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A 20-yr reanalysis Experiment in the Baltic Sea Using three Dimensional Variational (3DVAR) method

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Abstract

A 20-year retrospective reanalysis of the ocean state in the Baltic Sea is constructed using three dimensional variational (3DVAR) data assimilation combining an operational numerical model with available historical temperature (T) and salinity (S) profiles.

⁵ To determine the accuracy of the reanalysis, the authors present a series of comparisons with independent observations on a monthly mean basis. The performance of the assimilation in deep/shallow waters is investigated.

With assimilation, temperature and salinity in the reanalysis fit better than the free run with independent measurements at different depths. Overall, the mean biases of temperature and salinity are reduced by 0.32 °C and 0.34 psu, respectively. Similarly,

- the mean root mean square error (RMSE) of the reanalysis is decreased by 0.35 °C and 0.34 psu, respectively. Similarly, the mean root mean square error (RMSE) of the reanalysis is decreased by 0.35 °C and 0.3 psu compared to the free run. In space, the model error is inhomogeneous and strongly steered by the model error dynamics. Seasonally varying error of the modeled sea surface temperature is mainly controlled by the weather forcing, and shows the
- ¹⁵ least improvements due to sparse observations. Deep layers, on the other hand, witness significant and stable model error improvements. In particular, the salinity related to saline water intrusions into the Baltic Proper is largely improved in the reanalysis. The major inflow events such as in 1993 and 2003 are captured more accurately in the reanalysis as the model salinity in the bottom layer is increased by 2–3 psu. Sea level
- is also improved due to an improved density field. The correlation between model and observation is increased by 2%-5%, and the RMSE is generally reduced by 10 cm in the reanalysis compared to the free run. The reduction of RMSE is mainly due to the reduction of mean bias. Assimilation of *T/S* contributes little to the barotropic transport in the shallow Danish Transition zone.
- The mixed layer depth exhibits strong seasonal variations in the Baltic Sea. The basin-averaged value is about 10 m in summer and 30 m in winter. In addition, assimilation of T/S profiles results in changes of about 20 m for the mixed layer depth in the Baltic Proper region in winter. Comparisons of mixed layer depth show that the



assimilation induces more changes in deep water of winter time whereas the mixed layer depth is changed only about 2 m in summer time and shallow waters. One reason could be that the effect of the assimilation is counterbalanced by the effect of heating in summer and the dominant role of the surface forcing in shallow water. The significant impact in deep waters suggests that the T/S assimilation mainly adjusts the baroclinic transport by redistributing the density field.

1 Introduction

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Reanalysis combining state of the art models and assimilation methods with quality controlled observations has helped enormously in making the historical record more
homogeneous and useful for many purposes. For instance, ocean reanalysis data has been applied to research on ocean climate variability as well as on the variability of biochemistry, eco-systems (e.g. Bengtsson et al., 2004; Carton et al., 2005; Friedrichs et al., 2006; Kishi et al 2007). Ocean reanalysis can also provide benchmarks for comprehensive validation of model results in a wide range (e.g. Carton et al., 2008; Fu
et al., 2009; Fu et al., 2011a). Comparison of reanalysis and non-assimilated simulation could help to identify deficiencies of ocean assimilation and prediction systems. Moreover, reanalysis in the ocean is beneficial to the identification and correction of

deficiencies in the observational records and filling the gaps in observations.

The Baltic Sea is an intercontinental dilution basin with a total area of 415 000 km². A large amount of freshwater is supplied from rivers and net precipitation in the northeastern part of the sea. Saline water enters the Baltic Sea in the southwestern strait area where currents and mixing processes are strongly influenced by the narrow and shallow Danish straits. In the Baltic Proper, deep water exchange is restricted by submarine sills and channels connecting deep basins. As the mean depth is about 54 m, the dy-

namics of the Baltic Sea is largely controlled by the atmospheric forcing which causes strong temporal variability in motions and physical properties (e.g. Leppäranta and Myrberg, 2009). Modeling and data assimilation in the Baltic Sea pose great challenges



due to the complex bathymetry and bottom topography. In the subsurface, direct observations in this region are sparse and inhomogeneous both in space and time. Therefore, it has been necessary to develop novel techniques for increased homogeneity of ocean reanalysis. In the past few years, there has been a proliferation of data assimilation algorithms applied in the Baltic Sea. These algorithms fall into two categories in a broad sense: variational adjoint methods and sequential estimation. For instance, a simplified Kalman filter was employed for sea surface temperature (SST) assimilation using a two-way nested model (Larsen et al., 2006). The Optimal Interpolation

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(OI) method is applied for the operational ocean forecasting at the Swedish Meteoro logical and Hydrological Institute (SMHI) (Pemberton and Funkquist, 2006). A three dimensional variational (3DVAR) method with an anisotropic recursive filter is used for
 dealing with observed profiles of temperature and salinity (Liu et al., 2009; Zhuang et al., 2011). Fu et al. (2011b) attempted an Ensemble Optimal Interpolation (EnOI) to
 assimilate temperature and salinity profiles. Major objectives of these studies are: first,
 validating the assimilation schemes; second, enhancing the understanding of the state in the Baltic Sea; and third, examining the role of adjusting model parameters in the assimilation of coastal/shelf seas.

Assimilation of subsurface *T/S* profiles contributes greatly to modeling the ocean state and improving the ocean forecasts in the Baltic Sea. This has been demonstrated in previous studies (e.g. Liu et al., 2009; Fu et al., 2011b; Zhuang et al., 2011). Although results from these studies are shown to be beneficial and encouraging, the experiments usually cover relatively short periods ranging from months to a year. Assimilation experiments covering a long term period would be desirable in the Baltic Sea for climate related research e.g. detection climate change signals, testing the performance of cou-

²⁵ pled regional climate models and scenarios etc. Moreover, the reanalysis provides uniformly and regularly available samples of not only variables that are directly observed, but also indirect variables such as vertical velocity, water mass transformation and transport whose long-term variations can not be investigated with observations.



In this paper we present a multi-decadal reanalysis experiment to reconstruct the changing ocean state in the Baltic Sea. At present, a reanalysis experiment covering 1990–2009 has been conducted by assimilating available historical temperature and salinity profiles. Our goals are twofold: first, to explore and assess the effect of data assimilation on rectifying the model's deficiencies such as poor simulation of the saline water intrusion in the Baltic Proper region; second, to construct a long homogeneous analysis of the sea level, temperature and salinity of the Baltic Sea. We adopt a three dimensional variational (3DVAR) approach in which a numerical model provides a first guess of the ocean state at the update time and is modified by inserting corrections into the initial condition in an regular basis.

The rest of the paper is organized as follows: observations and data assimilation method are described in Sect. 2; Model description is given in Sect. 3; Sea level, temperature, salinity and mixed layer depth of the reanalysis are compared with various dataset in Sect. 4; Summary and conclusion are given in Sect. 5.

15 2 Data assimilation

2.1 3DVAR scheme

In this study, a 3DVAR is used to find the optimal solution of the model state \mathbf{x} which minimizes the following cost function:

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{B}^{-1} (\mathbf{x} - \mathbf{x}_b) + \frac{1}{2} (H(\mathbf{x}) - \mathbf{y}_o)^T \mathbf{R}^{-1} (H(\mathbf{x}) - \mathbf{y}_o)$$
(1)

²⁰ **x** is the model state to be estimated. x_b is the background state vector, y_o is the observation state vector. *H* is the non-linear observational operator with which the analysis equivalent of observation y = H(x) can be obtained to compare with the observation measurements. The superscript T denotes matrix transpose. In the cost function, background error covariance (**B**) and observational error covariance (**R**) weight the misfit



between analysis and background and the misfit between analysis and observation, respectively. Usually the optimal solution is found by minimizing the cost function J(x) with respect to x, in which its gradient is also needed for determining the search direction and iteration steps in the minimizing algorithm:

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$$\nabla J(\mathbf{x}) = \mathbf{B}^{-1}(\mathbf{x} - \mathbf{x}_b) + \nabla_{\mathbf{x}} H(\mathbf{x})^T \mathbf{R}^{-1}(H(\mathbf{x}) - \mathbf{y}_o)$$

An incremental method (Courtie et al., 1994) is used to transform Equation (1) and it is linearized around the background state into the following form:

$$J(\delta x) = \frac{1}{2} \delta x^{T} B^{-1} \delta x + \frac{1}{2} (H \delta x - d)^{T} R^{-1} (H \delta x - d)$$
(3)

where $d = y_o - H(x_B)$ is the innovation vector, *H* is the linearized observation operator veluated at $x = x_B$ and $\delta x = x - x_B$ is the analysis incremental vector.

In our current scheme, the state vector is composed of only temperature and salinity:

 $\boldsymbol{x} = \begin{bmatrix} T \ S \end{bmatrix}^T \tag{4}$

A preconditioned control variable transform (defined by $\delta x = Uv$) is used in the pro-¹⁵ cess of minimization (e.g. Lorenc, 1997) where *U* is chosen to approximately satisfy the relationship $B = UU^{7}$ and the control variable vector *v* is chosen as their errors are relatively uncorrelated. In this way, the minimization can be carried out without handling the inverse of **B**. For a typical coastal ocean data assimilation system, the order of original size of the background error covariance matrix **B** is about $10^{6} \sim 10^{7}$.

²⁰ A quasi-Newton L-BFGS algorithm (Byrd et al. 1995) is adopted to minimize the cost function. Due to its moderate memory requirement, the L-BFGS method is particularly well suited for optimization problems with a large number of variables.

The computation of **B** implicitly involves the transform of **U** which includes a sequence of linear operators:

 $_{25} \quad \boldsymbol{U} = \boldsymbol{U}_{\boldsymbol{P}}\boldsymbol{U}_{\boldsymbol{V}}\boldsymbol{U}_{\boldsymbol{H}}$



(2)

(5)

where U_H and U_V are the horizontal and vertical part of the control variable transform related to the modes of **B**, and U_P is the physical transform related to the multivariate dynamic or physical constraints (e.g. the relationship between sea surface height (SSH) error and temperature/salinity error). The horizontal part of background error covariance (B) is represented by recursive filter and the vertical part is represented with dominant

 (B) is represented by recursive filter and the vertical part is represented with dominant EOF modes to reduce computational expense. A more detailed description is given in Zhuang et al. (2011).

2.2 Data preparation for reanalysis

The main datasets to constrain the model forecast are the historical T and S profiles from the International Council for the Exploration of the Sea (ICES). The data were compiled and quality-controlled before beeing assimilated into the model. Some withheld profiles together with tide gauge sea level data and satellite Sea Surface Temperature (SST) data are used to validate the reanalysis and quantify the uncertainty. The tide gauge data are obtained from DMI data base which includes the historical observations at stations near the coast.

From 1990 to 2009, the ICES basic subsurface temperature and salinity observation data sets consist of approximately 139315 profiles. The ICES community now includes all coastal states bordering the North Atlantic and the Baltic Sea. The ICES Data Centre accepts a wide variety of marine data and meta-data types into its databases from its members. In general, the historical dataset comprises most of the measurements

- Its members. In general, the historical dataset comprises most of the measurements collected from the Baltic Sea region for the past many years. The data coverage as a function of space and time is presented in Fig. 1. The number of observations is ranging from 1200 to 4000 per month. One prominent feature is that it has significantly decreased since 1998.
- ²⁵ Most of the *T/S* profiles have already gone through a primary data quality control prior to the entry into the ICES Database. For further application in data assimilation, we have applied a simple quality control scheme in the 3DVAR in order to remove the data of "poor quality" and avoid sharp shocks to the model. In calculating the innovation



vector, i.e., the difference between the background field and the observations, an observation will be excluded when the differences exceed three standard deviations of the variability of analysis. For a long term experiment, one critical issue is to ensure a stable integration. To avoid strong shocks to the initial state, we empirically adjusted

- the errors of observations according to the innovations. By this definition, some observations were discarded because the innovations exceed a certain number. The criteria are set up empirically based on our past validation results of the model. For example, an observation will be discarded if the magnitude of innovation is larger than 3.0 °C or 2.5 psu.
- The above treatment is important for long time assimilation. For instance, Fu et al. (2011b) and Zhuang et al. (2011) carried out specific experiments to investigate the effect of initial condition on the subsequent forecast. The first experiment starting from initial condition with T/S profiles assimilated was compared to the second experiment starting from initial conditions with no data assimilation. In general, the bias and
- RMSE of *T/S* is shown to be obviously reduced in the first experiment in the nexe 2 or 3 weeks. It can be expected that the persistence time would be larger in the deep bottom layer of the Baltic Sea where the water masses are relatively stationary. In this sense, the model state cannot be drastically adjusted during the assimilation and a cold/warm eddy may be spuriously formed due to the large misfit between model and observation.
- ²⁰ The "shock" on model state caused by a "problematic" observation can be maintained in the following simulation and cause the model unstable. This problem can well happen at the beginning of the assimilation experiment because the model differs largely from the observations in some areas. As the model state is rendered close to observations with the continuously insertion of measurement information, the criteria based
- on innovations will be gradually loosened. In total, there are about 82 354 temperature and 79 148 salinity measurements combined into the model. About 2000 observations are withheld for validating the reanalysis as independent data. With the above quality control, about 8 % temperature and 9 % salinity measurements are discarded from the original dataset.



3 Model configuration

3.1 Physical model

The model used in this study is a two-way nested, free surface, hydrostatic threedimensional (3-D) circulation model HIROBM-BOOS (HBM). The model code forms

- the basis of a common Baltic Sea model for providing GMES Marine Core Service since 2009. The finite difference method is adopted for its spatial discretization in which a staggered Arakawa C grid is applied on a horizontally spherical and vertically zcoordinate. A detailed description of the model can be found in Berg and Poulsen (2011).
- In this study, the model is set up with a coarser resolution than the model's operational set up. It has a 6 nautical mile (nm) horizontal resolution for the Baltic-North Sea with a two-way nested 1nm resolution domain to resolve the narrow Danish Straits (Fig. 1). It should be noted that the two-way nesting facility is very important in making multi-decadal simulations in order to correctly resolve the Baltic-North Sea transport.
- The 3D models have in total 50 vertical layers. The top layer thickness is selected at 8 m in the coarse resolution Baltic-North Sea model in order to avoid tidal drying of the first layer in the English Strait. The rest of the layers in the upper 80 m have 2 m vertical resolution. The layer thickness below 80 m increases gradually from 4 m to 50 m. For the fine resolution domain, the vertical resolution is enhanced to resolve the strong stratification in the shallow inner Danish waters. The ten layer is 0 m and then with a
- stratification in the shallow inner Danish waters. The top layer is 2 m and then with a 1 m or 2 m layer thickness in the rest of 49 layers.

The meteorological forcing is based on a reanalysis using the regional climate model HIRHAM through a dynamic downscaling (including a daily re-initialization) from ERA-Interim Global reanalysis. HIRHAM is a regional atmospheric climate model (RCM)

²⁵ based on a subset of the HIRLAM and ECHAM models, combining the dynamics of the former model with the physical parameterization schemes of the latter. The HIRLAM model – High Resolution Limited Area Model - is a numerical short-range weather forecasting system developed by the international HIRLAM Programme (http://hirlam.org).



The ECHAM global climate model (GCM) is a general atmospheric circulation model developed at the Max Planck Institute of Meteorology (MPI) in collaboration with external partners. The original HIRHAM model was collaboration between DMI, the Royal Netherlands Meteorological Institute (KNMI) and MPI. A detailed description of HIRHAM Version 5 can be found in Christensen et al. (2006).

3.2 Experimental setup

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Two experiments spanning 1990–2009 have been carried out in this study. The surface momentum and heat fluxes in the model are calculated by using bulk formulations with inputs of hourly HIRHAM data of 10 m wind, 2 m air temperature, mean sea level pressure, surface humidity and cloud cover was used on the ocean model grid with a horizontal resolution of about 12 km. The surface heat flux was parameterized using bulk quantities of both atmosphere and sea or sea ice and taken into account only in the heat budget calculations. Change of water volume due to evaporation, precipitation and ice formation were ignored. River fresh water discharge was a daily averaged

- ¹⁵ data based on a combination of measurements and hydrological simulations. The lateral boundary condition in the North Sea contains three components: a tidal sea level derived from 17 major tidal constituents; a surge component derived from a Northeast Atlantic two-dimensional surge model (in 6 nm resolution) and a density profile derived from ICES *T/S* monthly climatology.
- The first experiment is a free run of the model without data assimilation while the second experiment is conducted with the same forcing but with assimilating ICES *T/S* profile data by using the 3DVAR Scheme described in Sect. 2.1. The assimilation is performed on a daily basis provided that any observations are available. Observations are combined into the initial state of the model at the end of a day and the updated model
- state will serve as a new initial state in a sequential way. The number of assimilated observations is shown in Fig. 1. The number is not necessarily increasing with time and ranging from 1000 to 4100 for different months. For the two experiments, hourly model output is saved for future applications that require high temporal resolution.



4 Results

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To present an overview of the quality of the reanalysis, we validate the monthly mean reanalysis against a variety of observations. Sea level measurements from tide gauge stations, satellite SST and independent in situ observations are used to assess the misfit between model and observations. The correlation coefficients, evolution of RMSE (Root Mean Square Error) and bias are presented for the period 1990–2009.

4.1 Temperature

4.1.1 SST verification

Monthly mean satellite SST maps were obtained from BSH, based on observations
from NOAA AVHRR measurements during 1990–2009. The monthly model SST errors against the satellite data were estimated and the results are shown in Fig. 3. For the free run, the model has a RMSE of 1.87 °C. A large part of this error is attributed to the SST biases, which vary seasonally ranging from 1 to 1.5 °C. The maximum warm bias occurs in winter and a cold bias in summer. The RMSE was reduced to 1.69 °C after the assimilation whereas the bias was only reduced by 0.09 °C. The large seasonal bias may be attributed to errors in the meteorological forcing and heat flux parameterization used in the ocean model. This bias cannot be eliminated by the assimilation of only sparse *T/S* profiles. An interesting feature is that the major SST error reduction due to the assimilation occurs in winter when fewer observations are found. It should be noted that the abave comparison is effected by the assimilation occurs in when fewer observations are found.

that the above comparison is affected by the quality of satellite SST, which also has biases compared to profile data according to Löptien and Meier (2011). The deviations between satellite data and in situ observations are strongest in spring and somewhat weaker during the other seasons.



4.1.2 Temperature profile verification using independent data

The time series of temperature is compared with independent observations located at (55.15° N, 15.92° E) in the Bornholm Basin and at (57.15° N, 19.92° E) in the Baltic Proper. These two locations are withheld from the assimilation because they have relatively complete records for the period 1990–2009. In the Bornholm Basin, the upper layer of the sea is subject to strong annual and semi-annual variations. According to Fu et al. (2011a), the annual and semi-annual cycles account for 70 percent of the total variance in the temperature. From Fig. 4, the characteristics in the observations are well reproduced by the model for the whole period. The temperature at 15 m exhibits strong annual and semi-annual variations. The temperature differs by about 10°C between winter and summer whereas the inter-annual variability is much weaker. The correlation coefficient between model and observation is very high (0.98) for the 20 yr period. By comparison, temperature in the reanalysis is slightly improved by 0.1–0.3°C at several months. The depth of 50 m can be a good representative of permanent halo-

- cline in the Bornholm basin which typically lies at about 40-60 m. At this depth, the temperature in the intermediate water is less subject to annual and semi-annual variations than at the surface. Notably, the effect of assimilation is more evident than at the depth of 15 m. The correlation coefficient is increased from 0.74 in the free run to 0.81 in the reanalysis while the mean RMSE is reduced from 1.27 °C to 0.98 °C. The temper-
- ature at the depth of 80 m can be representative of the temperature in the bottom layer. It is found that the reanalysis temperature is much closer to the observations than the free run. The misfit is substantially decreased from 1.20 °C to 0.49 °C while the correlation coefficients rise from 0.72 to 0.91. It suggests that the reanalysis reproduces more realistic variations of the temperature near the bottom layer.

²⁵ In the central Baltic Proper, the water column is permanently stratified and the halocline lies at about 60–80 m. The two models runs show similar error feature as in the Bornholm Basin station. The temperature at (57.15° N, 19.92° E) is well simulated by the model at the depth of 15 m (Fig. 5a) with a model-data correlation coefficient of



0.96. However, the free run overestimates the temperature at 50 m depth by ~1°C (Fig. 5b). As the model's resolution was inadequate to resolve the topography and eddies in this region, the halocline was deeper in the model than in the observations. In the reanalysis, this is largely improved where the temperature is much closer to the observations. The mean RMSE is reduced from 1.09°C to 0.45°C while the correlation coefficient is raised from 0.75 to 0.81. Still, there are years giving exceptions, e.g. 1994 and 2004. The temperature at the depth of 175 m represents conditions of deep layer, which is dominated by inter-annual variability (Fig. 5c). Changes of the water mass in this area are strongly linked to large-scale atmospheric variability (Stigebrandt and Gustafsson 2003). For instance, the temperature was 1°C higher from 1998 onward then the period 1000.

than the period 1990–1998. Similarly, the reanalysis data fitted better with the observations for most of the time. The RMSE is decreased from 0.42 °C to 0.17 °C whereas the correlation coefficient is noticeably increased from 0.79 to 0.96.

4.1.3 Temperature profile verification using all data

- facilitate the comparison. the observed profiles binned То are into 15 10 km × 10 km × 1 mon bins corresponding with the model grid. In addition, the bias and RMSE are also calculated below the permanent halocline depth in the central Baltic where the model tends to have large bias. The total RMSE and bias of both runs are shown in Fig. 6. In Fig. 6a, the model has clear warm bias in the Baltic Sea. The mean bias is about 0.69°C for the whole basin and all seasons. Notably the all season 20 warm bias is not consistent with the SST verification results in Sect. 4.1.1 where a strong cold bias is shown in summer. A possible explanation is that there is a significant
- warm bias in the subsurface layer of the model so that the cold bias in summer was compensated by the subsurface warm bias. In addition, the bias is smaller in winter then in summer for most verse. During summer, a very shallow account thermacline
- than in summer for most years. During summer, a very shallow seasonal thermocline develops in the Baltic Sea when the surface cold water is warmed. In the shallow western area, there is a change between stratification and well-mixed conditions. At present, modeling the seasonal thermocline is still a big challenge for high resolution



coastal models, which tend to result in big errors of the temperature in summer. In the reanalysis, the mean bias was typically less than the free run. For the whole Baltic Sea, it was reduced to 0.37 °C. In particular, the warm bias was significantly reduced from 0.78 °C to 0.20 °C below 60 m (Fig. 6c). This demonstrates the benefit
⁵ of data assimilation for systematic errors. It should be noted the comparison was not independent and may be affected by the number of available observations for each month.

Different from the bias, the RMSE of temperature appears to be dominated by seasonal variations in the Baltic Sea, about 2.0 °C in summer and 1.0 °C in winter. As
explained above, the model has large bias in summer time, which comprises a large portion of the RMSE. By comparison, the RMSE was generally reduced in the reanalysis for the 20 years. For example, the mean RMSE was 1.58 °C for the Baltic Sea for the free run while it was reduced to 1.37 °C in the reanalysis (Fig. 6c). Below 60 m, the RMSE was largely reduced from 1.38 °C to about 0.89 °C in the reanalysis (Fig. 6d).
Mean bias reflected the time-mean component of the systematic errors due to model deficiencies. Meanwhile, the time-varying components could result from inaccuracies in the time baltic sea for the systematic from inaccuracies.

in the time varying boundary forcing. This part is relatively difficult to rectify with the current assimilation scheme. For example, the total bias for the Baltic Sea was reduced from 0.69 °C to 0.37 °C while the RMSE was still about 1.37 °C in the reanalysis.

20 4.2 Salinity

4.2.1 Salinity profile verification using independent data

The time series of salinity is compared with independent observations for the same two stations as used for the verification of temperature. The comparison provides a good opportunity to examine the saline water intrusion (inflow) from the Bornholm Basin to the Baltic Proper. In the buffering Bornholm Basin, the incoming water may be trapped

the Baltic Proper. In the buffering Bornholm Basin, the incoming water may be trapped by the sill depth. According to classical descriptions (e.g. Grasshoff, 1975), there are three different modes of salt water intrusion: (1) regular inflow just below the primary



halocline interleaving on the level of neutral buoyancy; (2) occasional inflow of saline water, sinking to the bottom and exchanging the Bornholm Basin deep water; (3) rather infrequent occasional (major) inflow of large amounts of saline water, filling the whole Bornholm Basin above Stolpe Sill level (60 m) and exchanging the Gotland Deep water.

- ⁵ The model simulation played an important role in the Bornholm Basin because sinking or mixing of the incoming saline water will have large impact on the salinity in the central Baltic Sea. Figure 7 displays model-data salinity comparison at Bornholm Basin station (55.15° N, 15.92° E). As shown in Fig. 7, the observed salinity at 15 m depth displayed pronounced seasonal variation which is associated with the variation of fresh
- river runoff and net E-P (Evaporation-Precipitation) flux. The salinity is large in spring and small in summer. The observations also show a slightly decreasing trend from 1990 to 2002. After assimilation, the reanalysis is rendered closer to observations for most months. The mean RMSE is reduced from 0.18 psu in the free run to 0.09 psu while the correlation coefficient is increased from 0.60 to 0.73 (Fig. 7a). At 50 m depth
- (Fig. 7b), the reanalysis salinity is also closer to the observations than the free run. The strong inter-annual variations are better produced as the correlation coefficient with the observed time series is increased from 0.36 to 0.49. Meanwhile, the RMSE is slightly decreased from 1.20 psu to 1.12 psu. At the depth of 80 m, however, the free run is substantially lower than the observation by about 2 psu. This is probably caused by
- ²⁰ poor simulation of the saline water intrusion in this region. As stated above, the intrusion of saline water behaves in three different manners. It posed great challenges for model to tackle the dynamics of the inflow process, which is complex and contains internal fronts with fine-scale intrusions, surface and subsurface eddies etc. The benefit of data assimilation can be clearly seen from Fig. 7c. The mean RMSE is largely decreased
- ²⁵ from 4.33 psu to 1.34 psu. For the major inflow events in 1993 (Jacobsen, 2005) and 2003, the salinity in the reanalysis is much closer to the observations at 80 m than the free run. The correlation coefficient with the observations is about 0.68 and 0.74 for the free run and reanalysis, respectively.



The time series of salinity at Gotland Deep station $(57.15^{\circ} N, 19.92^{\circ} E)$ is shown in Fig. 8 for the upper, intermediate and bottom layer. At 15 m depth, salinity of the free run is typically improved by the assimilation (Fig. 8a). The mean RMSE is considerably decreased from 0.31 psu to 0.13 psu while the correlation coefficient is increased from

- 5 0.49 to 0.78. In addition, the decreasing tendency in the salinity of the free run is absent from the reanalysis and observation. At the depth of 80 m (Fig. 8b), the salinity was slightly increased from 1990 to 2009 in the observations, which could be associated with the saline water intrusion. However, the increasing trend is absent in the free run. In the reanalysis, the variations of salinity is much more consistent with the ob-
- servations than the free run as the correlation coefficient is significantly increased from 0.18 to 0.62. Further, the RMSE is reduced from 0.86 psu to 0.38 psu. Water below primary halocline of the Baltic Proper is comparatively steady and its natural variation is strongly related to the large-scale atmospheric variability and the accumulated freshwater inflow (Stigebrandt and Gustafsson 2003; Meier and Kauker 2003). This can be
- ¹⁵ demonstrated from the salinity at the depth of 175 m (Fig. 8c). The observations show a clear increasing trend from 1990 to 2009. The salinity reaches 12.5 psu in from 2004 to 2009, indicating strong saline water intrusion. Without assimilation, bottom saline water in the free run is gradually diluted which reflects the deficit of model in simulating inflow events. The salinity is about 2 psu lower than the observations. The effect of the
- assimilation could be sustained for long time because of the steady water masses in this region. Once the state of the bottom water is changed, it is maintained until another inflow intrudes. It can be seen from the reanalysis, which presents remarkable improvements as the salinity is generally increased by 2 psu. In addition, the major inflow events are more consistent with the observations except in 2006–2008. The RMSE
- is reduced from 2.31 psu to 0.27 psu while the correlation coefficient is increased from 0.78 to 0.89.

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4.2.2 Salinity profile verification using all data

To get an overall statistics of the improvement on salinity, we compared the total RMSE and bias of the reanalysis with those of the free run. The verification process is similar as made for temperature in Sect. 4.1.3. In Fig. 9, the modeled salinity is about 0.5 psu

- ⁵ lower than the observations in the Baltic Sea. In particular, the bias is more prominent below 60 m (about -1.07 psu) in the central Baltic Sea where salinity is largely influenced by the simulation of inflow from Bornholm basin to the Baltic Proper. In the reanalysis, the mean bias is typically reduced for the whole Baltic Sea and in the central Part. The mean bias is about -0.18 for the whole Baltic Sea compared to -0.52 in the
- free run. Meanwhile, the mean bias was significantly reduced from -1.07 to -0.21 psu in the central part of the Baltic Sea (Fig. 9c). Similar to the bias, the RMSE is also substantially reduced in the reanalysis. For example, the mean RMSE is 1.46 psu for the Baltic Sea in the free run (Fig. 9b) while it is reduced to 1.15 psu in the reanalysis. Below 60 m, the RMSE was largely reduced from 1.74 psu to about 0.83 psu in the reanalysis due to the improvement on the simulation of inflow (Fig. 9d).

4.3 Sea level

Since sea level is a very good indicator of the model behavior with respect to the barotropic dynamics of the system, it is one of the most important variables to be assessed in the reanalysis. Typically large-scale ocean models are judged against satel-²⁰ lite born altimeter data. The validation with altimeter data has severe limitations in relatively small semi-enclosed seas like the Baltic Sea due to the limited accuracy near the coast and their low spatial resolution. Meanwhile, the validations against observed sea level from tide gauge stations are of higher confidence than those against satellite sea level in the coastal region. In this study, the sea level from the 20yr reanalysis is ²⁵ compared to independent tide gauge data at 14 stations. RMSE and correlation coefficients are calculated with the data on monthly basis (Table 1). Since no sea level data



is assimilated, the comparison is completely independent.

From Table 1, most of the stations are located in the transition zone between the North Sea and the Baltic Sea. In this transition zone, a general estuarine circulation forms a regional scale frontal system from northern Kattegat to the Arkona Sea. Numerical modeling in this region requires high-resolution bathymetry usually achieved

- ⁵ by a nested model system (She et al., 2007). Compared with tide gauge, the correlation coefficient at 9 stations was larger than 0.8. At Rodby and Gedser, the coefficients were 0.52 and 0.67, respectively. These two stations were located near the Darss Sill where the sub-grid scale feature of narrow transport cannot be fully resolved even in high resolution nested model. In general, it was encouraging that the reanalysis was
- ¹⁰ better correlated with the tide gauge data than the free run by 2–5%. In addition, the mean bias of sea level was substantially reduced by about 0.1 m for all stations, indicating the impact of *T/S* assimilation. In fact, assimilation of temperature is equivalent of modifying thermal expansion while assimilation of salinity amounts to altering water volume. The induced variations in the density will cause regional changes in sea level.
- ¹⁵ However, we found that the redistributed density field mainly contributed to reducing the mean bias of the model. In Table 1, the RMSD was calculated similarly as the RMSE by using the residual of time series whose mean is subtracted. The reduction of RMSD could reflect the impact of assimilation on the time-varying component of the systematic errors. The changes in RMSD were less than 1 cm for the most stations. It suggests that the assimilation of sparse *T/S* profile data behaved more effectively in
- ²⁰ suggests that the assimilation of sparse *T/S* profile data behaved more effectively in rectifying the time-mean component of systematic errors.

The transition zone between the North Sea and the Baltic Sea is characterized by a brackish Baltic Sea outflowing in the upper layer and a saline North Sea in the bottom layer. Time series of sea level at Gedser and Hornbaek are presented in Figure 10. It is

shown that the free run produced sea levels generally higher than the tide gauge data. Sea level in the reanalysis was decreased after the assimilation and closer to observations. As shown in Table 1, the improvements were essentially due to the reduction of the mean bias. Sea level differences between Hornbæk and Gedser can be regarded as a barotropic transport index. The barotropic transport through the area is relatively



large, with instantaneous transport which can be an order of magnitude larger than the annually averaged estuarine flow (Bendtsen et al., 2009). This transport is forced by the water level difference between the northern Kattegat and the Arkona Sea. From Fig. 10c, the water level difference between Hornbæk and Gedser showed very minor
changes between the free run and reanalysis. The strong transport in 1993 was not captured in both experiments. The variations in the transport were well produced but the magnitude was underestimated. The assimilation of *T/S* seems ineffective to improve the barotropic transport. This may be related to that the density changes of the water mass that are caused by *T/S* assimilation largely act on the baroclinic transport through the Danish transition zone.

4.4 Mixing layer Depth (MLD)

The mixed layer depth is an important variable for determining seasonal climate signals, and primary biogeochemical features in marine ecosystems. With very deep mixed layers, the phytoplankton are unable to get enough light to maintain their ¹⁵ metabolism. The shallowing of the mixed layers during spring in the North Atlantic is therefore associated with a strong spring bloom of plankton. The mixed layer is characterized by being nearly uniform in properties such as temperature and salinity throughout the layer. The depth of the mixed layer is often determined by hydrographic measurements of water properties. Two criteria often used to determine the mixed layer ²⁰ depth are temperature and sigma-t (density) change from a reference value. In this study, the temperature criterion as used in Levitus (1982) is chosen to define the mixed

layer as the depth at which the temperature change from the surface value exceeds 0.5 °C.

The climatological mixed layer depth from both experiments is presented in Fig. 11 for winter (January) and summer (July). Two features could be found: first, the mixed layer depth is typically larger in winter than in summer; second, assimilating *T/S* profiles deepens MLD by up to 20m in winter and 2meter in summer (Fig. 11e–f). The first feature is associated with the magnitude of turbulent mixing that is weak in summer



because of strong heating and weak wind. The mixed layer is only a few meters thick in some areas in summer. From autumn to winter, mixing due to the wind is strengthened, leading to thickening of the mixed layer. Therefore, the mixed layer continues to thicken and becomes thickest in late winter. The mean mixed layer depth differs by 20 m be-

tween winter and summer. Particularly in the Baltic proper, the mixed layer depth is only about 10 m in summer but is considerably deepened to 40–60 m in winter (Fig. 11b). The water column of this area in winter is well mixed and vertically homogeneous down to the halocline (about 60–70 m in central Baltic Sea).

The large change of winter MLD after assimilation suggests that the model does not have enough vertical mixing during winter (Fig. 11e). This can be caused by either the vertical mixing scheme in the ocean model or surface stress parameterization. Weather forcing is unlikely the cause as the reanalysis winds are quite accurate. There are little changes in the MLD of summer after the assimilation of *T/S* profiles (Fig. 11f), which indicates that either the MLD in summer is simulated properly in the free-run or the cauterling affect of weather is too strong to alter via the assimilation.

- ¹⁵ controlling effect of weather is too strong to alter via the assimilation. This is mainly because the state of upper sea in summer depends primarily upon the surface Ekman flow. The model simulation of the upper layer would thus depend almost entirely upon the accuracy of the meteorological forcing used to force the system. The surface forcing could quickly dissipate the changes of temperature and salinity caused by the data as-
- similation. Another important factor is the effect of gradually increasing heating, which contributes to the formation of a seasonal thermocline at about 10–20 m depth from spring. In summer, the heating is strongest and plays a dominant role in the formation of the mixed layer. The mixed layer is largely confined to the surface several meters above the thermocline. In this case, mixed layer may not benefit substantially from the
- assimilation when the role of meteorological forcing is dominant. The effect of assimilation is weak in shallow coastal water such as the Danish transition zone because the entire water column can be a turbulent boundary layer through the year. For instance, deep mixed layer in summer mainly occur near the coast, like the southern coast of central Baltic Sea, in southern Skagerrak and in the Archipelago Sea.



Evolution of the MLD at (57.15° N, 19.92° E) and mean simulated MLD for the Baltic Sea are presented in Fig. 12. As explained above, the MLD displays a pronounced seasonal cycle and is typically larger in winter than in summer for the mean value in the Baltic or at the given location. Both the free run and the reanalysis MLD at (57.15° N, 19.92° E) are in good agreement with the observations in summer, which supports

the findings in Fig. 11f. The most significant differences between the free run and the reanalysis occur in winter time, which is consistent with Fig. 11e which represents an improvement of simulating winter MLD. It is noted that even after assimilation, the model MLD in winter is still shallower than observations.

10 5 Summary and conclusion

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In this paper, a 3DVAR scheme is used to construct a retrospective analysis of temperature, salinity, and sea level in the Baltic Sea during the past 20 years. The goal of this reanalysis is two-fold: first, the performance of 3DVAR scheme can be assessed in a long term integration and provide more experience for future operational applications; second, the analysis can provide a uniformly gridded dataset for use in studies of model intercomparison, physical processes and other purposes in the Baltic Sea. The accuracy of the reanalysis is quantified by direct comparison against independent water level, temperature and salinity measurements from the region. Particular attention is focused on the effect of assimilation on reducing bias and RMSE in the model forecast.

We begin with a comparison to time series of temperature and salinity with relatively complete records in the Bornholm Basin and Baltic Proper. For these two locations, time series of temperature and salinity are generally improved in the reanalysis and fit better with the observations than the free run. The RMSE of temperature and salinity is substantially required for different deaths while the correlation coefficients between

is substantially reduced for different depths while the correlation coefficients between model and observation are largely increased. In particular, the salinity related to the saline water intrusion in this region is largely improved in the reanalysis. Major inflow



events such as in 1993 and 2003 are captured more accurately in the reanalysis as the salinity in the bottom layer is increased by 2-3 psu. Statistically, the mean bias of temperature is reduced from 0.69 to 0.37 °C for the whole Baltic Sea while the mean bias of salinity is reduced from -0.52 psu about -0.18 psu. Similarly, the mean RMSE is generally reduced in the reanalysis by 0.25 °C and 0.3 psu, respectively. In the central Baltic region, the errors associated with the simulation of saline water intrusion are significantly reduced in the reanalysis with mean RMSE and bias of salinity reduced by 0.86 psu and 0.91 psu.

The reanalysis is further validated against sea level data from 14 tide gauge stations. By comparison, the reanalysis is better correlated with the measurements than the free run as the correlation coefficients are increased by 2%–5% for most stations. In addition, the RMSE is generally reduced by 10 cm in the reanalysis. The reduction of RMSE is mainly due to the reduction of mean bias since the mean bias of the reanalysis is substantially decreased by 10 cm as well. After the mean is subtracted from the time

- series of sea level, root-mean-square differences are also shown to be slightly reduced (within 1 cm). It suggests the assimilation of *T/S* profiles contributes mainly to reducing the time-mean component of systematic errors of the model. Through the Danish Straits, there is a relatively large barotropic transport maintained by the water level difference between the northern Kattegat and the Arkona Sea. Differences of sea level
- ²⁰ between Gedser and Hornbaek are sometimes used as a barotropic transport index. The reduction of the mean bias contributes little to improve the barotropic transport. It appears that the assimilation helps to raise the whole water column in the Danish waters other than the distribution of the water mass. Assimilation of *T/S* profiles could play more important role in deep waters where changes in density filed due to assimilation ²⁵ would adjust the baroclinic transport and redistribute the water mass.

The mean mixed layer depth is compared between the reanalysis and free run for the 20 year period. In the Baltic Sea, the mixed layer is important for marine environment and fishery as its depth determines the average level of light seen by marine organisms. It is found that the mixed layer depth is typically large in winter than in summer,



differing by 20 m on average. In addition, changes in mixed layer depth due to the assimilation appear to be minor in summer time and shallow waters. The effect of heating in summer and dominant surface forcing could be linked to the relatively small effect of the assimilation. In deep waters, however, the effect of the assimilation is significant in winter time. In the Baltic Proper and Bothnian Sea the mixed layer is deepened by

⁵ In winter time. In the Baltic Proper and Bothnian Sea the mixed layer is deepened by 20 m in the reanalysis. In the Danish transition Zone to the Bornholm Basin, the mixed layer depth has small variations throughout the year because the whole water column can be regarded as a turbulent boundary layer.

The results of the reanalysis are encouraging because it is generally better than the run without assimilation for those comparisons with different observations. In addition, the assimilation helps to mitigate some model deficiencies such as the simulation of saline water intrusion in the Baltic Proper. The reanalysis can be regarded as a good surrogate data for process studies in the Baltic Sea. Furthermore, the long term reanalysis helps to identify problems in assimilation. For instance, the assimilation is less effective in shallow water such as the Danish transition water where the barotropic

transport is barely improved. The reduction of RMSE is largely due to the reduction of model's mean bias. The random error is only slightly reduced according to the correlation coefficients. Finally, this reanalysis may be further improved by assimilating more surface observations in addition to *T/S* profiles. But for this reanalysis, surface
 observations such as SST and SSH can easily be used for independent comparisons.

Some problems need to be further addressed in the reanalysis in the future: first, there is a significant seasonal SST bias, warm in winter and cold in summer. The improvement of SST by assimilating the ICES T/S profile data is very much limited due to a combined steering of the weather forcing and heat flux parameterization in the ocean

²⁵ model. Second, significant improvement is found in the intermediate and deep layers. This is related to the longer time scale in these layers. Spatially varing correlation scales may be more effective for the 3DVAR and will be implemented for the next step. Third, the MLD in the reanalysis is in good agreement with observations in summer but underestimates in winter. The underestimation in the Gotland Deep station is still up



to 10–40 m. Finally, assimilation of T/S profiles improves mean sea level by 10 cm but not the transient component of the sea level. For the next step, the reanalysis will be further improved by assimilating more surface observations particularly from satellite that is shown to play a complementary role to the subsurface in situ observations.

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Table 1. The correlation coefficients and RMSD of the model compared to observed tide gauge data in 14 stations. The RMSD is calculated with the residual of time series after the mean is subtracted.

	r collion (Bogicco)	Reanalysis			Free run		
		Corr Coef	RMSD	Bias	Corr Coeff	RMSD	Bias
rhus	56.15° N, 10.22° E	0.785	0.0668	0.1044	0.7453	0.0692	0.2069
ederikshavn	57.43° N, 10.57° E	0.827	0.0641	0.1569	0.8033	0.0661	0.2621
pshavn	55.28° N, 10.83° E	0.783	0.0605	0.1084	0.7501	0.0611	0.2100
rsor	55.33° N, 11.13° E	0.7255	0.0691	0.0922	0.7124	0.0667	0.1934
rnbaek	56.10° N, 12.47° E	0.8776	0.0581	0.1712	0.8588	0.0608	0.2728
dby	54.65° N, 11.35° E	0.5268	0.1014	0.0644	0.5367	0.0989	0.1655
dser	54.57° N, 11.93° E	0.6794	0.0869	0.1035	0.6766	0.0854	0.2045
n	55.25° N, 14.83° E	0.8775	0.0656	0.2353	0.8756	0.0649	0.3349
lix	65.68° N, 23.13° E	0.9153	0.0858	0.3847	0.9159	0.0856	0.4916
agshamn	55.52° N, 12.75° E	0.8626	0.0578	0.2231	0.8358	0.0618	0.3241
ngsholmsfort	56.08° N, 15.54° E	0.9001	0.0609	0.2700	0.8844	0.0644	0.3716
ngsvik	58.78° N, 11.13° E	0.9008	0.0526	0.1594	0.8848	0.0564	0.2646
tan	63.98° N, 20.88° E	0.9496	0.0622	0.3771	0.9480	0.0636	0.4835
sby	57.63° N, 18.28° E	0.9378	0.0540	0.2970	0.9318	0.0559	0.3971
rhus ederikshavn pshavn rsor rnbaek dby edser n lix agshamn ngsholmsfort ngsvik tan sby	56.15° N, 10.22° E 57.43° N, 10.57° E 55.28° N, 10.83° E 55.33° N, 11.13° E 56.10° N, 12.47° E 54.65° N, 11.35° E 54.57° N, 11.93° E 55.25° N, 14.83° E 65.68° N, 23.13° E 55.52° N, 12.75° E 56.08° N, 15.54° E 58.78° N, 11.13° E 63.98° N, 20.88° E 57.63° N, 18.28° E	Corr Coef 0.785 0.827 0.783 0.7255 0.8776 0.5268 0.6794 0.8775 0.9153 0.8626 0.9001 0.9008 0.9496 0.9378	RMSD 0.0668 0.0641 0.0605 0.0691 0.0581 0.1014 0.0869 0.0656 0.0858 0.0578 0.0609 0.0526 0.0622 0.0540	Bias 0.1044 0.1569 0.1084 0.0922 0.1712 0.0644 0.1035 0.2353 0.3847 0.2231 0.2700 0.1594 0.3771 0.2970	Corr Coeff 0.7453 0.8033 0.7501 0.7124 0.8588 0.5367 0.6766 0.8756 0.9159 0.8358 0.8844 0.8848 0.9480 0.9318	RMSD 0.0692 0.0661 0.0611 0.0667 0.0608 0.0854 0.0854 0.0649 0.0856 0.0618 0.0644 0.0564 0.0559	Bias 0.200 0.262 0.210 0.193 0.272 0.165 0.204 0.334 0.334 0.334 0.324 0.337 0.264 0.397

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Fig. 1. The model domain with depth contours used in the DMI- BSHCmod.





Fig. 2. The **(a)** spatial locations of the T/S profiles and **(b)** actual number of records being assimilated into the model for each month from 1990 to 2009.



















Fig. 5. The time series of temperature at $(57.15^{\circ} \text{ N}, 19.92^{\circ} \text{ E})$ for the depth of **(a)** 15 m, **(b)** 80 m, and **(c)** 175 m. The red is from experiment without data assimilation, the blue denotes assimilation experiment, and the black is for observations.











Fig. 7. The time series of salinity at $(55.15^{\circ} \text{ N}, 15.92^{\circ} \text{ E})$ for the depth of **(a)** 15 m, **(b)** 50 m and **(c)** 80 m. The red is from experiment without data assimilation, the blue denotes assimilation experiment, and the black is for observations.



Fig. 8. The time series of salinity at $(57.15^{\circ} \text{ N}, 19.92^{\circ} \text{ E})$ for the depth of **(a)** 15 m, **(b)** 80 m and **(c)** 80 m. The red is from experiment without data assimilation, the blue denotes assimilation experiment, and the black is for observations.





Fig. 9. The rmse and bias of salinity caculated with monthly mean data from 1990 to 2009 for **(a)** bias for all levels, **(b)** RMSE for all levels, **(c)** bais below 60 m and **(d)** RMSE below 60 m. The red is from experiment without data assimilation, the blue denotes assimilation experiment.



















