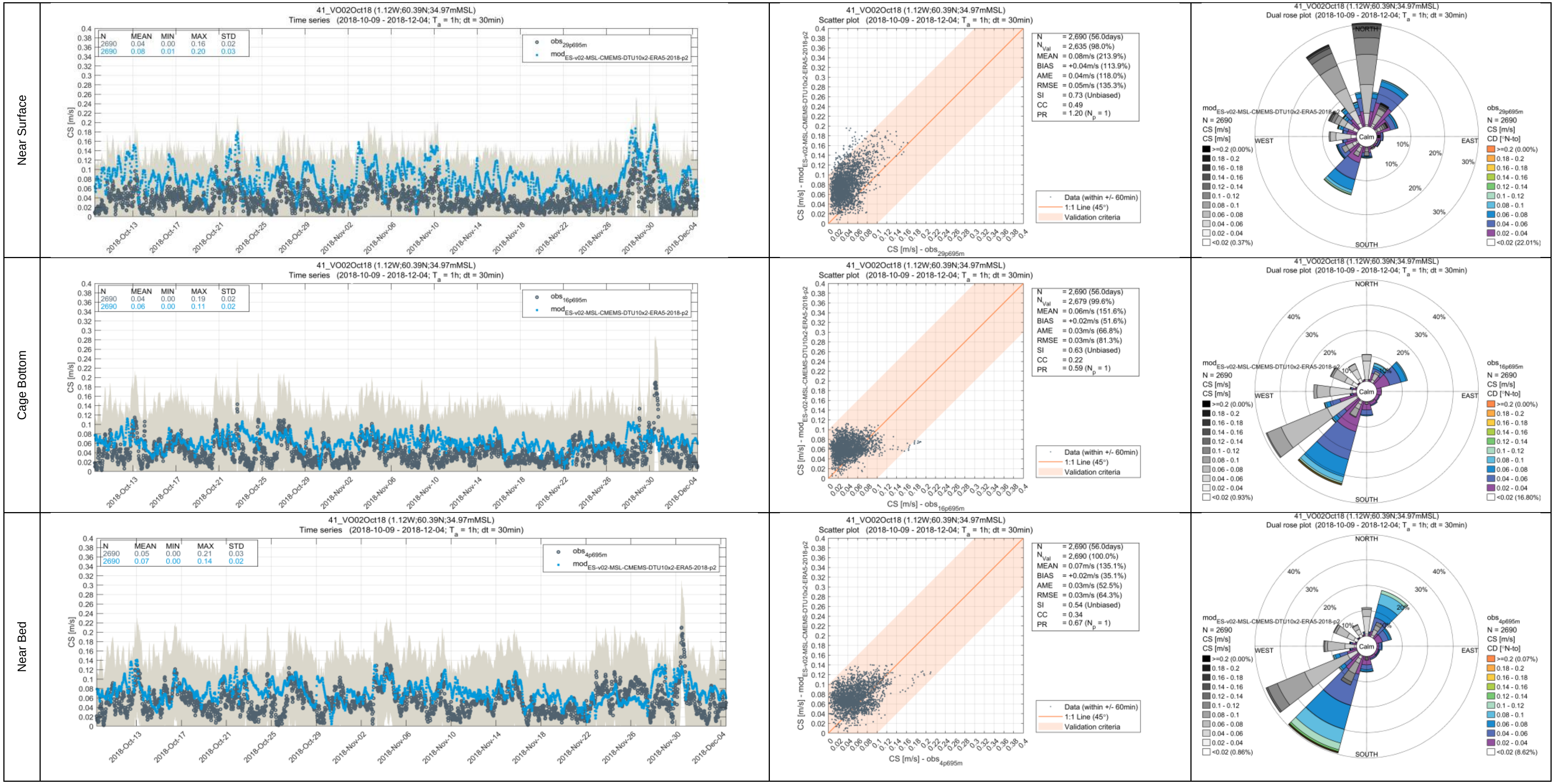


Figure 5.9 Station **41_VO02Oct18**. Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons for near surface (top row), cage bottom (middle row) and near bed (bottom row) current speed and directions, see Table 5.1. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

5.2 Model Validation

The East of Shetland hydrodynamic hindcast model was validated against observed hydrographic data (water levels and 3D currents) from four (4) measurement campaigns in Taing of Kelswick, Setterness and Fish Holm.

The model validation periods were selected based primarily on the spatial relevance of the available data. These are detailed in Table 5.1 and Figure 5.1.

Section 5.3 details the results from these sites for the validation period. All validation images are included as a digital appendix to this report (Appendix C). Validation plots for Taing of Kelswick, Setterness and Fish Holm are shown in the following section.

In addition, SEPA's hydrodynamic model criteria as in [8], p.34, Table 3 are presented along with the timeseries and scatterplots.

5.2.1 Water Levels

The velocity field scaling used to increase current speeds in the model has resulted in a time delay between the peak of a tidal force and the resulting peak of the tidal response (phase lag error). This delay has affected the validation of the model against in-situ data collected at numerous locations throughout the model domain. It is important to consider this delay when analysing the results of the model and to further monitor and assess its impact on the accuracy of the model.

Figure 5.10 and Figure 5.11 present timeseries and scatterplot comparisons of observed and modelled water levels at Taing of Kelswick, Setterness North, and Fish Holm. At Taing of Kelswick, two ADCPs were deployed. The first was deployed on May 09, 2021, and the second ADCP was deployed on June 10, 2021. During the second deployment, the first ADCP was lifted out the water and redeployed at approximately the same location. However, this redeployment resulted in the device being placed into shallower water, which caused a 0.5m drop in water level. This change can be observed in the time series plot in Figure 5.10 and affects the validation statistics of water levels at this site (site reference 56_ToK02).

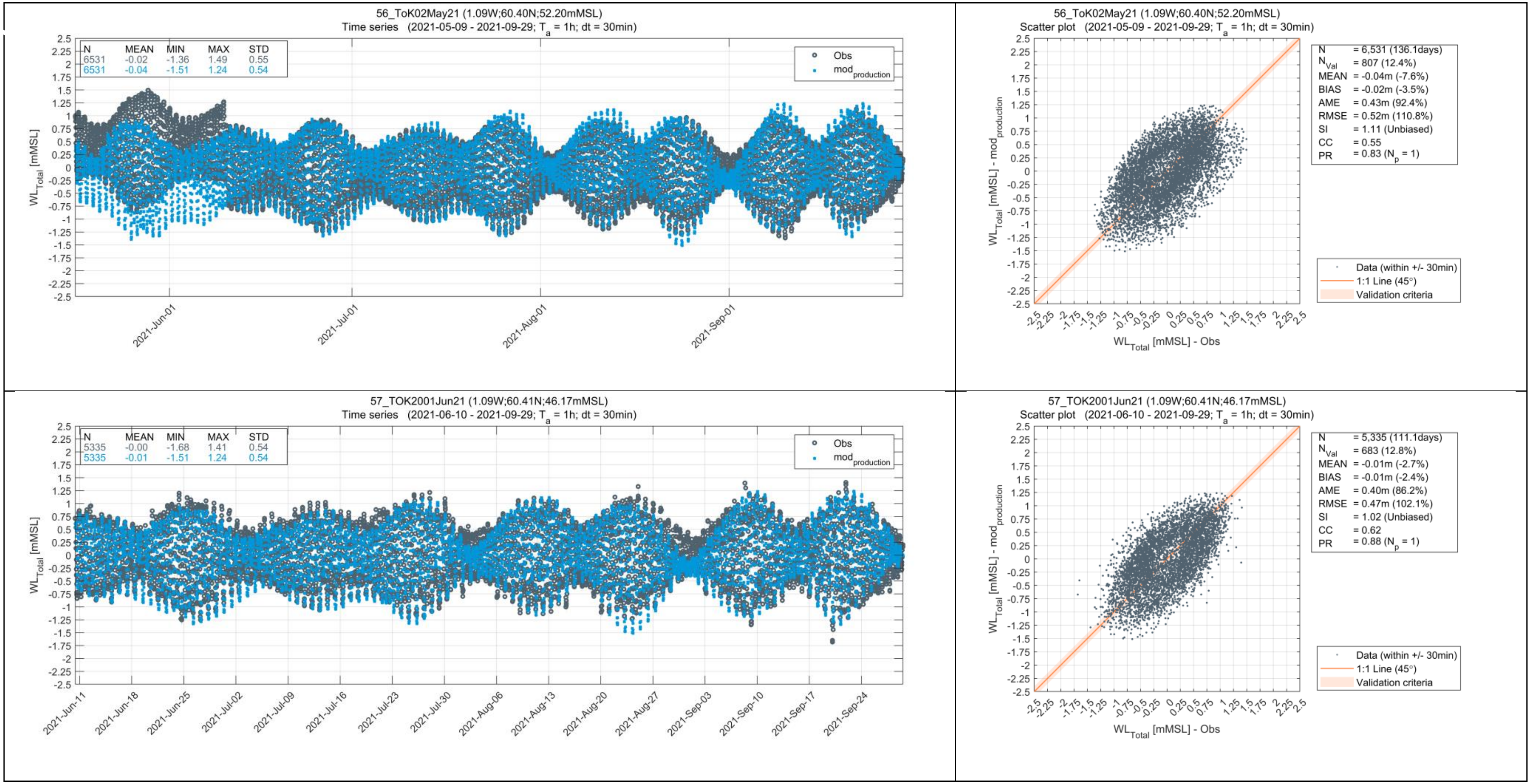


Figure 5.10 Timeseries (left) and scatterplot (right) comparisons of observed and modelled water levels at SSF's **Taing of Kelswick** ADCP locations, see also Table 5.1.

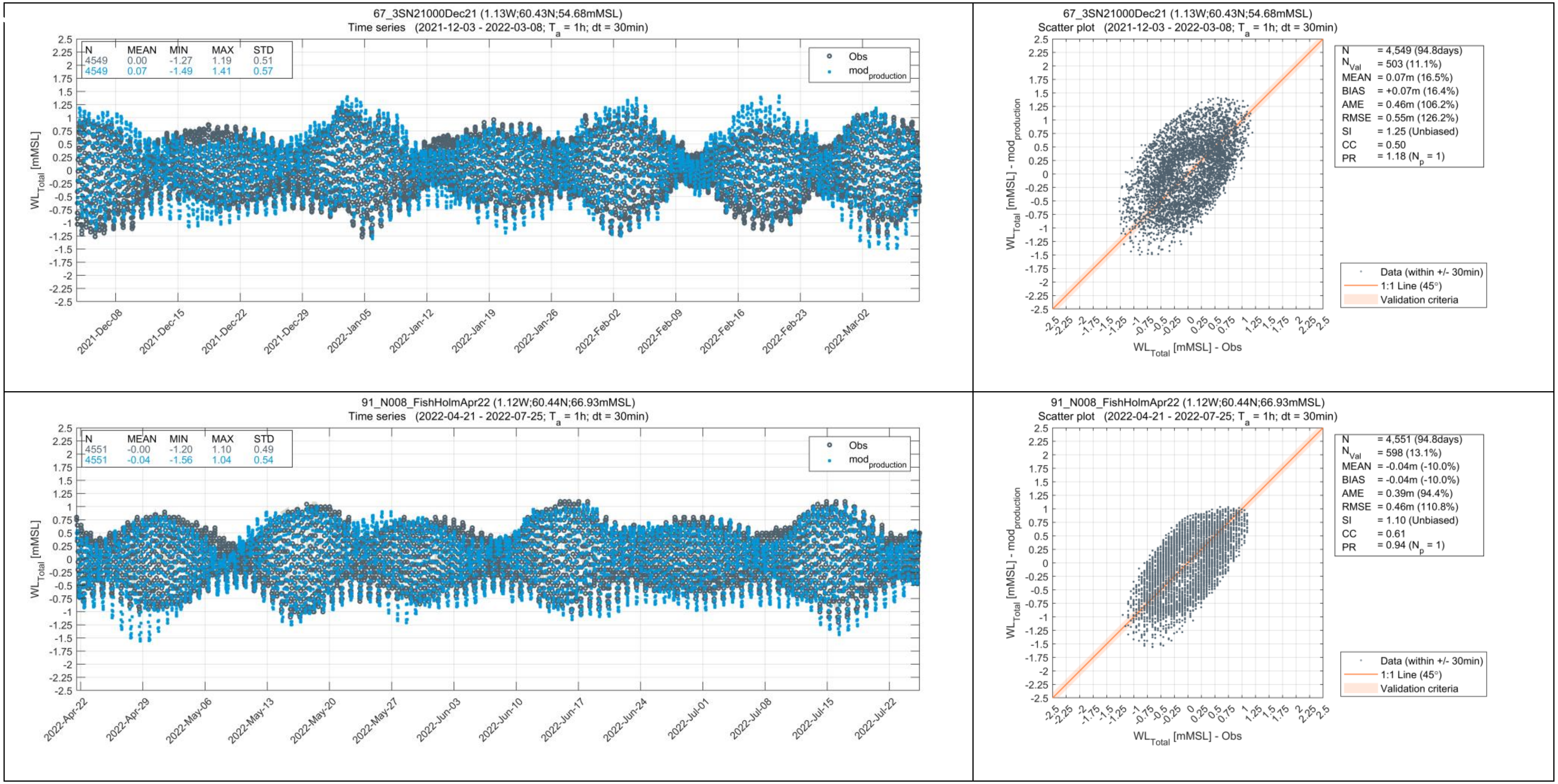


Figure 5.11 Timeseries (left) and scatterplot (right) comparisons of observed and modelled water levels at SSF's **Setterness North** and **Fish Holm** ADCP locations, see also Table 5.1.

5.2.2 Currents

The $HD_{ES\_Hindcast}$ model was validated against several stations, and the results indicate that it provides a good replication of current conditions at Taing of Kelswick sites. However, the model's performance is less satisfactory at North Setterness and Fish Holm, where it replicates current conditions accurately about 60 – 76 % of the time. For these sites, the model is considered to depict the mean status of current speed and direction but to a lesser degree the instantaneous variability, in terms of magnitude, exhibited by the observational record. A more detailed description of validation results for each site is given below and summarised in Figure 5.12 to Figure 5.15.

Taing of Kelswick

At the first Taing of Kelswick site (56_ToK02) the model performs well in terms of current speed, meeting SEPA guidelines. Validation against observations representing cage bottom showed good representation of current direction and magnitude, although the near-surface region was less well represented. At the second site (57_TOK2001), the same general trends were observed, with some variation in the representation of cage bottom. Modelled currents at the near the bed level show less favourable agreement to the ones derived from the observational record to an almost reverse predominant direction but replicated within criteria as in [8] for 98% of the time.

Setterness North

The $HD_{ES\_Hindcast}$ model generally captured the predominant current directions in the range 330° to 60°, albeit with less success for currents within the 90° to 270° degree range. At all vertical levels examined, the model consistently overpredicted currents flowing to the North-East. In terms of current speed, the model was within SEPA's criteria 61% of cases at the surface, mainly due to the exhibited model bias attributed here to the wind driven currents, 74% of cases at the cage-bottom, and 79% of cases near the bed. However, some deviations were found, with the model biased towards faster current speeds at the surface (+0.05m/s) and somewhat slower current speeds at the cage bottom (-0.01m/s).

Fish Holm

For the Fish Holm site, the model predicts reasonably well current directions at most vertical levels. However, there is a negative bias in the model's current speed prediction, consistently underpredicting magnitudes by 0.06 m/s to 0.07 m/s throughout the water column. The model's validation metric against SEPA's criteria in terms of current speed is 67% at the near surface, 70% at the cage bottom, and 66% at the near bed.

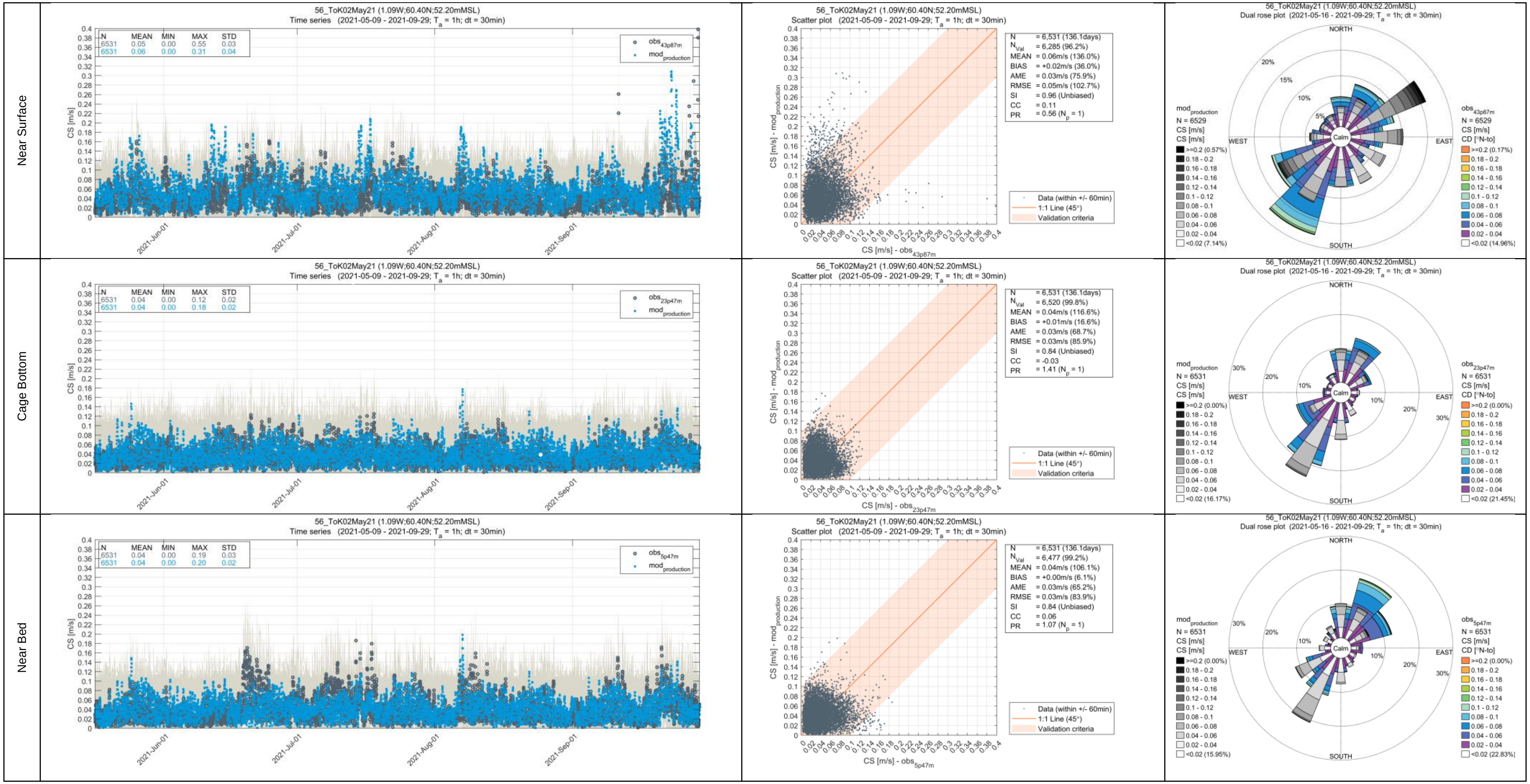


Figure 5.12 Station **Taing of Kelswick** (reference **T0K02**). Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons of observed and modelled 3D currents at near surface (top row), cage bottom (middle row) and near bed (bottom row) depths. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

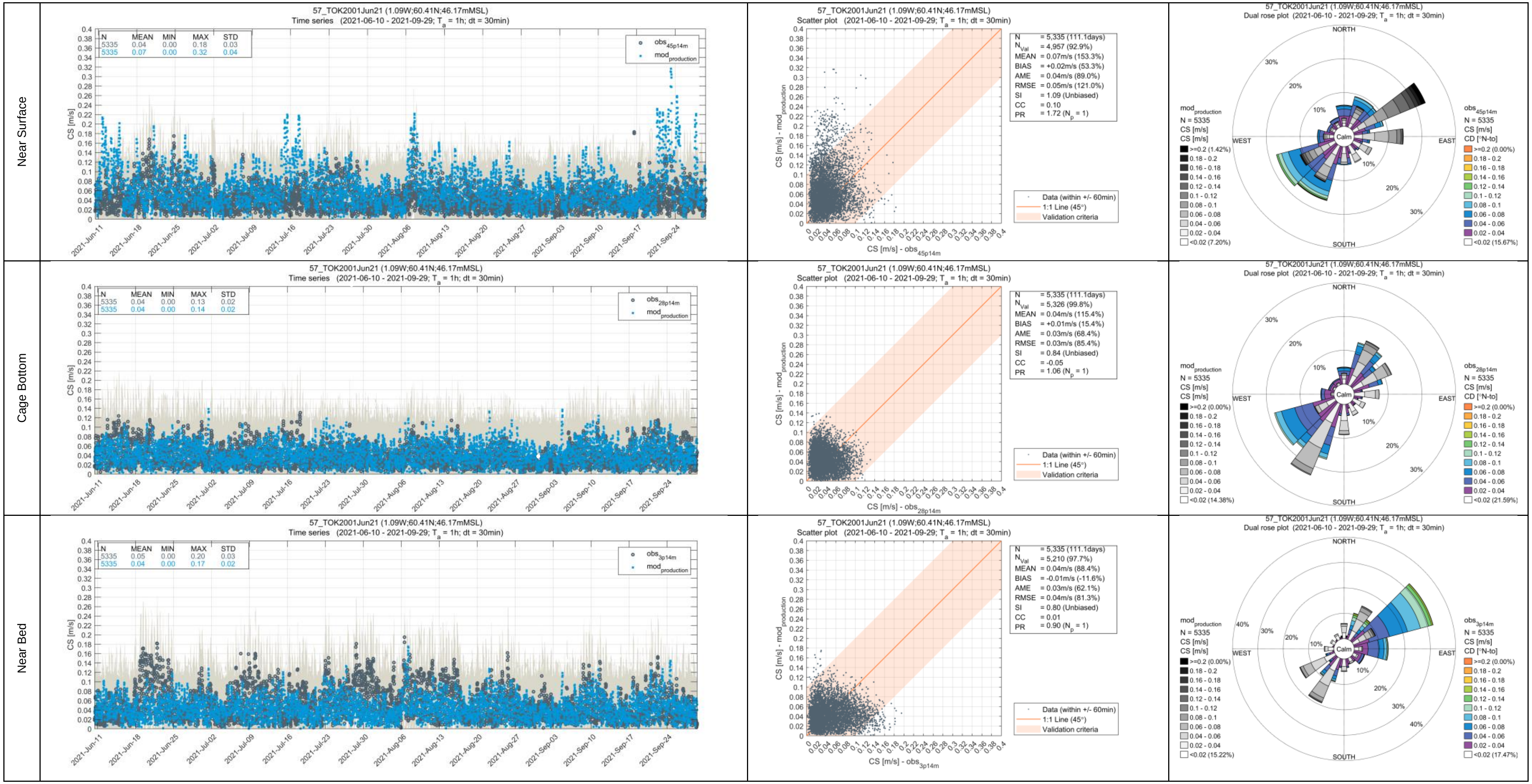


Figure 5.13 SSF's **Taing of Kelswick** site (reference **TOK2001**). Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons of observed and modelled 3D currents at near surface (top row), cage bottom (middle row) and near bed (bottom row) depths. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

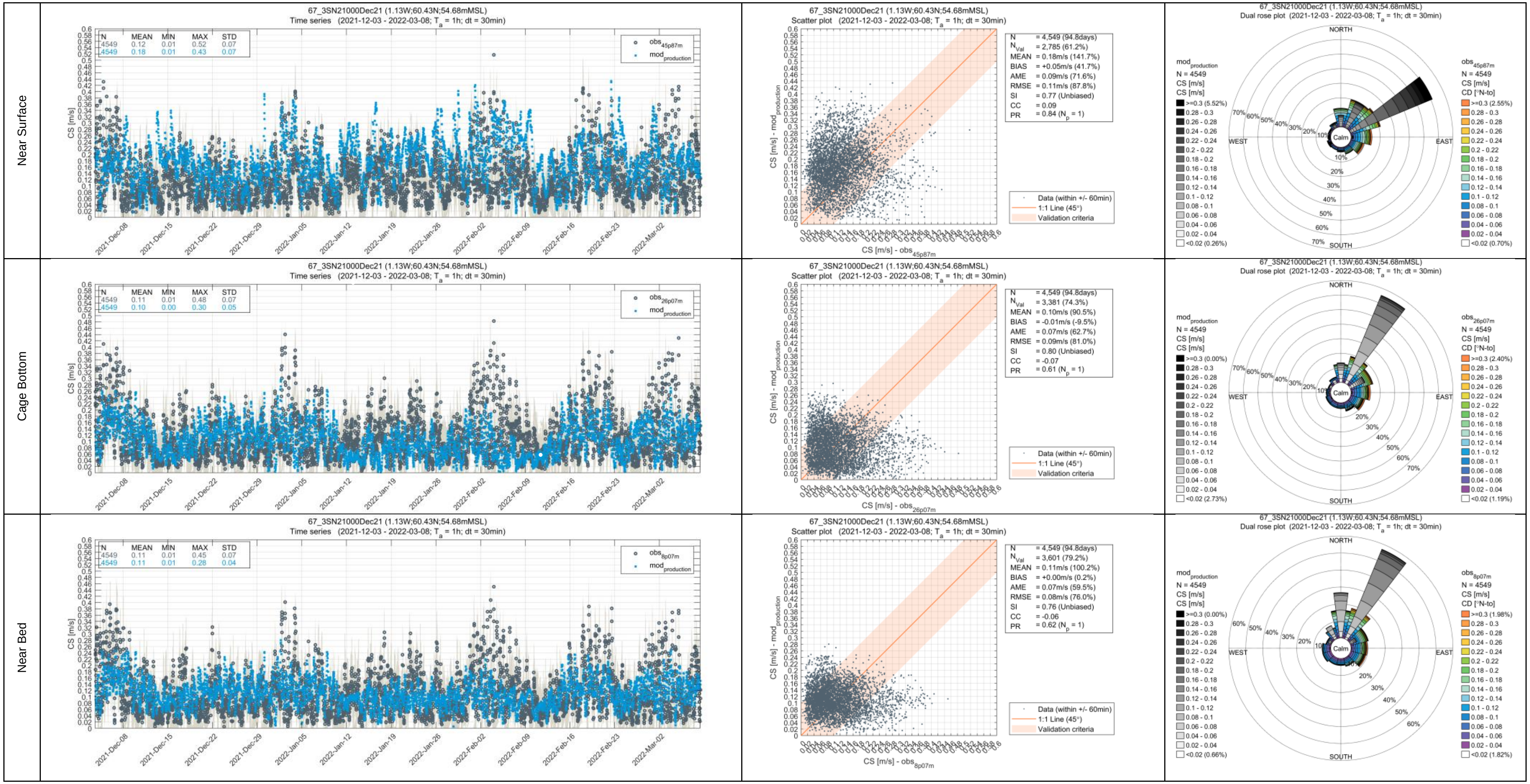


Figure 5.14 SSF's **Setterness North** site. Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons of observed and modelled 3D currents at near surface (top row), cage bottom (middle row) and near bed (bottom row) depths. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

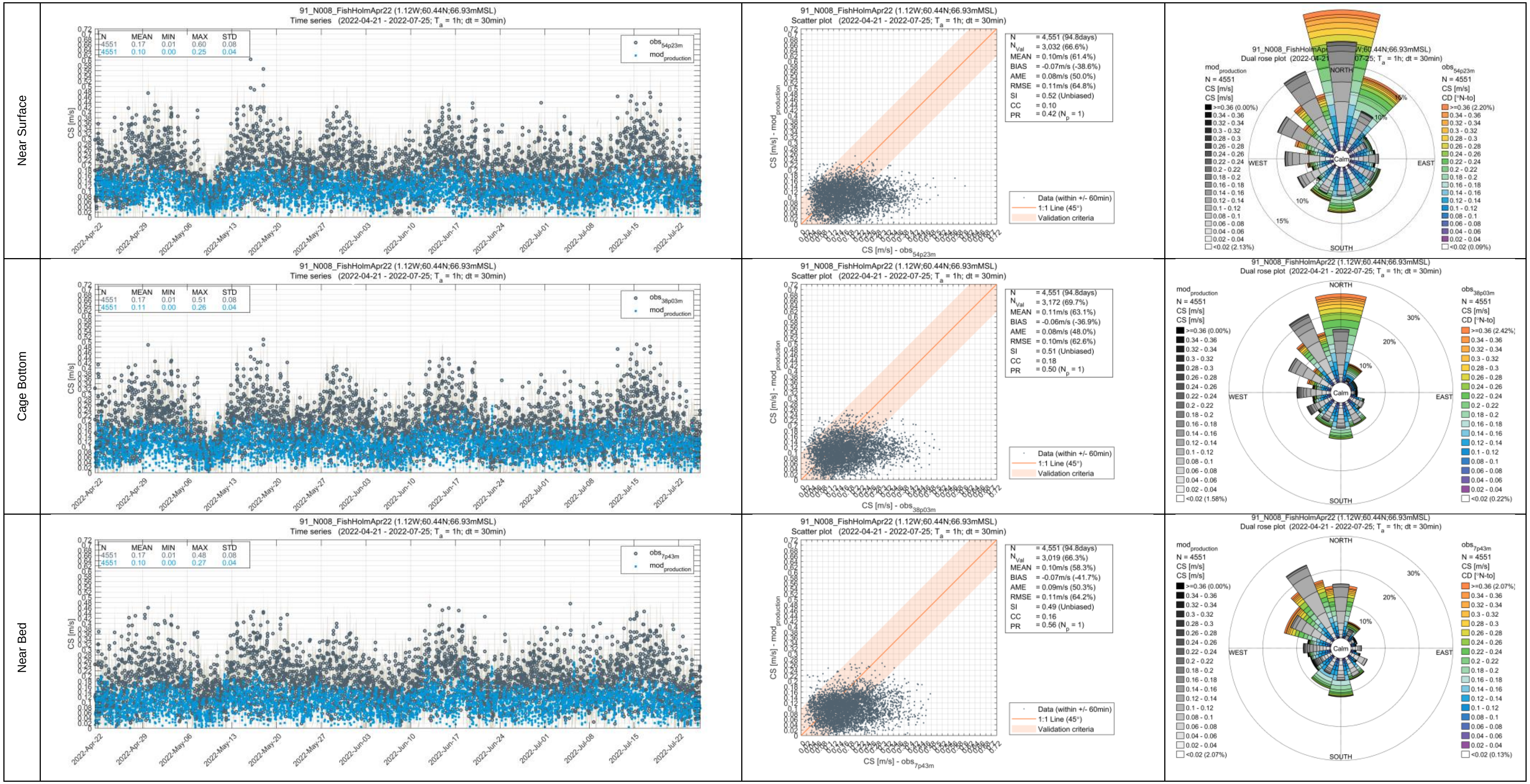


Figure 5.15 SSF's **Fish Holm** site. Timeseries (left-column panels) , scatter (mid-column panels) and dual rose (right-column panels) plots comparisons of observed and modelled 3D currents at near surface (top row), cage bottom (middle row) and near bed (bottom row) depths. SEPA's regulatory criteria for current speeds [8] shown as shaded area with percentage of conformity as N_{val} (only at scatterplots).

5.3 Summary of model quality indices

Below a summary of quality indices for the calibration and validation periods is presented for water level (WL) and current speed (CS) for all observational records used during the calibration and validation stages of the hydrodynamic database development.

5.3.1 Water Level (WL)

Table 5.3 Summary of the East of Shetland hydrodynamic hindcast model against calibration/validation sites, water level (WL) quality indices with conformity percentage (Nval %) to SEPA's criteria as in [8].

CALIBRATION																								
			WL - Obs				WL - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018																								
53SS02	2343	48.8	-0.00	-1.49	1.13	0.54	-0.41	-1.56	0.81	0.49	79	3.4	-0.41	-89.6	-0.41	-89.6	0.41	89.9	0.45	98.5	0.41	0.94	0.72	Np = 1
49BELL01	2298	47.9	-0.00	-1.43	1.11	0.53	-0.41	-1.57	0.81	0.50	73	3.2	-0.41	-92.1	-0.41	-92.0	0.42	92.3	0.45	100.9	0.41	0.94	0.73	Np = 1
54SS03	2331	48.6	0.00	-1.21	1.15	0.52	-0.44	-1.48	0.55	0.48	16	0.7	-0.44	-100.0	-0.44	-99.9	0.44	99.9	0.46	104.3	0.30	0.97	0.48	Np = 1
50BEL02	2307	48.1	0.00	-1.21	1.11	0.52	-0.44	-1.49	0.56	0.49	16	0.7	-0.44	-99.9	-0.44	-99.8	0.44	99.8	0.46	104.2	0.30	0.97	0.50	Np = 1
40VO01	2349	48.9	-0.00	-1.14	1.22	0.55	-0.51	-1.52	0.73	0.48	16	0.7	-0.51	-107.7	-0.51	-107.6	0.51	107.7	0.53	110.8	0.26	0.98	0.59	Np = 1
44VN	2348	48.9	-0.00	-1.17	1.20	0.55	-0.51	-1.52	0.73	0.48	23	1.0	-0.51	-107.6	-0.51	-107.6	0.51	107.6	0.53	111.0	0.27	0.98	0.60	Np = 1
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018-p2																								
45VN04	2177	45.4	-0.00	-1.27	1.19	0.54	-0.30	-1.38	0.76	0.47	184	8.5	-0.30	-66.8	-0.30	-66.8	0.30	67.0	0.34	74.6	0.33	0.96	0.64	Np = 1
41VO02	2690	56.0	-0.00	-1.32	1.15	0.54	-0.28	-1.38	0.76	0.48	313	11.6	-0.28	-61.7	-0.28	-61.6	0.29	63.2	0.33	71.6	0.36	0.95	0.66	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018																								
53SS02	1335	27.8	-0.02	-1.49	1.08	0.52	-0.33	-1.50	0.81	0.42	248	18.6	-0.33	-74.7	-0.31	-70.1	0.37	83.9	0.45	102.2	0.74	0.78	0.75	Np = 1
49BELL01	1290	26.9	-0.00	-1.43	1.08	0.50	-0.33	-1.52	0.82	0.43	219	17.0	-0.33	-78.2	-0.33	-77.2	0.37	86.3	0.44	103.9	0.70	0.81	0.76	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018-p2																								
45VN04	2177	45.4	-0.00	-1.27	1.19	0.54	-0.29	-1.45	0.90	0.52	253	11.6	-0.29	-63.0	-0.29	-63.0	0.52	113.7	0.61	135.2	1.20	0.47	0.76	Np = 1
41VO02	2690	56.0	-0.00	-1.32	1.15	0.54	-0.26	-1.45	0.90	0.53	292	10.9	-0.26	-57.7	-0.26	-57.7	0.53	115.5	0.63	137.4	1.25	0.42	0.79	Np = 1

VALIDATION																							
			WL - SSM				WL - MIKEClima																
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
PRODUCTION RUN																							
56ToK02	6531	136.1	-0.02	-1.36	1.49	0.55	-0.04	-1.51	1.24	0.54	807	12.4	-0.04	-7.6	-0.02	-3.5	0.43	92.4	0.52	110.8	1.11	0.55	0.83	Np = 1
57TOK2001	5335	111.1	-0.00	-1.68	1.41	0.54	-0.01	-1.51	1.24	0.54	683	12.8	-0.01	-2.7	-0.01	-2.4	0.40	86.2	0.47	102.1	1.02	0.62	0.88	Np = 1
673SN21000	4549	94.8	0.00	-1.27	1.19	0.51	0.07	-1.49	1.41	0.57	503	11.1	0.07	16.5	+0.07	16.4	0.46	106.2	0.55	126.2	1.25	0.50	1.18	Np = 1
91N008	4551	94.8	-0.00	-1.20	1.10	0.49	-0.04	-1.56	1.04	0.54	598	13.1	-0.04	-10.0	-0.04	-10.0	0.39	94.4	0.46	110.8	1.10	0.61	0.94	Np = 1

5.3.2 Current Speed (CS)

Table 5.4 Summary of the East of Shetland hydrodynamic hindcast model against calibration/validation sites, current speed (CS) model quality indices with conformity percentage (Nval %) to SEPA's criteria as in [8] at Near Surface.

CALIBRATION																								
			CS@NS - Obs				CS@NS - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018																								
53SS02	2343	48.8	0.30	0.00	0.12	0.02	0.04	0.00	0.12	0.02	2342	100.0	0.04	126.6	+0.01	26.6	0.02	60.2	0.02	80.6	0.76	0.42	0.97	Np = 1
49BELL01	2292	47.8	0.11	0.00	0.56	0.08	0.03	0.00	0.09	0.01	1583	68.9	0.03	23.8	-0.08	-76.2	0.09	78.1	0.12	107.4	0.76	-0.07	0.16	Np = 1
54SS03	2331	48.6	0.03	0.00	0.15	0.02	0.04	0.00	0.09	0.02	2322	99.6	0.04	146.2	+0.01	46.2	0.02	89.6	0.03	111.3	1.01	-0.09	0.57	Np = 1
50BEL02	2307	48.1	0.10	0.00	0.54	0.09	0.02	0.00	0.09	0.01	1633	70.8	0.02	22.4	-0.08	-77.6	0.08	80.7	0.12	115.3	0.85	0.00	0.17	Np = 1
40VO01	2349	48.9	0.03	0.00	0.15	0.02	0.03	0.00	0.15	0.02	2349	100.0	0.03	111.4	+0.00	11.4	0.02	49.4	0.02	64.1	0.63	0.65	0.97	Np = 1
44VN	2348	48.9	0.03	0.00	0.15	0.02	0.04	0.00	0.09	0.02	2347	100.0	0.04	128.5	+0.01	28.5	0.02	77.9	0.03	97.6	0.93	0.12	0.62	Np = 1
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018-p2																								
45VN02	2177	45.4	0.03	0.00	0.17	0.02	0.05	0.00	0.13	0.03	2175	99.9	0.05	143.0	+0.01	43.0	0.02	65.2	0.03	85.9	0.74	0.51	0.79	Np = 1
41VO02	2690	56.0	0.06	0.00	0.22	0.02	0.06	0.00	0.22	0.04	2601	96.7	0.06	166.2	+0.03	66.2	0.04	93.1	0.05	119.2	0.99	0.33	1.34	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018																								
53SS02	1335	27.8	0.03	0.00	0.12	0.02	0.02	0.00	0.07	0.01	1334	99.9	0.02	83.0	-0.01	-17.0	0.02	54.8	0.02	72.6	0.71	0.27	0.59	Np = 1
49BELL01	1285	26.8	0.10	0.00	0.56	0.07	0.09	0.01	0.23	0.04	1068	82.8	0.09	88.7	-0.01	-11.3	0.06	57.9	0.08	79.9	0.79	0.17	0.41	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018-p2																								
45VN02	2177	45.4	0.03	0.00	0.17	0.02	0.03	0.00	0.09	0.02	2172	99.8	0.03	90.1	-0.00	-9.9	0.02	51.5	0.02	70.3	0.70	0.17	0.53	Np = 1
41VO02	2690	56.0	0.04	0.00	0.16	0.02	0.08	0.01	0.20	0.03	2635	98.0	0.08	213.9	+0.04	113.9	0.04	118.0	0.05	135.3	0.73	0.49	1.20	Np = 1

VALIDATION																								
			CS@NS - Obs				CS@NS - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
PRODUCTION RUN																								
56ToK02	6531	136.1	0.05	0.00	0.55	0.00	0.06	0.00	0.31	0.04	6285	96.2	0.06	136.0	+0.02	36.0	0.03	75.9	0.05	102.7	0.96	0.11	0.56	Np = 1
57TOK2001	5335	111.1	0.04	0.00	0.18	0.03	0.07	0.00	0.32	0.04	4957	92.9	0.07	153.3	+0.02	53.3	0.04	89.0	0.05	121.0	1.09	0.10	1.72	Np = 1
673SN21000	4549	94.8	0.12	0.01	0.52	0.07	0.18	0.01	0.43	0.07	2785	61.2	0.18	141.7	+0.05	41.7	0.09	71.6	0.11	87.8	0.77	0.09	0.84	Np = 1
91N008	4551	94.8	0.17	0.01	0.60	0.08	0.10	0.00	0.25	0.04	3032	66.6	0.10	61.4	-0.07	-38.6	0.08	50.0	0.11	64.8	0.52	0.10	0.42	Np = 1

Table 5.5 Summary of the East of Shetland hydrodynamic hindcast model against calibration/validation sites, current speed (CS) model quality indices with conformity percentage (Nval %) to SEPA's criteria as in [8] at Cage Bottom.

CALIBRATION																								
			CS@CB-Obs				CS@CB - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018																								
53SS02	2343	48.8	0.03	0.00	0.15	0.02	0.03	0.00	0.10	0.02	2343	100.0	0.03	108.7	+0.00	8.7	0.01	52.2	0.02	68.4	0.68	0.41	0.70	Np = 1
49BELL01	2298	47.9	0.11	0.01	0.57	0.08	0.02	0.00	0.09	0.01	1539	67.0	0.02	20.9	-0.09	-79.1	0.09	80.5	0.12	109.6	0.76	-0.08	0.16	Np = 1
54SS03	2331	48.6	0.03	0.00	0.10	0.02	0.05	0.02	0.08	0.01	2331	100.0	0.05	207.9	+0.03	107.9	0.03	119.3	0.04	133.9	0.79	-0.17	0.80	Np = 1
50BEL02	2307	48.1	0.11	0.00	0.53	0.09	0.02	0.00	0.09	0.01	1579	68.4	0.02	18.8	-0.09	-81.2	0.09	82.6	0.12	115.2	0.82	0.07	0.16	Np = 1
40VO01	2349	48.9	0.03	0.00	0.15	0.02	0.03	0.00	0.15	0.02	2349	100.0	0.03	111.4	+0.00	11.4	0.02	49.4	0.02	64.1	0.63	0.65	0.97	Np = 1
44VN	2348	48.9	0.03	0.00	0.13	0.02	0.03	0.00	0.09	0.02	2348	100.0	0.03	126.3	+0.01	26.3	0.02	77.6	0.03	98.8	0.95	0.02	0.65	Np = 1
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018-p2																								
45VN02	2177	45.4	0.03	0.00	0.17	0.02	0.05	0.00	0.13	0.03	2175	99.9	0.05	143.0	+0.01	43.0	0.02	65.2	0.03	85.9	0.74	0.51	0.79	Np = 1
41VO02	2690	56.0	0.03	0.00	0.18	0.02	0.05	0.00	0.24	0.04	2660	98.9	0.05	159.9	+0.02	59.9	0.02	72.7	0.03	99.5	0.79	0.64	1.33	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018																								
53SS02	1335	27.8	0.03	0.00	0.15	0.02	0.02	0.00	0.07	0.01	1331	99.7	0.02	72.8	-0.01	-27.2	0.02	56.3	0.02	77.7	0.73	0.14	0.44	Np = 1
49BELL01	1290	26.9	0.10	0.01	0.57	0.07	0.09	0.00	0.23	0.04	1082	83.9	0.09	88.8	-0.01	-11.2	0.06	56.7	0.08	78.5	0.78	0.20	0.41	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018-p2																								
45VN02	2177	45.4	0.03	0.00	0.17	0.02	0.03	0.00	0.09	0.02	2170	99.7	0.03	96.4	-0.00	-3.6	0.02	55.7	0.02	74.6	0.74	0.11	0.56	Np = 1
41VO02	2690	56.0	0.03	0.00	0.18	0.02	0.06	0.01	0.10	0.01	2676	99.5	0.06	164.9	+0.02	64.9	0.03	82.8	0.03	98.1	0.74	0.12	0.57	Np = 1

VALIDATION																								
			CS@CB-Obs				CS@CB - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
PRODUCTION RUN																								
56ToK02	6531	136.1	0.04	0.00	0.12	0.02	0.04	0.00	0.18	0.02	6520	99.8	0.04	116.6	+0.01	16.6	0.03	68.7	0.03	85.9	0.84	-0.03	1.41	Np = 1
57TOK2001	5335	111.1	0.04	0.00	0.13	0.02	0.04	0.00	0.14	0.02	5326	99.8	0.04	115.4	+0.01	15.4	0.03	68.4	0.03	85.4	0.84	-0.05	1.06	Np = 1
673SN21000	4549	94.8	0.11	0.01	0.48	0.07	0.10	0.00	0.30	0.05	3381	74.3	0.10	90.5	-0.01	-9.5	0.07	62.7	0.09	81.0	0.80	-0.07	0.61	Np = 1
91N008	4551	94.8	0.17	0.01	0.51	0.08	0.11	0.00	0.26	0.04	3172	69.7	0.11	63.1	-0.06	-36.9	0.08	48.0	0.10	62.6	0.51	0.18	0.50	Np = 1

Table 5.6 Summary of the East of Shetland hydrodynamic hindcast model against calibration/validation sites, current speed (CS) model quality indices with conformity percentage (Nval %) to SEPA's criteria as in [8] at Near Bed.

CALIBRATION																								
			CS@NB-Obs				CS@NB - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018																								
53SS02	2343	48.8	0.03	0.00	0.13	0.02	0.05	0.00	0.16	0.03	2333	99.6	0.05	133.8	+0.01	33.8	0.03	75.0	0.03	96.2	0.90	0.30	1.23	Np = 1
49BELL01	2298	47.9	0.10	0.01	0.49	0.07	0.04	0.00	0.10	0.02	1733	75.4	0.04	34.8	-0.07	-65.2	0.07	69.6	0.10	99.4	0.75	-0.02	0.21	Np = 1
54SS03	2331	48.6	0.03	0.00	0.16	0.02	0.02	0.00	0.08	0.02	2321	99.6	0.02	72.9	-0.01	-27.1	0.02	62.4	0.02	84.9	0.80	0.24	0.50	Np = 1
50BEL02	2307	48.1	0.10	0.00	0.50	0.08	0.03	0.00	0.11	0.02	1683	73.0	0.03	26.9	-0.07	-73.1	0.08	78.7	0.11	113.4	0.87	-0.03	0.21	Np = 1
40VO01	2349	48.9	0.04	0.00	0.20	0.03	0.04	0.00	0.15	0.02	2349	100.0	0.04	98.0	-0.00	-2.0	0.02	55.4	0.03	69.9	0.70	0.55	0.75	Np = 1
44VN	2348	48.9	0.03	0.00	0.18	0.03	0.04	0.00	0.12	0.02	2332	99.3	0.04	117.7	+0.01	17.7	0.02	69.3	0.03	90.2	0.88	0.29	0.64	Np = 1
ES-v02rev-MSL-CMEMS-DTU10plusERA5-2018-p2																								
45VN04	2177	45.4	0.05	0.00	0.19	0.03	0.06	0.00	0.17	0.04	2167	99.5	0.06	125.0	+0.01	25.0	0.02	46.5	0.03	61.4	0.56	0.63	0.89	Np = 1
41VO02	2690	56.0	0.05	0.00	0.21	0.03	0.06	0.00	0.23	0.04	2682	99.7	0.06	117.0	+0.01	17.0	0.03	46.9	0.03	61.3	0.59	0.56	1.10	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018																								
53SS02	1335	27.8	0.03	0.00	0.13	0.02	0.03	0.00	0.11	0.02	1335	100.0	0.03	91.6	-0.00	-8.4	0.02	51.0	0.02	65.7	0.65	0.42	0.79	Np = 1
49BELL01	1290	26.9	0.09	0.01	0.47	0.07	0.08	0.00	0.21	0.04	1088	84.3	0.08	87.9	-0.01	-12.1	0.05	59.1	0.08	81.7	0.81	0.11	0.44	Np = 1
ES-v02rev-MSL-CMEMS-DTU10x2plusERA5-2018-p2																								
45VN04	2177	45.4	0.05	0.00	0.19	0.03	0.05	0.00	0.12	0.02	2172	99.8	0.05	88.8	-0.01	-11.2	0.02	44.0	0.03	56.2	0.55	0.45	0.61	Np = 1
41VO02	2690	56.0	0.05	0.00	0.21	0.03	0.07	0.00	0.14	0.02	2690	100.0	0.07	135.1	+0.02	35.1	0.03	52.5	0.03	64.3	0.54	0.34	0.67	Np = 1

VALIDATION																								
			CS@NB-Obs				CS@NB - Mod																	
	N	Ndays	Mean	Min	Max	STD	Mean	Min	Max	STD	Nval	Nval %	Mean	Mean %	Bias	Bias %	AME m	AME %	RMSE m	RMSE %	SI	CC	PR	
PRODUCTION RUN																								
56ToK02	6531	136.1	0.04	0.00	0.19	0.03	0.04	0.00	0.20	0.02	6477	99.2	0.04	106.1	+0.00	6.1	0.03	65.2	0.03	83.9	0.84	0.06	1.07	Np = 1
57TOK2001	5335	111.1	0.05	0.00	0.20	0.03	0.04	0.00	0.17	0.02	5210	97.7	0.04	88.4	-0.01	-11.6	0.03	62.1	0.04	81.3	0.80	0.01	0.90	Np = 1
673SN21000	4549	94.8	0.11	0.01	0.45	0.07	0.11	0.01	0.28	0.04	3601	79.2	0.11	100.2	+0.00	0.2	0.07	59.5	0.08	76.0	0.76	-0.06	0.62	Np = 1
91N008	4551	94.8	0.17	0.01	0.48	0.08	0.10	0.00	0.27	0.04	3019	66.3	0.10	58.3	-0.07	-41.7	0.09	50.3	0.11	64.2	0.49	0.16	0.56	Np = 1

6 Hydrodynamic climatology model verification

As mentioned previously, the underlying concept of a climatology model is the assumption that the conditions at a particular location for a particular day do not change significantly from one year to the next. Unfortunately, no long-term (multi-year) records of currents or water properties are available to assess model performance, and it is unreasonable to compare model predictions against short-term measurement data, which reflect a specific set of conditions during which the measurements were made. Instead, an assessment of the regional Shetland hydrodynamic climatology is performed in the following ways:

- Deriving tidal constituents at Lerwick from the regional climatological model (HD_{ES_Clima}) and comparing against those derived from long-term tide gauge observations.
- Comparing model prediction of water level, currents speed, current direction, water temperature, and water salinity at offshore locations. Here we are verifying the model downscaling from shelf scale to local domain (SSM→HD_{ES_Clima})

6.1.1 Tidal constituents at Lerwick

Long-term water level observations of the water level at Lerwick were obtained from the UK National Tide Gauge Network[16] for the period 1993-2014. Modelled water levels at Lerwick (-1.1403; 60.1541) were also extracted from HD_{ES_Clima}. Astronomical water levels (tidal levels) were then calculated using harmonic tidal analysis to separate the tidal and non-tidal (residual) components of the total water level time series. The harmonic analysis was conducted using the U-tide toolbox, see [7], which is based on the IOS tidal analysis method defined by the Institute of Oceanographic Sciences as described by [25], and integrates the approaches defined in [26] and [27]. The residual water level was calculated by subtracting the predicted tidal level from the total water level.

Figure 6.1 (top panel) shows the derived tidal constituents from HD_{ES_Clima} and their amplitude, period, and phase at Lerwick. The largest constituent is the principal lunar semi-diurnal *M2* component (0.60m amplitude), followed by the principal solar semi-diurnal *S2* component (0.21m amplitude).

Figure 6.1 (bottom panel) shows a time series plot of modelled water levels (total, tidal, and residual) at Lerwick. The semidiurnal and spring-neap tidal cycle is prominent in the total and tidal signal. One can also clearly see the seasonal variability in the residual water levels, but low variability on shorter timescales which reflects the climatologically averaged meteorological conditions (see Section 4.3.1.1). In the legend also shown are the astronomical water levels which are defined as follows:

- HAT — Maximum predicted WL
- MHWS: — Average of the two successive high waters reached during the 24 hours when the tidal range is at its greatest (spring tide)
- MHWN: — Average of the two successive high waters reached during the 24 hours when the tidal range is at its lowest (neap tide)
- MSL: — Mean predicted WL
- MLWN: — Average of the two successive low waters reached during the 24 hours when the tidal range is at its lowest (neap tide)

[16] UK Tide Gauge Network accessed May 2021

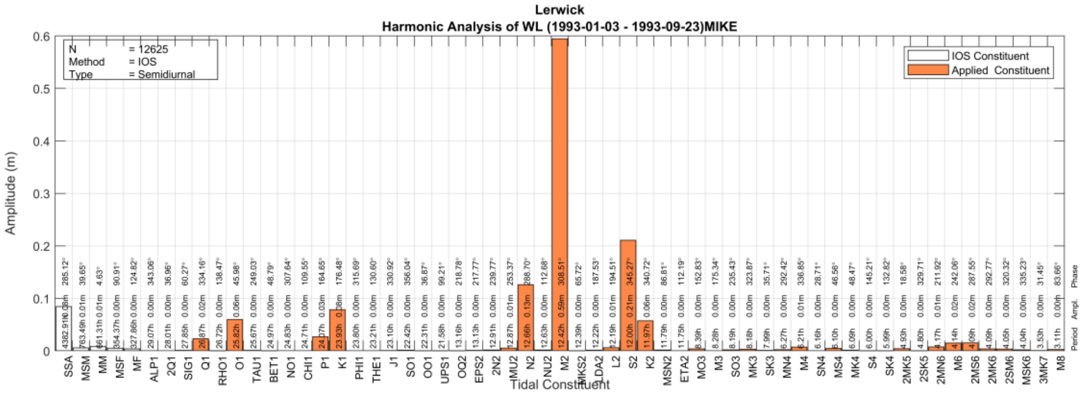
- MLWS: Average of the two successive low waters reached during the 24 hours when the tidal range is at its greatest (spring tide)
- LAT: Minimum predicted WL

Table 6.1 compares the main tidal constituents derived from HD_{ES_Clima} with those derived from the Lerwick tide gauge. There is an overall very good agreement in the prediction of tidal amplitude with approximately a phase error of about 20º.

Figure 6.2 and Figure 6.3 show respectively a timeseries/frequency and scatter comparison plots of the tidal signals (following analysis described above) between the observed BODC Lerwick tide gauge and the extracted timeseries at the same location from the HD_{ES_Clima} over the period January 1993 to September 1993 (the climatological run covers the calendar year of 1993). On overall there is very good agreement in tidal water level signal representation in the downscaled East of Shetland climatology. The QQ fit in Figure 6.3 is close to 1:1 with a bias of 0.01m. RMSE is 0.15m and due mainly to the phase error, previously also reported when examining individual tidal constituents, and depicted by the slight oval shape of the scatter points in Figure 6.3.

Table 6.1 Comparison of the amplitude [m] and phase [°] of selected tidal constituents at Lerwick based on tide gauge measurements and HD_{ES_Clima} model for the period Jan 1993 – Sep 1993

Consituent	Lerwick tide gauge		Lerwick, HD_{ES_Clima}	
	Amplitde [m]	Phase [°]	Amplitde [m]	Phase [°]
M2	0.57	291.22	0.59	308.51
S2	0.20	328.42	0.21	345.27
N2	0.12	268.68	0.13	288.70
K1	0.07	148.11	0.08	176.48
O1	0.08	21.49	0.06	45.98
K2	0.07	334.28	0.06	340.72



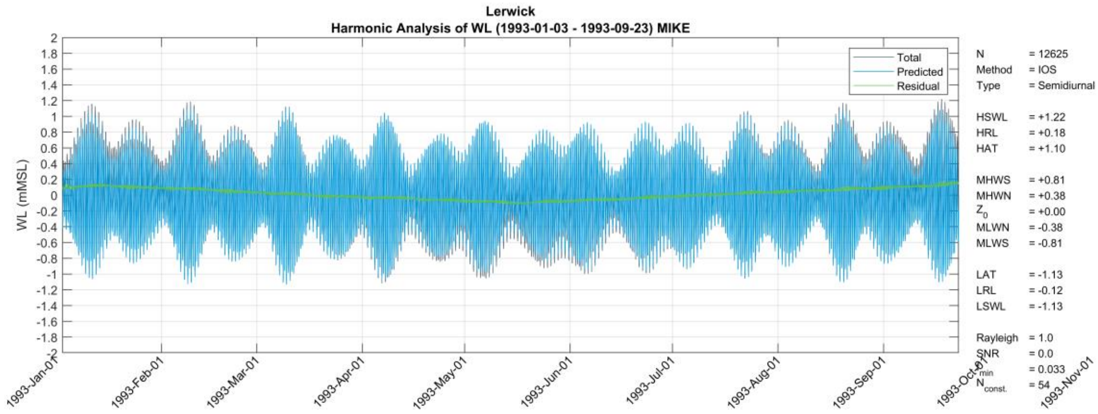


Figure 6.1 (top panel) Amplitude, period, and phase of tidal constituents and (bottom panel) timeseries of modelled water levels (total, tidal, and residual) and astronomical water levels derived at Lerwick location from HD_{ES_Clima}

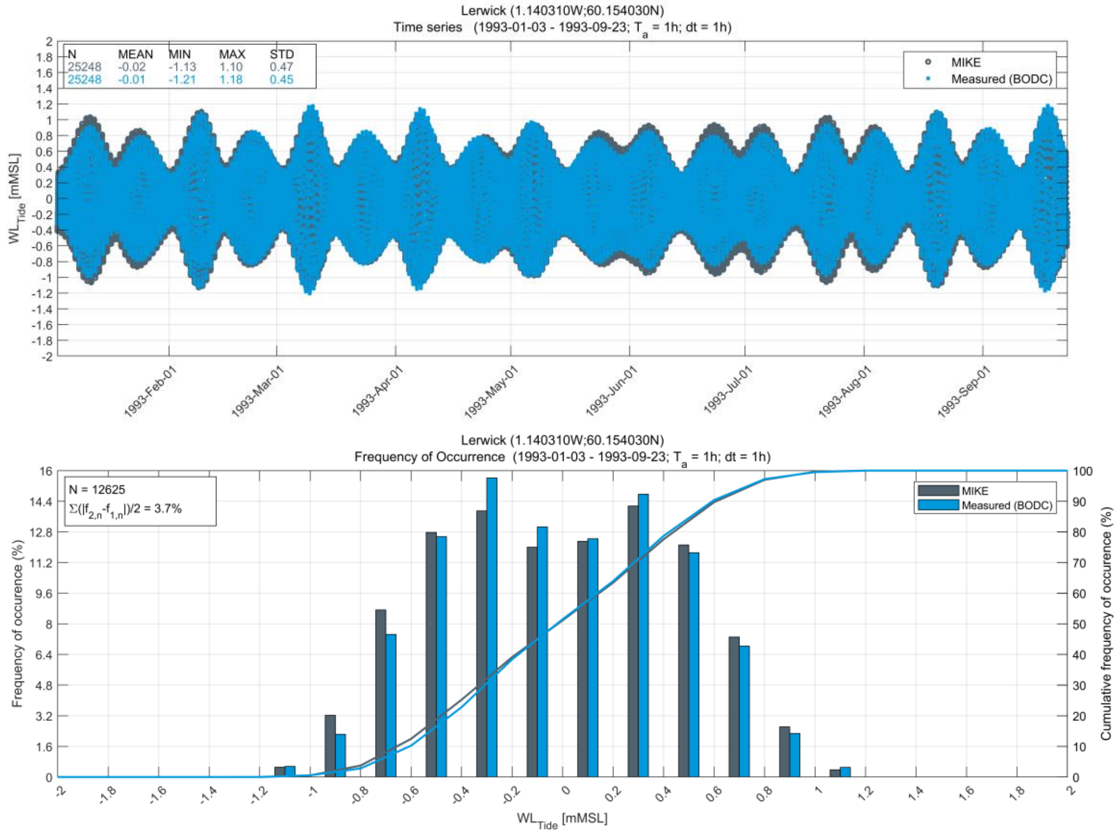


Figure 6.2 Timeseries (top) and frequency (bottom) comparison plots for tidal signal at the Lerwick tide gauge location.

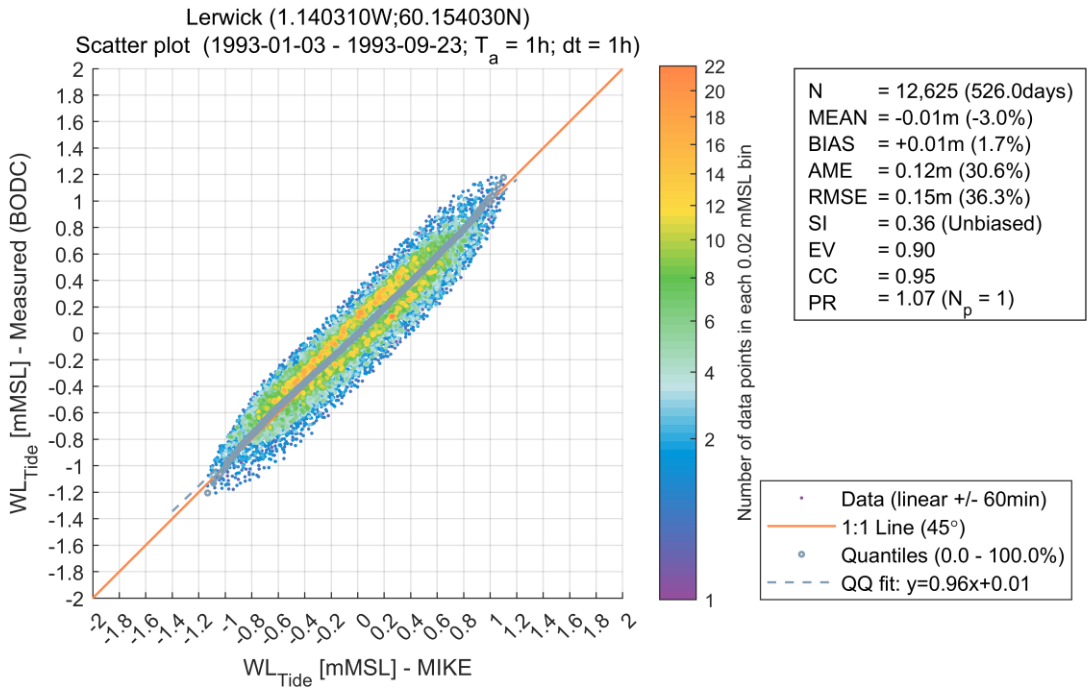


Figure 6.3 Scatter plot comparison of tidal signals between HD_{ES_Clima} and BODC tidal record at Lerwick tide gauge

6.1.2 Offshore comparisons to SSM

The regional Shetland hydrodynamic climatology model is a down-scaled version of the SSM shelf-wide domain model; it is forced by SSM derived boundary conditions with consistent meteorological inputs, but with higher spatial resolution in and around Shetland. To verify the model down-scaling (SSM → HD_{ES_Clima}) comparisons of model predictions have been performed at five offshore locations (P01-09 in Figure 6.4). These locations are approximately equidistant between the model boundaries and Shetland itself and in relatively deep water (100mMSL to 120mMSL). The five (5) offshore should not be influenced by the changes in model resolution and bathymetry in and around the islands from HD_{ES_Clima}. The four (4) nearshore points depict the effect of downscaling (increase in model resolution, coastal features/islands and high-resolution bathymetry) of SSM in and around the islands from HD_{ES_Clima} in the main areas of interest with regards to SSF's operations.

Model parameters including current speed, current direction, sea water temperature, and salinity were extracted from both the SSM and HD_{ES_Clima} at location P01 to P09 for depths of 5m, 10m, 20m, 40m, and 80m below SWL. Water levels relative to MSL were also extracted at each location. A comparison between the two models time-series was then performed, consisting of time-series, scatter plot, histogram, and rose plot comparisons. Statistical model quality indices (QI's) were also determined. For more information on model QI's please see Appendix B (note that these indices are more commonly used to compare measurement, but we herein use the SSM model as the baseline reference).

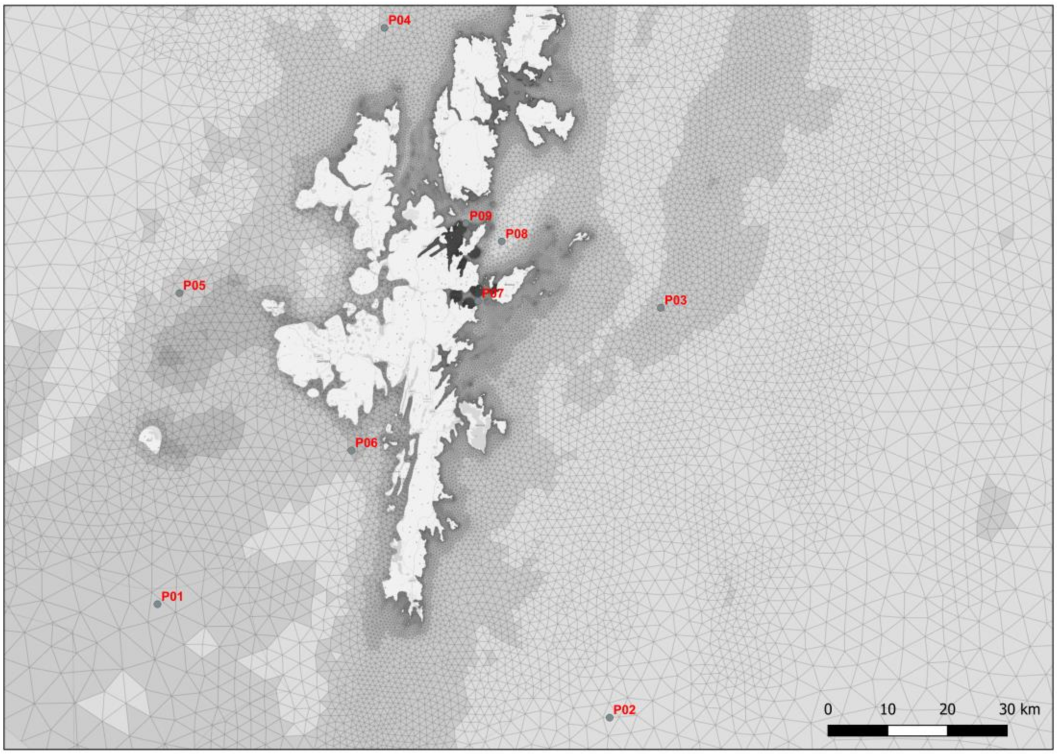


Figure 6.4 HD_{ES_Clima} model domain showing locations of verification points including offshore locations P01 to P05) and locations nearshore in main areas of SSF's aquaculture activities and areas of interest.

Verification plots of water levels at location P03 are shown in Figure 6.5, while comparison of current speed, current direction and salinity with sea water temperature at 5, 20 and 80 m below SWL at P03 are shown in Figure 6.6 and Figure 6.7 respectively. SSM climatological conditions are well replicated by HD_{ES_Clima}. Equivalent plots showing the verification at all locations (P01 to P09) and water depths are provided in digital format accompanying this report (see Appendix C).

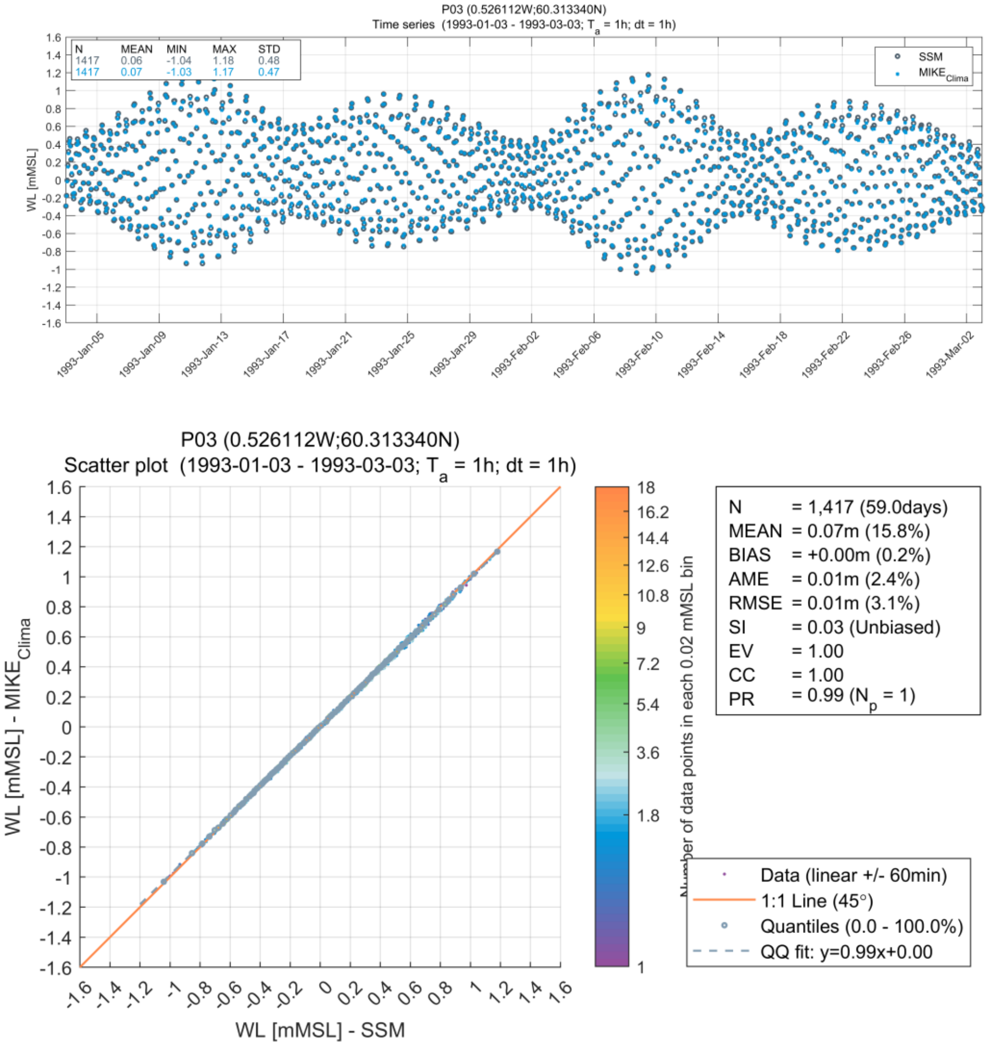


Figure 6.5 Time-series comparison (upper panel) and scatter plot (bottom panel) comparison of SSM and HD_{ES_Clima} modelled water levels (*WL*) at point P03

Comparison of HD$_{ES_Clima}$ (MIKE$_{Clima}$) versus SSM climatology at P03 and at a depth of 5m (top), 20m (middle) and 80m (bottom) below still water level (BSWL)

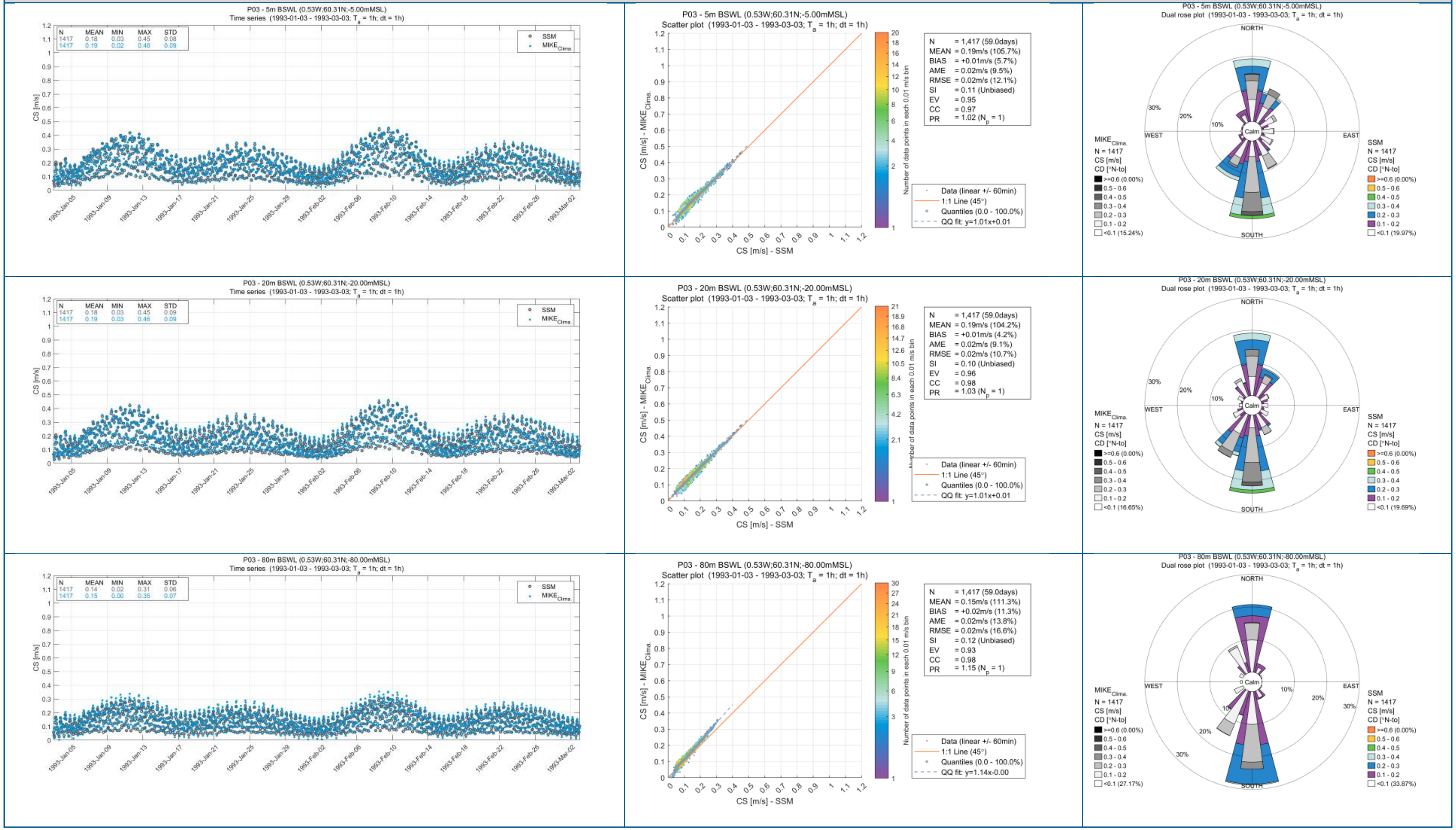
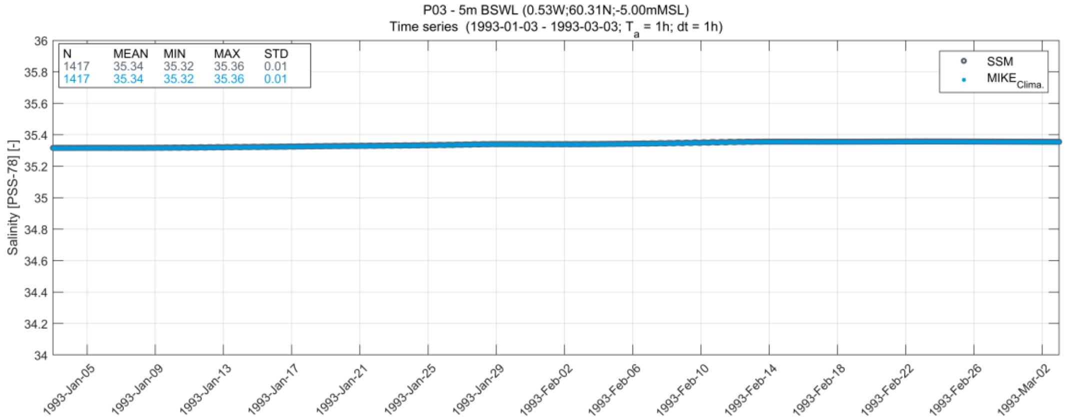
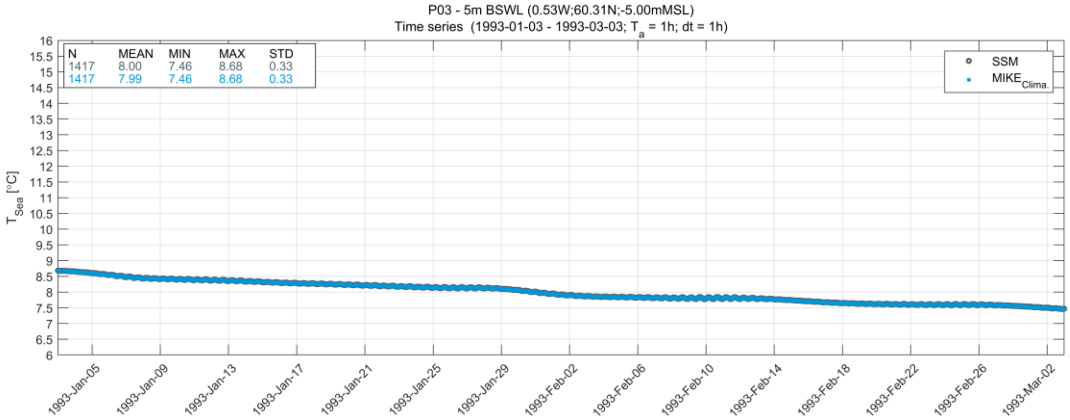
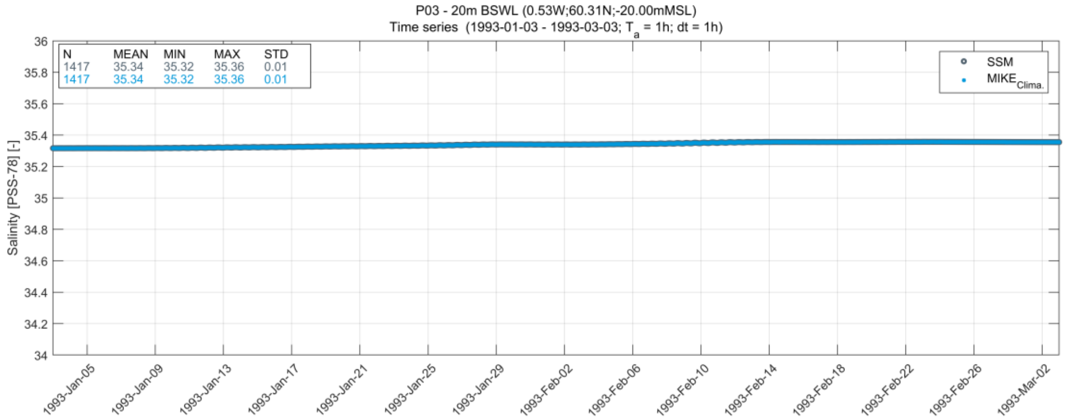
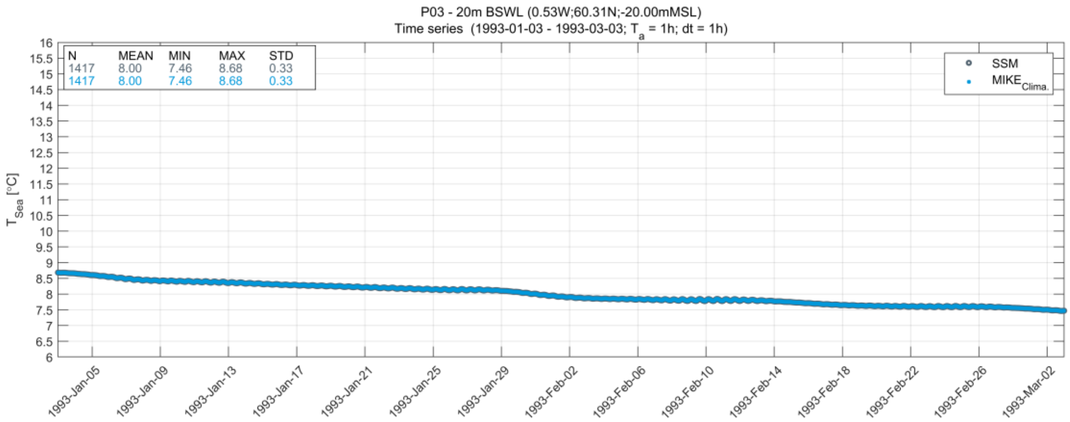


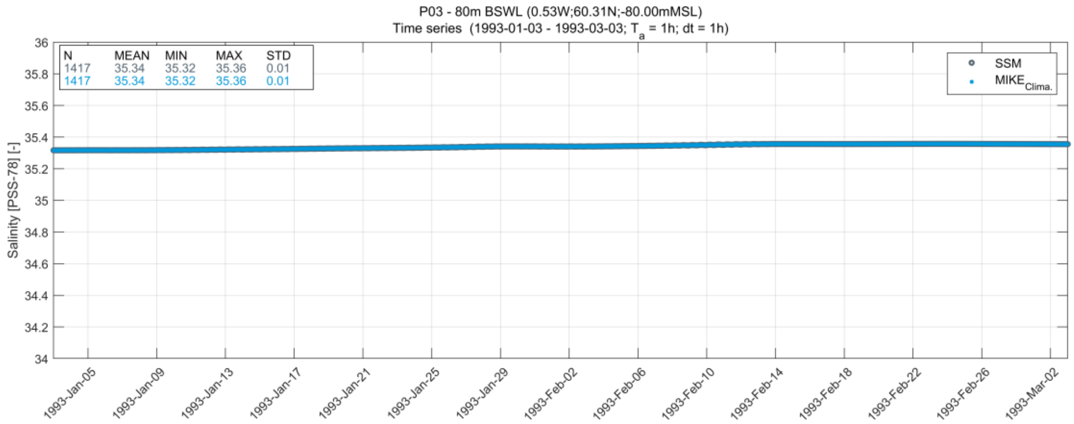
Figure 6.6 Current speed timeseries, scatter and rose plots of model versus SSM climatology for P03 at selected vertical levels of 5, 20 and 80 m


P03 - 5m BSWL (0.53W;60.31N;-5.00mMSL)
Time series (1993-01-03 - 1993-03-03; T_a = 1h; dt = 1h)
N MEAN MIN MAX STD
1417 35.34 35.32 35.36 0.01
1417 35.34 35.32 35.36 0.01
SSM
MIKE Clima.
Salinity [PSS-78] [-]


P03 - 5m BSWL (0.53W;60.31N;-5.00mMSL)
Time series (1993-01-03 - 1993-03-03; T_a = 1h; dt = 1h)
N MEAN MIN MAX STD
1417 8.00 7.46 8.68 0.33
1417 7.99 7.46 8.68 0.33
SSM
MIKE Clima.
T Sea [°C]


P03 - 20m BSWL (0.53W;60.31N;-20.00mMSL)
Time series (1993-01-03 - 1993-03-03; T_a = 1h; dt = 1h)
N MEAN MIN MAX STD
1417 35.34 35.32 35.36 0.01
1417 35.34 35.32 35.36 0.01
SSM
MIKE Clima.
Salinity [PSS-78] [-]


P03 - 20m BSWL (0.53W;60.31N;-20.00mMSL)
Time series (1993-01-03 - 1993-03-03; T_a = 1h; dt = 1h)
N MEAN MIN MAX STD
1417 8.00 7.46 8.68 0.33
1417 8.00 7.46 8.68 0.33
SSM
MIKE Clima.
T Sea [°C]



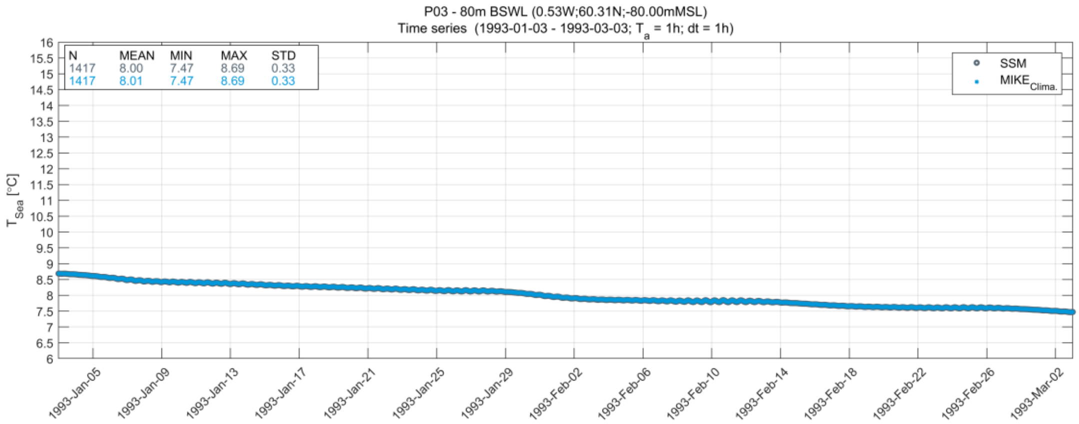


Figure 6.7 Salinity and temperature comparison of modelled versus SSM climatology at P03 and selected vertical levels of 5, 20 and 80 m (top to bottom).

7 Model Results

In this section, the results of the 3D hydrodynamic models are presented. This includes a qualitative verification of the climatological model against the hindcast version, and a brief description of modelled hydrodynamics over the area of interest.

7.1 Model outputs

The residual (net) circulation as derived from the depth-averaged currents in HD_{ES_Clima} and $HD_{ES\_hindcast}$ are shown in Figure 7.1, Figure 7.2 and Figure 7.3. Strong residual currents are found where the flow is constrained around the headlands and in narrow channels driven in principle by asymmetries mainly in the barotropic tidal and secondary in the baroclinic circulation.

At all SSF's sites the net circulation is considered to be 'weak' (white to light blue areas Figure 7.2 - Figure 7.3) which would also suggest a reduced net dispersion capacity outside of the semi-diurnal tidal cycles. Exception are the Fish Holm and Dragon's Ness sites, see Figure 7.2 and Figure 7.3, with significant net circulation indicating a high dispersion capacity from the sites themselves.

Figure 7.2 also shows one prominent cyclonic recirculation feature of the residual current field, located north-east of Fish Holm and extending throughout the whole width of the straights between the Yell Island and the Shetland Mainland. This cyclonic pattern, associated with net upwelling, has a distinct cold core footprint in the temperature field in both the climatology and reanalysis realisations. This cold core eddy itself probably also plays a significant role in the dispersion of depositional and/or other passive material introduced to the nearby marine environment acting as an effective pathway to redistribution of material in nearby receptors[17].

The consistency in residual circulation[18], both in terms of current speed and direction between the climatology and hindcast version supports the dominant tidal character of the area and demonstrates that the atmospheric forcing is perhaps of secondary importance. Still, the observational record shows significant contribution from a non-tidal component that the $HD_{ES\_hindcast}$ fails to replicate in many instances. Thus, the significance of variability and seasonal signals in meteorological conditions in the area and how they affect and/or drive episodic events, potentially also affecting dispersion, at shorter timescales - similar to usual storm durations at these latitudes for example - should not be negated and/or diminished in their effect in any dispersion assessment for the locations in question.

[17] This study does not move forward with characterising/identifying in the velocity field the presence of coherent structures that would act as barriers to mixing and straining of material lines as a metric of the dispersion capacity approached here as a ratio of area of dispersed material over a user defined time unit.

[18] having in mind the adjustment of the tidal component for the hindcast version

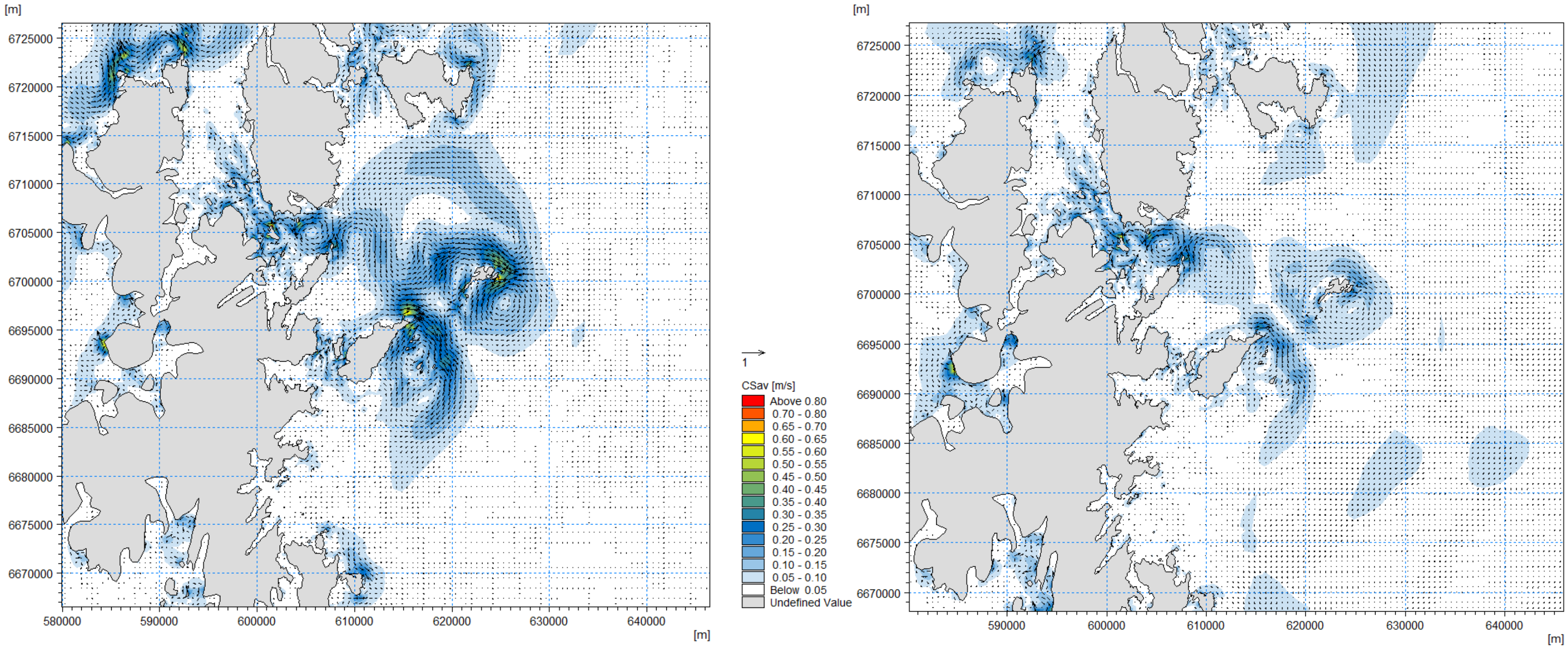


Figure 7.1 Residual circulation for East of Shetland area of interest based on the reanalysis $HD_{ES\_hindcast}$ (left panel) and climatological HD_{ES_Clima} (right panel) realisations. While the general circulation patterns are consistent between the two databases the residual velocity field is significantly enhanced in the hindcast version due to the adjustment of the velocity field in order to match the observational record. A similar comparison (not shown herein) has been performed versus the HYCOM and CMEMS forcing with similar to the SSM climatology underestimation of the velocity field in the areas of question.

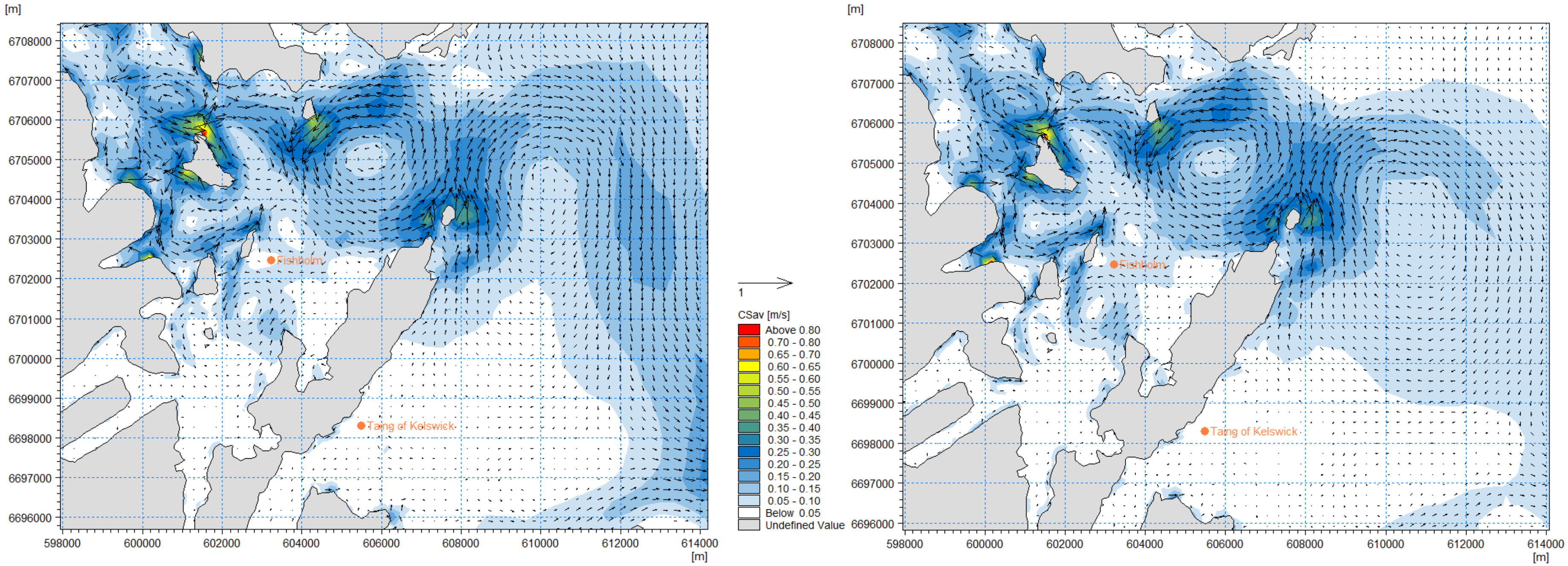


Figure 7.2 Residual circulation focused on Fish Holms and Taign of Kelswick for areas of interest based on the reanalysis $HD_{ES\_hindcast}$ (left panel) and climatological HD_{ES_Clima} (right panel) realisations. The main recirculation feature (cyclonic eddy) isolating the Voe is present in both HD realisations and in fact being depicted with similar intensity rendering the climatology suitable for dispersion experiments without loss of integrity in the accuracy of hydrodynamics versus the hindcast version.

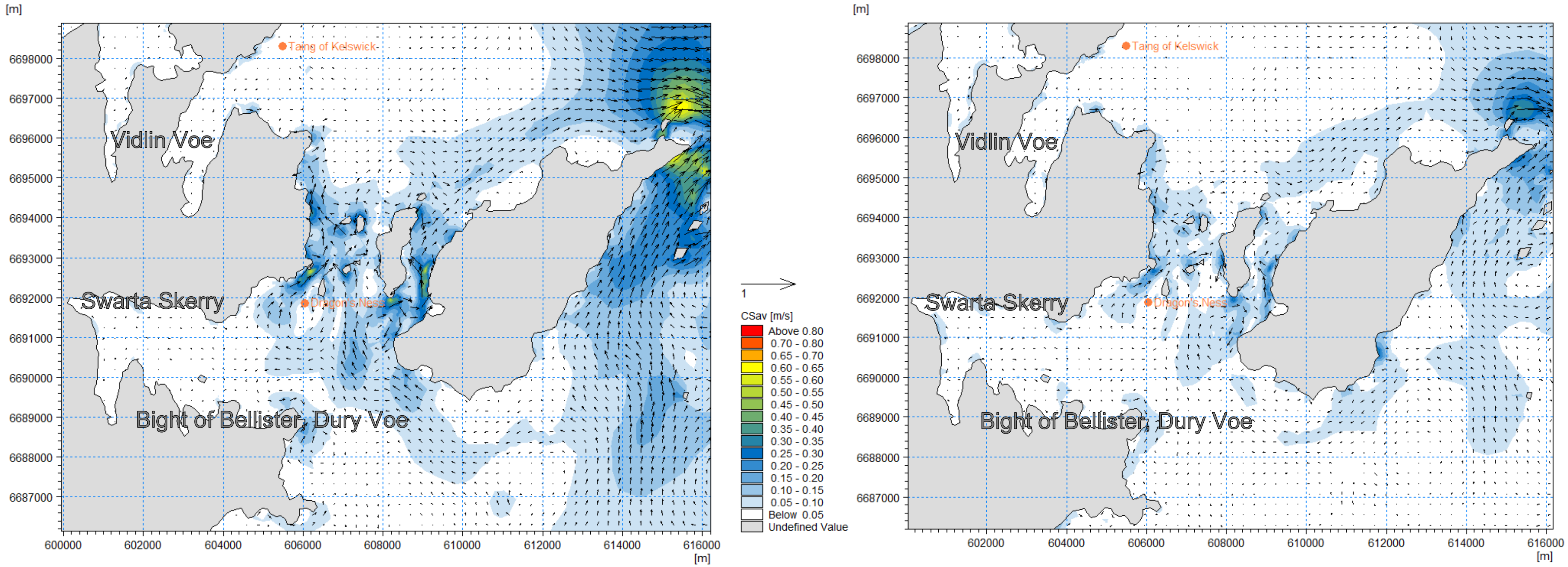


Figure 7.3 Residual circulation focused on Vidlin Voe, Bellister and Swarta Skerry areas of interest based on the reanalysis $HD_{ES\_hindcast}$ (left panel) and climatological HD_{ES_Clima} (right panel) realisations. While main circulation features are represented consistently in both HD realisations there is a discernible difference in the hindcast version in the depiction of the velocity field at the most energetic locations.

8 Summary

A 3-dimensional hydrodynamic hindcast and climatology model database for the East of Shetland domain has been developed to support marine pen fin fish aquaculture projects in Shetland islands, Scotland. The model database has been established using DHI's MIKE 3 FM numerical engine. The climatology version was based on upon the existing SSM climatology developed for Marine Scotland Science.

The hydrodynamic database includes a regional hydrodynamic climatology, and a hindcast version, with a resolution of approximately <150m at the coastline and ~20-40m at all designated SSF aquaculture sites (main areas of interest) gradually increasing to 150-200m at 1km from pen locations. The model has refined resolution of down to 150-200m around existing marine sensitive areas (PMFs).

The hydrodynamic hindcast and climatology model databases provide a basis for future modelling to support regulatory applications such as: assessing connectivity between fish farms sites located within the East of Shetland domain; site selection and site screening; dispersion modelling of waste solids and bath treatment medicines.

In general, the model exhibits good skill in terms of current speeds, replicates water level range sufficiently at all stations and mean current directions are in general terms consistent with the observational records (depending on the examined directions at the respective depths where model skill is assessed). Current speeds especially are well within regulatory modelling criteria as set in [8]. At all stations examined, as stated in section 5.1, the tidal signal propagation is sufficiently replicated.

The initial tidal forcing was adjusted as, while the model was well capturing sites with current speeds < 0.3m/s was nonetheless failing to fully capture full range of conditions at more energetic sites such as Bellister. This discrepancy guided final calibration efforts towards adjusting the velocity field that was being used as boundary forcing. The adjustment was based on the bias of the tidal current speed signal used as forcing versus the inferred one following tidal analysis of the observational records at the stations in question.

9 References

[1] R. J. Shucksmith, “Shetland Islands Marine Region State of the Environment Assessment,” NAFC Marine Centre UHI. Report for the Shetland Islands Marine Planning Partnership. pp 172, 2017.

[2] S. Governmant, “Scotland's Marine Atlas: Information for The National Marine Plan,” 16 03 2011. [Online]. Available: https://www.gov.scot/publications/scotlands-marine-atlas-information-national-marine-plan/pages/. [Accessed 19 02 2021].

[3] M. Office, “Nortern Scotland: climate,” 10 10 2016. [Online]. Available: https://www.metoffice.gov.uk/binaries/content/assets/metofficegovuk/pdf/weather/learn-about/uk-past-events/regional-climates/northern-scotland_-climate---met-office.pdf. [Accessed 01 03 2021].

[4] S. P. Neill, A. Vögler, A. Goward-Brown, S. Baston, M. J. Lewis, P. A. Gillibrand, S. Waldman and D. K. Woolf, “The wave and tidal resource of Scotland,” *Vögler,* vol. 114, no. Part A, pp. 3-17, 2017.

[5] R. Halliday, “Shetland Islands Wave and Tidal Resource,” Natural Power for Shetland Island Council (805-NPC-SIC-004), 2001.

[6] Marine Scotland Science, “Scottish Fish Farm Production Survey 2021,” The Scottish Government, October 2022.

[7] D. L. Codiga, “Unified Tidal Analysis and Prediction Using the UTide Matlab Functions. Technical Report 2011-01,” Graduate School of Oceanography, University of Rhode Island, Narragansett, RI. 59pp, 2011.

[8] SEPA, “Regulatory Modelling Guidance for the Aquaculture Sector, Version 1.1,” Scottish Environment Protection Agency, July 2019.

[9] DHI, “MIKE 21 & MIKE 3 Flow Model FM, Hydrodynamic and Transport Module, Scientific Documentation,” 2020. [Online]. Available: https://manuals.mikepoweredbydhi.help//2021/Coast_and_Sea/MIKE3HD_Scientific_Doc.pdf. [Accessed February 2021].

[10] M. Scotland, “The Scottish Shelf Model,” [Online]. Available: http://marine.gov.scot/themes/scottish-shelf-model. [Accessed 01 03 2021].

[11] J. Wolf, N. Yates, A. Bereton, H. Buckland, M. De Dominicis, A. Gallego and R. O'Hara Murray, “The Scottish Shelf Model. Part 1: Shelf-Wide Domain,” *Scottish Marine and Freshwater Science,* vol. 7, no. 3, 2016.

[12] M. De Dominicis, J. Wolf and R. O'Hara Murry, “Comparative Effects of Climate Change and Tidal Stream Energy Extraction in a Shelf Sea,” *JGR Oceans,* vol. 123, no. 7, pp. 5041-5067, 2018.

[13] C. Chen, H. Liu and R. C. Beardsley, “An unstructured grid, finite-volume, three-dimensional, primitive equations ocean model: Application to coastal ocean and estuaries,” *Journal of Atmospheric and Oceanic Technology,* vol. 20, no. 1, pp. 159-186, 2003.

[14] K. P. Edwards, R. Barciels and M. Butenschön, “Validation of the NEMO-ERSEM operational ecosystem model for the North West European Continental Shelf,” *Ocean Science,* vol. 8, no. 6, pp. 983-1000, 2012.

[15] E. J. O'Dea, A. K. Arnold, K. P. Edwards, R. Furner, P. Hyder and M. J. Martin, “An operational ocean forecast system incorporating NEMO and SST data assimilation for the tidally driven European North-West shelf,” *Journal of Operational Oceanography,* vol. 5, no. 1, 2012.

[16] D. P. Dee, S. M. Uppala, A. J. Simmons, P. Berrisford, P. Poli and S. Kobayashi, “The ERA-Interim reanalysis: configuration and performance of the data assimilation system,” *Quarterly Journal of the Royal Meteorological Society,* vol. 137, no. 656, pp. 553-597, 2011.

[17] V. A. Bell, A. L. Kay, R. G. Jones and R. J. Moore , “Development of a high resolution grid-based river flow model for use with regional climate model output,” *Hydrology and Earth System Sciences,* vol. 11, no. 1, pp. 532-549, 2007.

[18] S. J. Cole and R. J. Moore, “Distributed hydrological modelling using weather radar in gauged and ungauged basins,” *Advances in Water Resources,* vol. 32, no. 7, pp. 1107-1120, 2009.

[19] DHI, “MIKE 21 Toolbox Global Tide Model, https://www.mikepoweredbydhi.com/-/media/shared%20content/mike%20by%20dhi/flyers%20and%20pdf/product-documentation/mike-21-toolbox-global-tide-model.pdf,” 2022.

[20] R. A. Flather, “A tidal model of the northwest European continental shelf,” *Memories de la Societe Royale des Sciences de Liege,* vol. 6, no. 10, pp. 141-164, 1976.

[21] ECMWF, *ERA5 - Reanalysis Datasets.,* European Centre for Medium-Range Weather Forecasts, 2019.

[22] DHI, “MIKE 21 & MIKE 3 Flow Model FM, Hydrodynamic and Transport Module, Scientific Documentation,” 2022. [Online]. Available: https://manuals.mikepoweredbydhi.help//2022/Coast_and_Sea/MIKE3HD_Scientific_Doc.pdf. [Accessed February 2022].

[23] DHI, “MIKE 3 Flow Model FM, Hydrodynamic and Transport Module, Scientific Documentation,” 2021. [Online]. Available: https://manuals.mikepoweredbydhi.help//2021/Coast_and_Sea/MIKE_3_Flow_FM_Scientific_Doc.pdf. [Accessed 03 2021].

[24] R. Pawlowicz, B. Beardsley and S. Lentz, “Classical tidal harmonic analysis including error estimates in MATLAB using T-TIDE,” *Computers & Geosciences 28,* pp. 929-937, 2002.

[25] M. G. G. Foreman, J. Y. Cherniawsky and V. A. Ballantyne, “Versatile Harmonic Tidal Analysis: Improvements and Applications.,” *J. Atmos. Oceanic Tech. 26,* pp. 806-817. DOI: 810.1175/2008JTECHO1615.1171, 2009.

[26] K. E. Leffler and D. A. Jay, “Enhancing tidal harmonic analysis: Robust (hybrid L-1/L-2) solutions,” *Cont. Shelf Res. 29,* pp. 78-88. DOI: 10.1016/j.csr.2008.1004.1011, 2009.

[27] D. Price, C. Stuiver, H. Johnson, A. Galledo and R. O'Hara Murray, “The Scottish Shelf Model. Part 3: St Magnus Bay Sub-Domain,” *Scottish Marine and Freshwater Science,* vol. 7, no. 5, 2016.

[28] M. Niazy, “Pentland Firth & Orkney Water (PFOW) Tidal Array Stronsay Firth, between Shapinsay and Stronsay,” 2019.

APPENDICES

APPENDIX A

Hydrodynamic Model Database Files

A Hydrodynamic model database files

The hydrodynamic climatology models are supplied on a portable hard drive alongside this report. This includes the mesh files, offshore boundary conditions, meteorological conditions, model setup files, and the model results files. The data are provided in DHI MIKE format and can be used to generate boundary conditions for local climatology modelling or as input for scenario modelling.

Table A.1 summarises the model files provided for the HD_{ES_clima} model.

Table A.2 summarises the model files provided for the $HD_{ES\_hindcast}$ model.

Table A.1 Hydrodynamic climatology files (HD_{ES_Clima})

Folder	File name	File type	File size	Description
0_MetForcing	Climatology_swona_metforcing_TAU_M21_v2.dfsu	MIKE Zero Data Manager (.dfsu)	1.56 GB	SSM climatologically averaged meteorological forcing (6-hourly resolution) • U_{10} (wind u-velocity [m/s]) • V_{10} (wind v-velocity [m/s]) • Air pressure [hPa] • Air temperature [°C] • Evaporation [m/s] • Downwards longwave radiation [W/m^2] • Precipitation [m/s] • Relative humidity [%] • Downwards shortwave radiation [W/m^2]

Table A.1 Hydrodynamic climatology files (HD_{ES_Clima})

Folder	File name	File type	File size	Description
ES_SSMclimatology_production.m3fm - Result Files	area.dfsu	MIKE Zero Data Manager (.dfsu)	30.0 GB	2-Dimensional model outputs from 1-year model run (0.5-hour temporal resolution) • Surface elevation [mMSL] • Total water depth [m] • Depth-averaged u-velocity [m/s] • Depth-averaged v-velocity [m/s] • P (power) flux [$m^3s^{-1}m^{-1}$] • Q (volume) flux [$m^3s^{-1}m^{-1}$]
	volume.dfsu	MIKE Zero Data Manager (.dfsu)	331.5GB	3-Dimensional model outputs from 1-year model run (0.5-hour temporal resolution) • U-velocity component [m/s] • V-velocity component [m/s] • W-velocity component [m/s] • Density [kg/m^3] • Temperature [degrees Celsius] • Salinity [psu]

Table A.2 Hydrodynamic hindcast files ($HD_{ES\_hindcast}$)

Folder	File name	File type	File size	Description
ES_hindcast_MSL_CMEMS_DTU10plusERA5_TS_nudging_2021_2022_production.m3fm - Result Files	Elmnt_area.dfsu	MIKE Zero Data Manager (.dfsu)	4.55 MB	• Still water depth [mMSL] • Element area [m^2]
	area.dfsu	MIKE Zero Data Manager (.dfsu)	36.5 GB	2-Dimensional model outputs from 1-year model run (0.5-hour temporal resolution) • Surface elevation [mMSL] • Total water depth [m] • Depth-averaged u-velocity [m/s] • Depth-averaged v-velocity [m/s] • P (power) flux [$m^3s^{-1}m^{-1}$] • Q (volume) flux [$m^3s^{-1}m^{-1}$]
	volume.dfsu	MIKE Zero Data Manager (.dfsu)	644.4GB	3-Dimensional model outputs from 1-year model run (0.5-hour temporal resolution) • U-velocity component [m/s] • V-velocity component [m/s] • W-velocity component [m/s] • Density [kg/m^3] • Temperature [degrees Celsius] • Salinity [psu] • Turbulent Kinetic Energy (TKE) [m^2/s^2] • Dissipation of TKE [m^2/s^3] • Horizontal eddy viscosity [m^2/s] • Vertical eddy viscosity [m^2/s]
decoupled_production	ES_hindcast_MSL_CMEMS_DTU10plusERA5_TS_nudging_2021_2022_production_Decoupled.m3fm	Setup (.m21fm)		
	ES_hindcast_MSL_CMEMS_DTU10plusERA5_TS_nudging_2021_2022_production_DecouplingArea.dfsu	MIKE Zero Data Manager (.dfsu)	6.3GB	• Total water depth [m]

Table A.2 Hydrodynamic hindcast files ($HD_{ES\_hindcast}$)

Folder	File name	File type	File size	Description
	ES_hindcast_MSL_CMEMS_DTU10plusERA5_TS_nudging_2021_2022_production_DecouplingVolume.dfsu	MIKE Zero Data Manager (.dfsu)	478 GB	• U-velocity component [m/s] • V-velocity component [m/s] • W-velocity component [m/s] • Temperature [degrees Celsius] • Salinity [psu] • Turbulent Kinetic Energy (TKE) [m^2/s^2] • Dissipation of TKE [m^2/s^3]
	ES_hindcast_MSL_CMEMS_DTU10plusERA5_TS_nudging_2021_2022_production_DecouplingFlux.dfsu		167 GB	• Flux [undefined]

APPENDIX B

Definition of model quality indices

B Definition of model quality indices

To obtain an objective and quantitative measure of how well the model data compared to the observed data, a number of statistical parameters so-called quality indices (QI's) are calculated.

Prior to the comparisons, the model data are synchronised to the time stamps of the observations so that both time series had equal length and overlapping time stamps. For each valid observation, measured at time t, the corresponding model value is found using linear interpolation between the model time steps before and after t. Only observed values that had model values within ± the representative sampling or averaging period of the observations are included (e.g. for 10-min observed wind speeds measured every 10 min compared to modelled values every hour, only the observed value every hour is included in the comparison).

The comparisons of the synchronised observed and modelled data are illustrated in (some of) the following figures:

- Time series plot including general statistics
- Scatter plot including quantiles, QQ-fit and QI's (dots coloured according to the density)
- Histogram of occurrence vs. magnitude or direction
- Histogram of bias vs. magnitude
- Histogram of bias vs. direction
- Dual rose plot (overlapping roses)
- Peak event plot including joint (coinciding) individual peaks

The quality indices are described below, and their definitions are listed in Table B.1. Most of the quality indices are based on the entire dataset, and hence the quality indices should be considered averaged measures and may not be representative of the accuracy during rare conditions.

The MEAN represents the mean of modelled data, while the BIAS is the mean difference between the modelled and observed data. AME is the mean of the absolute difference, and RMSE is the root mean square of the difference. The MEAN, BIAS, AME and RMSE are given as absolute values and relative to the average of the observed data in percent in the scatter plot.

The scatter index (SI) is a non-dimensional measure of the difference calculated as the unbiased root-mean-square difference relative to the mean absolute value of the observations. In open water, an SI below 0.2 is usually considered a small difference (excellent agreement) for significant wave heights. In confined areas or during calm conditions, where mean significant wave heights are generally lower, a slightly higher SI may be acceptable (the definition of SI implies that it is negatively biased (lower) for time series with high mean values compared to time series with lower mean values (and same scatter/spreading), although it is normalised).

EV is the explained variation and measures the proportion [0 - 1] to which the model accounts for the variation (dispersion) of the observations.

The correlation coefficient (CC) is a non-dimensional measure reflecting the degree to which the variation of the first variable is reflected linearly in the variation of the second variable. A value close to 0 indicates very limited or no (linear) correlation between the two datasets, while a value close to 1 indicates a very high or perfect correlation. Typically, a CC above 0.9 is considered a high correlation (good agreement) for wave heights. It is noted that CC is 1 (or -1) for any two fully linearly correlated variables, even if they are not 1:1. However, the slope and intercept of the linear relation may be different from 1 and 0, respectively, despite CC of 1 (or -1).

The Q-Q line slope and intercept are found from a linear fit to the data quantiles in a least-square sense. The lower and uppermost quantiles are not included on the fit. A regression line slope different from 1 may indicate a trend in the difference.

The peak ratio (PR) is the average of the N_{peak} highest model values divided by the average of the N_{peak} highest observations. The peaks are found individually for each dataset through the Peak-Over-Threshold (POT) method applying an average annual number of exceedance of 4 and an inter-event time of 36 hours. A general underestimation of the modelled peak events results in PR below 1, while an overestimation results in a PR above 1.

An example of a peak plot is shown in Figure B.1. 'X' represents the observed peaks (x-axis), while 'Y' represents the modelled peaks (y-axis), based on the POT methodology, both represented by circles ('o') in the plot. The joint (coinciding) peaks, defined as any X and Y peaks within ±36 hours[19] of each other (i.e. less than or equal to the number of individual peaks), are represented by crosses ('x'). Hence, the joint peaks ('x') overlap with the individual peaks ('o') only if they occur at the same time exactly. Otherwise, the joint peaks ('x') represent an additional point in the plot, which may be associated with the observed and modelled individual peaks ('o') by searching in the respective X and Y-axis directions, see example with red lines in Figure B.1. It is seen that the 'X' peaks are often underneath the 1:1 line, while the 'Y' peaks are often above the 1:1 line.

[19] 36 hours is chosen arbitrarily as representative of an average storm duration. Often the observed and modelled storm peaks are within 1-2 hours of each other.

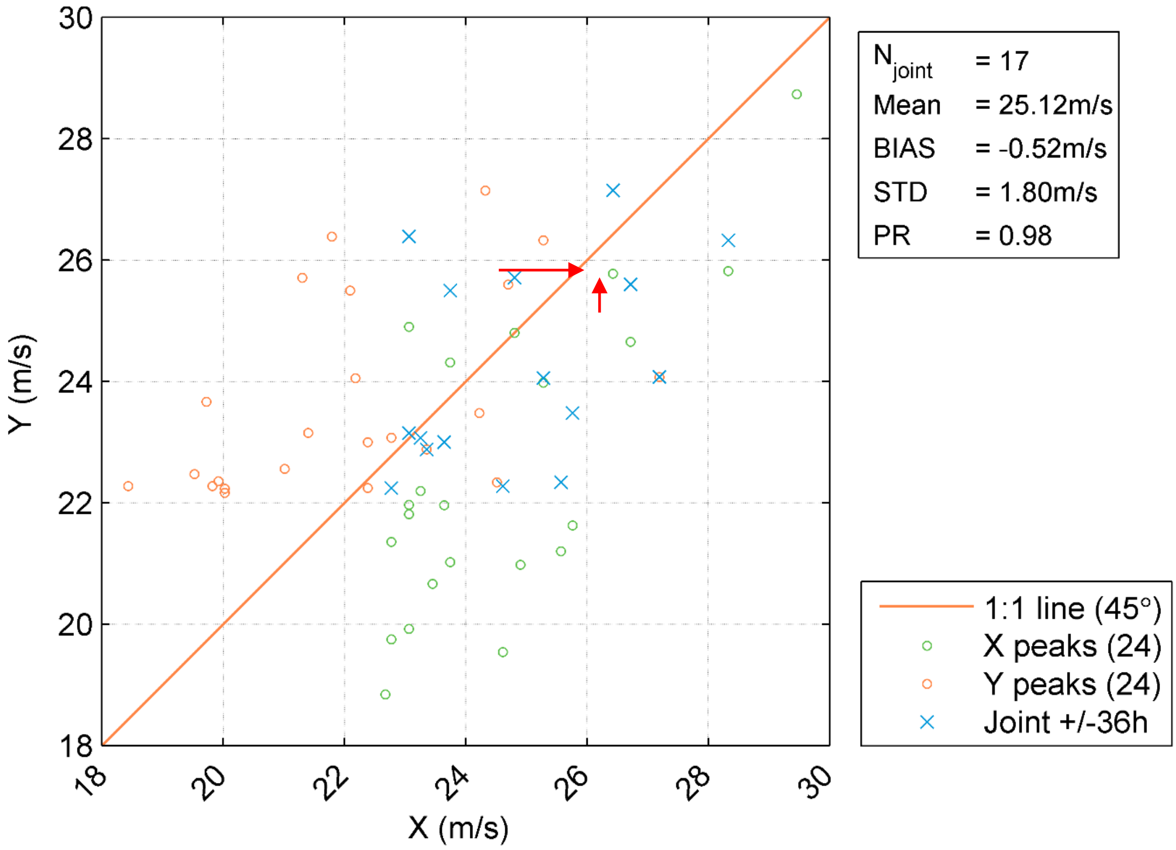


Figure B.1 Example of peak event plot (wind speed).

Table B.1 Definition of model quality indices (X = Observation, Y = Model).

Abbreviation	Description	Definition
N	Number of data (synchronised)	–
MEAN	Mean of Y data, Mean of X data	$\frac{1}{N}\sum_{i=1}^{N} Y_i \equiv \overline{Y}$, $\frac{1}{N}\sum_{i=1}^{N} X_i \equiv \overline{X}$
STD	Standard deviation of Y data Standard deviation of X data	$\sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(Y-\overline{Y})^2}$, $\sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(X-\overline{X})^2}$
BIAS	Mean difference	$\frac{1}{N}\sum_{i=1}^{N}(Y-X)_i = \overline{Y}-\overline{X}$
AME	Absolute mean error	$\frac{1}{N}\sum_{i=1}^{N}(\lvert Y-X\rvert)_i$
RMSE	Root mean square error	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y-X)_i^{\,2}}$
SI	Scatter index (unbiased)	$\frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y-X-BIAS)_i^{\,2}}}{\frac{1}{N}\sum_{i=1}^{N}\lvert X_i\rvert}$
EV	Explained variance	$\frac{\sum_{i=1}^{N}(X_i-\overline{X})^2-\sum_{i=1}^{N}[(X_i-\overline{X})-(Y_i-\overline{Y})]^2}{\sum_{i=1}^{N}(X_i-\overline{X})^2}$
CC	Correlation coefficient	$\frac{\sum_{i=1}^{N}(X_i-\overline{X})(Y_i-\overline{Y})}{\sqrt{\sum_{i=1}^{N}(X_i-\overline{X})^2\sum_{i=1}^{N}(Y_i-\overline{Y})^2}}$
QQ	Quantile-Quantile (line slope and intercept)	Linear least square fit to quantiles
PR	Peak ratio (of N_{peak} highest events)	$PR = i = 1NpeakY_i \sum_{i=1}^{N_{peak}} X_i$

APPENDIX C

Digital container of calibration/validation plots

C Digital container of calibration/validation plots