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A 20-year 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 by assimilating available historical temperature and salinity profiles into an operational numerical model with three-dimensional variational (3DVAR) method. To determine the accuracy of the reanalysis, the authors present a series of comparisons to independent observations on a monthly mean basis.

In the reanalysis, temperature (T) and salinity (S) fit better with independent measurements than the free run at different depths. Overall, the mean biases of temperature and salinity for the 20 year period are reduced by 0.32 °C and 0.34 psu, respectively. Similarly, the mean root mean square error (RMSE) is decreased by 0.35 °C for temperature and 0.3 psu for salinity compared to the free run. The modeled sea surface temperature, which is mainly controlled by the weather forcing, shows the least improvements due to sparse in situ 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 as the model salinity in the bottom layer is increased by 2–3 psu. Compared to independent sea level at 14 tide gauge stations, the correlation between model and observation is increased by 2 %–5 %, while the RMSE is generally reduced by 10 cm. It is found that the reduction of RMSE comes mainly from the reduction of mean bias. In addition, the changes in density induced by the assimilation of T/S contribute 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. By comparison, the assimilation induces a change of 20 m to the mixed layer depth in deep waters and wintertime, whereas small changes of about 2 m occur in summer and shallow waters. It is related to the strong heating in summer and the dominant role of the surface forcing in shallow water, which largely offset the effect of the assimilation.

1 Introduction

Reanalysis combining state-of-the-art models and assimilation methods with quality controlled observations has helped enormously to generate homogeneous historical data. Ocean reanalysis data serves many purposes. For instance, it has been applied to researches on ocean climate variability as well as on the variability of biochemistry and ecosystems (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 and Giese, 2008; Fu et al., 2009, 2011). Comparison of reanalysis and non-assimilated simulation could help to identify the deficiencies of ocean assimilation and prediction systems. Moreover, reanalysis in the ocean is beneficial to the identification and correction of deficiencies in observational records.

The Baltic Sea is an intercontinental dilution basin with a total area of 415 000 km^2. 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, the deep water exchange is restricted by submarine sills and channels connecting deep basins. Because the mean depth is about 54 m, the dynamics of the Baltic Sea are largely controlled by the atmospheric forcing, which causes strong temporal variability in motions and physical properties (e.g., Leppäranta and Myrberg, 2009). Thus, modeling and data assimilation in the Baltic Sea present great challenges due to the complex bathymetry and bottom topography. Subsurface measurements in this region are sparse and inhomogeneous in space and time. Therefore, there have been growing requirements to develop novel techniques for increased homogeneity of ocean state analysis. 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., 2007). The optimal interpolation (OI) method is applied for the operational ocean forecasting at the Swedish Meteorological and Hydrological Institute (SMHI) (Pemberton, 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. (2011) attempted an Ensemble Optimal Interpolation (EnOI) to assimilate temperature and salinity profiles in two-way nested model. Major objectives of these studies are as follows: first, validating the assimilation schemes; second, enhancing the understanding of the ocean state in the Baltic Sea; and third, examining the role of adjusting model parameters in the assimilation of coastal/shelf seas.

Assimilation of subsurface temperature and salinity profiles contributes greatly to modeling the ocean state and improving the ocean forecasts in the Baltic Sea. This has been demonstrated in some previous studies (e.g., Liu et al., 2009; Fu et al., 2011; Zhuang et al., 2011). Although results from these studies are encouraging, the experiments usually cover a relatively short period ranging from months to a year. Therefore, the usage of the results is limited for climate studies that focus on long-term variability and trends. Multi-decadal reanalysis would be desirable in the Baltic Sea for climate related research, e.g., to study daily to interannual variations, to validate the performance of coupled regional climate models and scenarios, even to identify fundamental errors in the physical processes that create climate model biases, etc. However, there is no such reanalysis published until now as far as we know. Another advantage of the reanalysis is that it 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 are difficult to investigate from sparse observations.

In this paper we carry out a multi-decadal reanalysis experiment to reconstruct the changes of the ocean state in the Baltic Sea. At present, available historical T/S profiles are assimilated in the reanalysis for the period 1990–2009. The goals are twofold: first, to explore and assess the impact of data assimilation on rectifying the model's deficiencies such as the poor simulation of saline water intrusion in the Baltic Proper region; second, to construct a long homogeneous analysis of sea level, temperature and salinity of the Baltic Sea. A three-dimensional variational (3DVAR) approach is adopted in which the numerical model provides the first guess of the ocean state at each update time and is modified by inserting corrections into the initial condition on an regular basis.

The rest of the paper is organized as follows: data assimilation method and the preparation of observations are described in Sect. 2; model description and experimental setup are introduced in Sect. 3; comparisons of the reanalysis with various datasets are presented in Sect. 4; conclusion and discussion are given in Sect. 5.

2 Data assimilation

2.1 3DVAR scheme

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

$$J(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_\mathrm{b})^\mathrm{T}\mathbf{B}^{-1}(\boldsymbol{x}-\boldsymbol{x}_\mathrm{b}) + \frac{1}{2}(H(\boldsymbol{x})-\boldsymbol{y}_\mathrm{o})^\mathrm{T}\mathbf{R}^{-1}(H(\boldsymbol{x})-\boldsymbol{y}_\mathrm{o}), \quad (1)$$

$\boldsymbol{x}$ is the model state to be estimated. $\boldsymbol{x}_\mathrm{b}$ is the background state vector, $\boldsymbol{y}_\mathrm{o}$ is the observation state vector. H is the nonlinear observational operator with which the analysis equivalent of observation $\boldsymbol{y} = H(\boldsymbol{x})$ can be obtained to compare with the observation measurements. The superscript "T" denotes matrix transpose. In the cost function, background error covariance ($\mathbf{B}$) and observational error covariance ($\mathbf{R}$) 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 $J(\boldsymbol{x})$ with respect to $\boldsymbol{x}$, in which its gradient is also needed for determining the search direction and iteration steps in the minimizing algorithm:

$$\nabla J(\boldsymbol{x}) = \boldsymbol{B}^{-1}(\boldsymbol{x}-\boldsymbol{x}_\mathrm{b}) + \nabla_\mathrm{x} H(\boldsymbol{x})^\mathrm{T}\boldsymbol{R}^{-1}(H(\boldsymbol{x})-\boldsymbol{y}_\mathrm{o}), \quad (2)$$

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

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

where $\boldsymbol{d} = \boldsymbol{y}_\mathrm{o} - \boldsymbol{H}(\boldsymbol{x}_\mathrm{b})$ is the innovation vector, H is the linearized observation operator evaluated at $\boldsymbol{x} = \boldsymbol{x}_\mathrm{b}$ and $\boldsymbol{\delta x} = \boldsymbol{x} - \boldsymbol{x}_\mathrm{b}$ is the analysis incremental vector.

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

$$\boldsymbol{x} = \left[T \;\; S \right]^{\mathrm{T}}. \tag{4}$$

A preconditioned control variable transform (defined by $\boldsymbol{\delta x} = \mathbf{U}\boldsymbol{v}$) is used in the process of minimization (e.g., Lorenc, 1997), where $\mathbf{U}$ is chosen to approximately satisfy the relationship $B = \mathbf{U}\mathbf{U}^{\mathrm{T}}$ and the control variable vector $\boldsymbol{v}$ is chosen as their errors are relatively uncorrelated. In this way, the minimization can be carried out without handling the inverse of $\mathbf{B}$. For a typical coastal ocean data assimilation system, the order of original size of the background error covariance matrix $\mathbf{B}$ is about $10^6 \sim 10^7$. 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 $\mathbf{B}$ implicitly involves the transform of $\mathbf{U}$ which includes a sequence of linear operators:

$$\mathbf{U} = \mathbf{U}_{\mathrm{P}}\mathbf{U}_{\mathrm{V}}\mathbf{U}_{\mathrm{H}}, \tag{5}$$

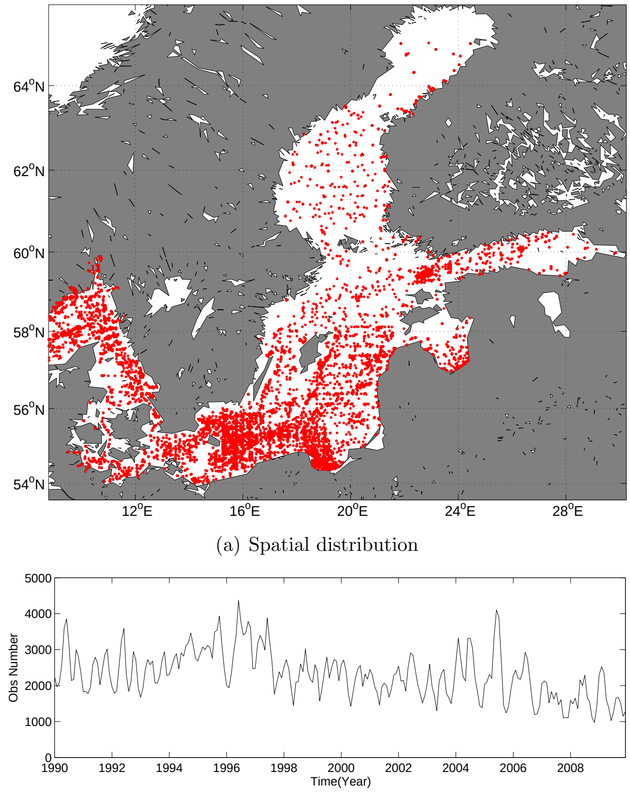
where $\mathbf{U}_{\mathrm{H}}$ and $\mathbf{U}_{\mathrm{V}}$ are the horizontal and vertical part of the control variable transform related to the modes of $\mathbf{B}$, and $\mathbf{U}_{\mathrm{P}}$ is the physical transform related to the multivariate dynamic or physical constraints (e.g., the relationship between sea surface height (SSH) error and temperature/salinity error).

Similar to Dobricic and Pinardi (2008), the horizontal part of the background error covariance ($\mathbf{B}$) is represented by an isotropic recursive filter. The vertical correlation is approximated by an empirical function. In addition, the covariance is represented with dominant EOF modes to reduce computational expense. More details of other parameters used in the recursive filter and empirical function can be found in Zhuang et al. (2011).

2.2 Data preparation for reanalysis

The main dataset to constrain the model forecast is the historical T and S profiles from the International Council for the Exploration of the Sea (ICES). The original data are compiled and quality-controlled before assimilated into the model. To validate the reanalysis, some profiles with relative complete records are withheld. Tide gauge sea level data and satellite sea surface temperature (SST) data are also used to quantify the uncertainty. Measurements from tide gauges near the coast are extracted from both DMI and SMHI databases.

From 1990 to 2009, the ICES basic subsurface temperature and salinity observation datasets consist of approximately 139 315 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 metadata types into its databases from its members. In general, the historical dataset comprises most of the measurements collected from the Baltic Sea region for the past 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 noticeable feature is that the number of observations per year has significantly decreased since 1998.



(a) Spatial distribution

(b) temporal evolution

Fig. 1. The **(a)** spatial locations and **(b)** actual number of records of the T/S profiles assimilated into the model for each month from 1990 to 2009.

Most of the T/S profiles have already gone through a preliminary data quality control prior to the entry into the ICES database. For further application in the data assimilation, we have applied a simple quality control scheme in the 3DVAR in order to remove questionable records and avoid sharp shocks to the model. The innovation vector, i.e., the difference between the background field and the observations, is used as one criterion. We exclude those observations when the innovations exceed triple standard deviations of the variability of analysis. For a long-term experiment, one critical issue is to ensure a stable integration. To avoid large shocks to the initial state, we empirically adjust the errors of observations according to the innovations. By this definition, some observations are 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.

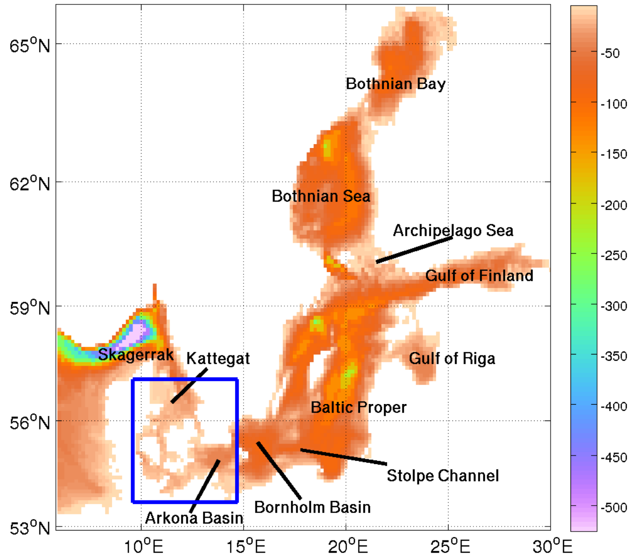


Fig. 2. The HBM model domain with depth contours (in m) used for the reanalysis.

The above treatment is crucial for the multi-decadal assimilation experiment. As shown in Fu et al. (2011) and Zhuang et al. (2011), the initial condition with data assimilation could reduce the RMSE of the subsequent prediction and the impact generally endures for 2–3 weeks. The persistence time scale is larger in the deep bottom layer of the Baltic Sea where the water masses are relatively stationary. Hence, the model state cannot be drastically adjusted during the assimilation, which will form a spurious cold/warm eddy if there is a large misfit between model and observation. The altered initial state due to one "questionable" measurement will cause spikes in the vertical stratification or even instability of the model. This problem can well happen at the beginning of the assimilation experiment because the model differs largely from the observations in the bottom layer. As the model state is gradually rendered close to observations with the continuous insertion of measurement information, the criteria based on innovations will be 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

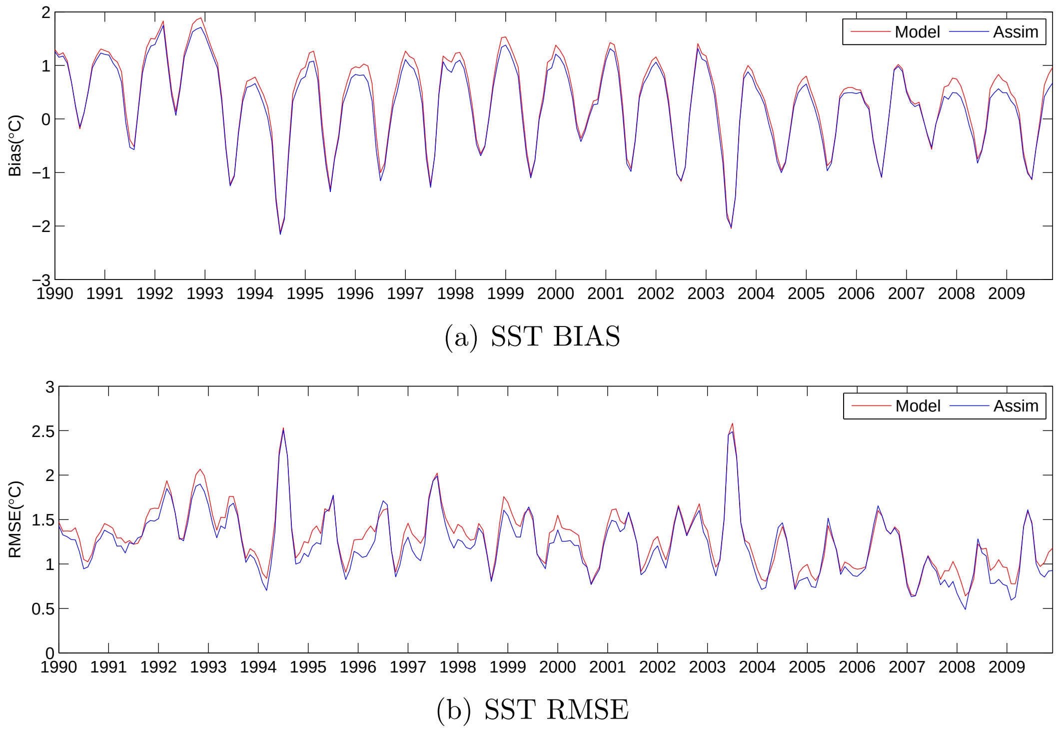
The model used in this study is a two-way nested, free surface, hydrostatic three-dimensional (3-D) circulation model HIROBM-BOOS (HBM). The model code forms the basis of a common Baltic Sea model for providing GMES Marine Core Service since 2009. The finite difference method is adopted for its spatial discretization in which a staggered Arakawa C grid is applied on a horizontally spherical and vertically z-coordinate. 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. In the Danish Water, a domain with 1 nm resolution is two-way nested with the Baltic Sea (Fig. 2). A high resolution model in the Danish water is very important for multi-decadal simulations because it helps to more realistically reproduce the narrow deep transports between the North Sea and Baltic Sea. The 3-D model for the Baltic–North Sea has 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. In the nested domain, the vertical resolution is increased to 52 levels to resolve the complex bathymetry in the shallow inner Danish waters. The top layer is 2 m thick and then with a 1 m or 2 m layer thickness for the rest of 51 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) 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 a 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. (2007).

3.2 Experimental setup

Two experiments spanning 1990–2009 have been carried out in this study. The surface momentum and heat fluxes in the



(a) SST BIAS

(b) SST RMSE

Fig. 3. The evolution of basin-averaged **(a)** bias and **(b)** RMSE calculated against monthly mean satellite SST from 1990 to 2009.

model are calculated by using bulk formulations. The thermodynamics of the ice is built on Semtner's layer model (Semtner, 1976). 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. River fresh water discharge data was averaged daily 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. Though the model domain covers the whole Baltic–North Sea, the results in the North Sea are not the focus of this paper. Compared to the Baltic Sea, the North Sea has different hydrographic features. This renders it difficult to cover all detailed comparisons and discussions of both seas in a single paper.

The experiment without data assimilation is referred to as the free run. A second experiment is carried out with the same forcing but the ICES T/S profile data was assimilated with the 3DVAR scheme described in Sect. 2.1. Assimilation time window is 1 day, i.e., the assimilation is performed daily provided that any observations are available. During the assimilation, observations for one day are combined into the initial state of the model at the end of a day and the updated model state will serve as the new initial state. The number of assimilated observations is shown in Fig. 2. The number ranges from 1000 to 4100 for different months, not necessarily increasing with time. For both experiments, model output is saved hourly to meet the requirements in applications that need high temporal resolution.

4 Results

To present an overview of the quality of the reanalysis, we validate the monthly mean reanalysis against a variety of observations. The misfit between model and observation is assessed with sea level measurements from tide gauge stations, satellite SST and independent in situ 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 is estimated and the results are shown in Fig. 3. For the free run, the model has a RMS error of 1.87 °C. A large part of this error is attributed to a seasonally

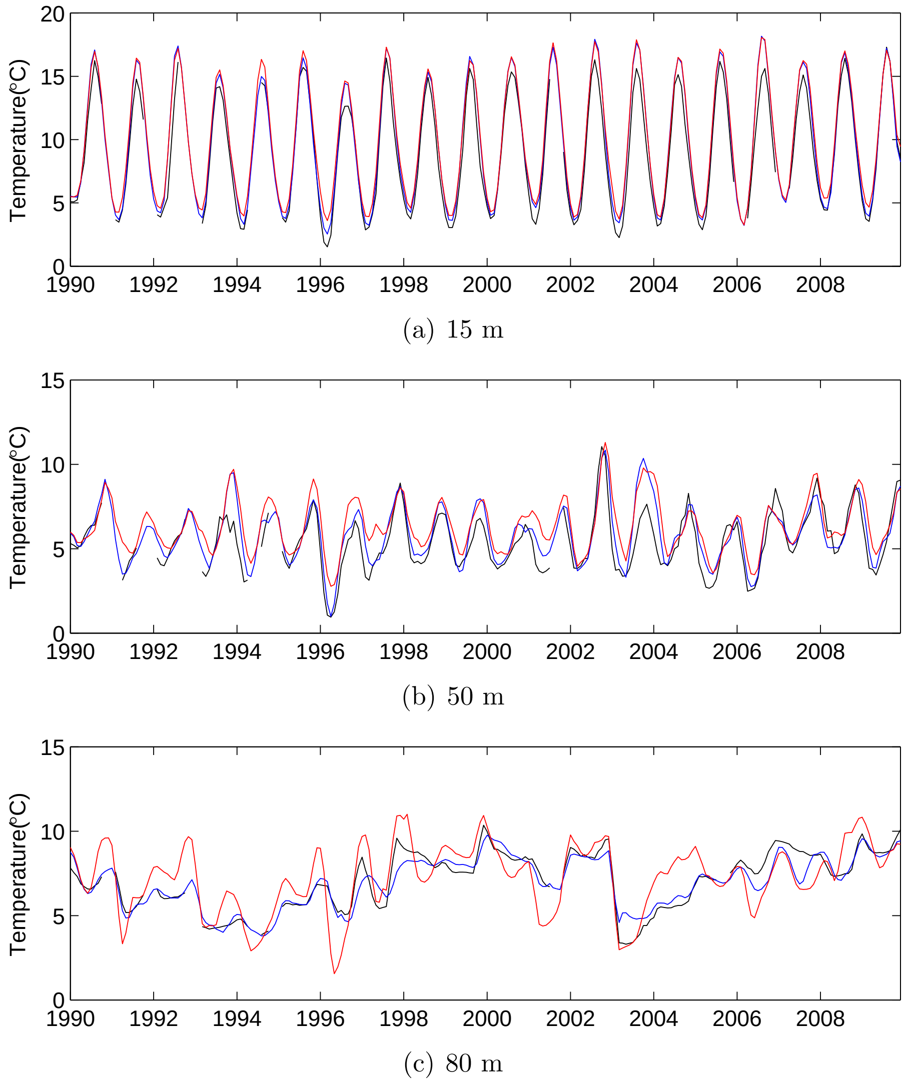


Fig. 4. The time series of temperature at 55.15° N, 15.92° E for the depth of **(a)** 15 m, **(b)** 50 m, and **(c)** 80 m. The red is the free run, the blue is the reanalysis and the black is for observations.

varying bias of 1–1.5 °C, with the peak in the winter and cold bias in the summer. The RMSE is reduced to 1.69 °C after the assimilation, whereas the bias is only reduced by 0.09 °C. From our previous validations (Høyer and She, 2007), the large seasonal bias in the free run can be largely attributed to the errors in the forcing and/or 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.

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 were 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. (2011), 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 year period. By comparison, temperature in the reanalysis is slightly improved by 0.1–0.3 °C in several months. The depth of 50 m can be

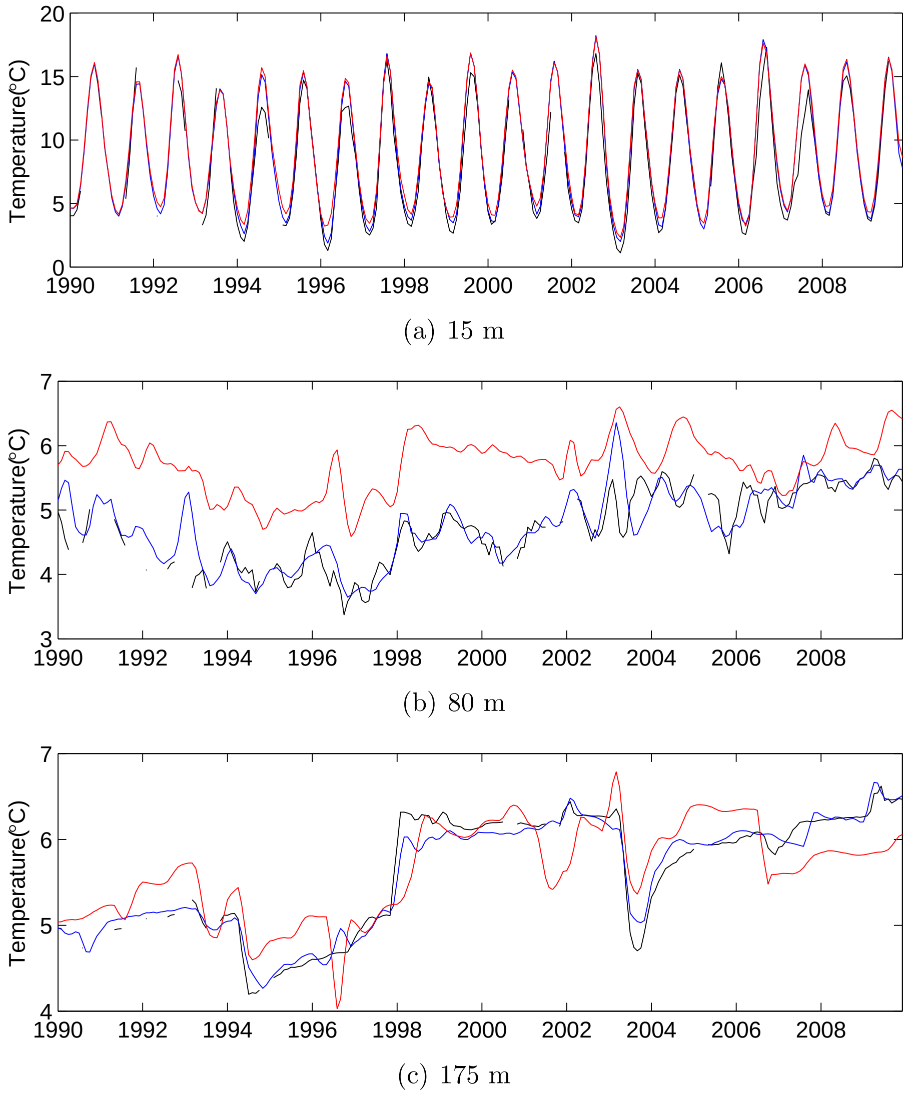
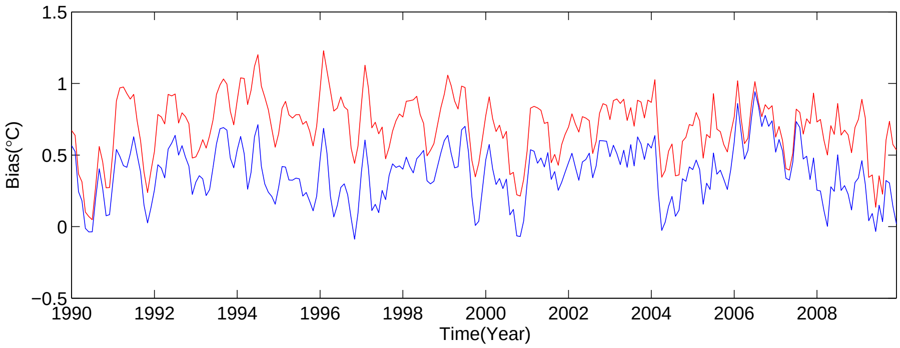


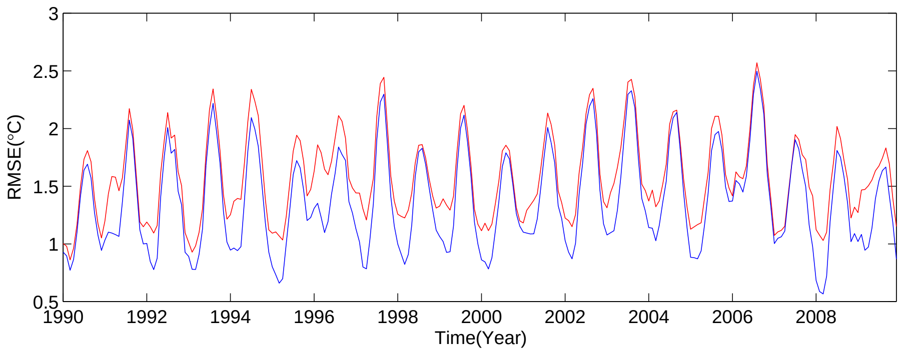
Fig. 5. The time series of temperature at 57.15° N, 19.92° E for the depth of **(a)** 15 m, **(b)** 80 m, and **(c)** 175 m. The red is the free run, the blue is the reanalysis and the black is for observations.

a good representation of primary halocline in the Bornholm basin that 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 temperature at the depth of 80 m may represent the temperature at the bottom layer. It is found that the reanalysis temperature is much closer to the observations than the free run. The misfit substantially drops from 1.20 °C to 0.49 °C while the correlation coefficients increase from 0.72 to 0.91. It suggests that the reanalysis reproduces more realistic variations of the temperature near the bottom layer.

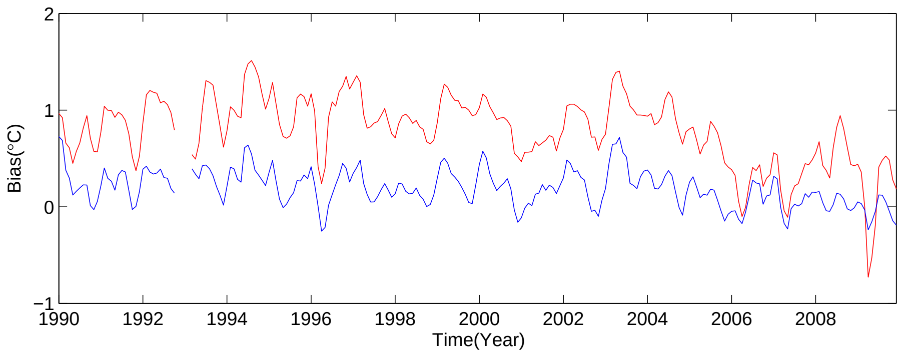
In the central Baltic Proper, the water column is permanently stratified and the halocline lies at about 60–80 m. The two model run show similar error features as in the Bornholm Basin station. The temperature at 57.15° N, 19.92° E is well simulated by the model at the depth of 15 m (Fig. 5a) with a 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 is inadequate to resolve the topography and eddies in this region, the halocline is 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 increased from 0.75 to 0.81. However, there are a few years with exceptions, for instance, in 1994 and 2004. The temperature at the depth of 175 m indicates the conditions



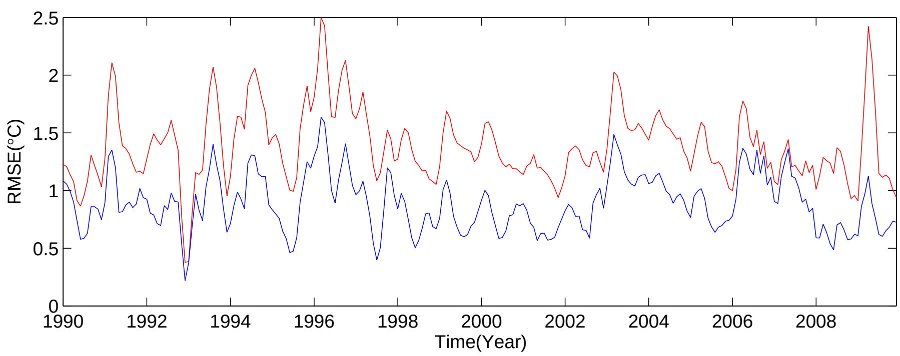
(a) total mean bias



(b) total mean RMSE



(c) bias below 60 m



(d) RMSE below 60 m

Fig. 6. The mean RMSE and bias of temperature caculated with monthly mean data from 1990 to 2009: **(a)** total mean bias, **(b)** total mean RMSE, **(c)** mean bias below 60 m, and **(d)** mean RMSE below 60 m. The red is the free run and the blue is the reanalysis.

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 is 1 °C higher from 1998 onward than the period 1990–1998. Similarly, the reanalysis data fit 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

To facilitate the comparison, the observed profiles are binned into 10 km × 10 km × 1 month bins corresponding to 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 a 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 on all seasons. Notably, the seasonal 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 model subsurface layer so that the cold bias in summer is compensated by the subsurface warm bias. In addition, the bias is smaller in winter than in summer for most years, which is consistent with our previous validations. During summer, a very shallow seasonal thermocline develops in the Baltic Sea when the surface cold water is heated. In the shallow western area, there is a change between stratification and well-mixed conditions. At present, modeling the seasonal thermocline is still a challenging problem even for the high resolution coastal models, which tend to result in big errors of the temperature in summer. In the reanalysis, the mean bias is typically less than the free run. For the whole Baltic Sea, it is reduced to 0.37 °C. In particular, the warm bias is significantly reduced from 0.78 °C to 0.20 °C below 60 m (Fig. 6c). This demonstrates the benefit of data assimilation for systematic errors. It should be noted, the comparison is 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 bias in the summertime, which forms a large portion of the RMSE. By comparison, the RMSE is generally reduced in the reanalysis for the 20 years. For example, the mean RMSE is 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 is markedly reduced from 1.38 °C to about 0.89 °C in the reanalysis (Fig. 6d). Mean bias reflects the time-mean component of the systematic errors due to model deficiencies. Meanwhile, the time-varying components could result from inaccuracies in the time varying boundary forcing. This part is relatively difficult to be remedied with the current assimilation scheme. For example, the total bias for the Baltic Sea is reduced from 0.69 °C to 0.37 °C while the RMSE is still about 1.37 °C in the reanalysis.

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, 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. The model simulation played an important role in the Bornholm Basin because sinking or mixing of the incoming saline water will have a 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 slight decreasing trend from 1990 to 2002. After assimilation, the reanalysis is rendered closer to observations for most of the 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 reproduced 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 poor simulation of the saline water intrusion in this region. As stated above, the intrusion of saline water behaves in three different manners. It poses great challenges for models 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 demonstrated in Fig. 7c. The mean RMSE is largely decreased from 4.33 psu to 1.34 psu. For the major inflow events in 1993 and 2003,

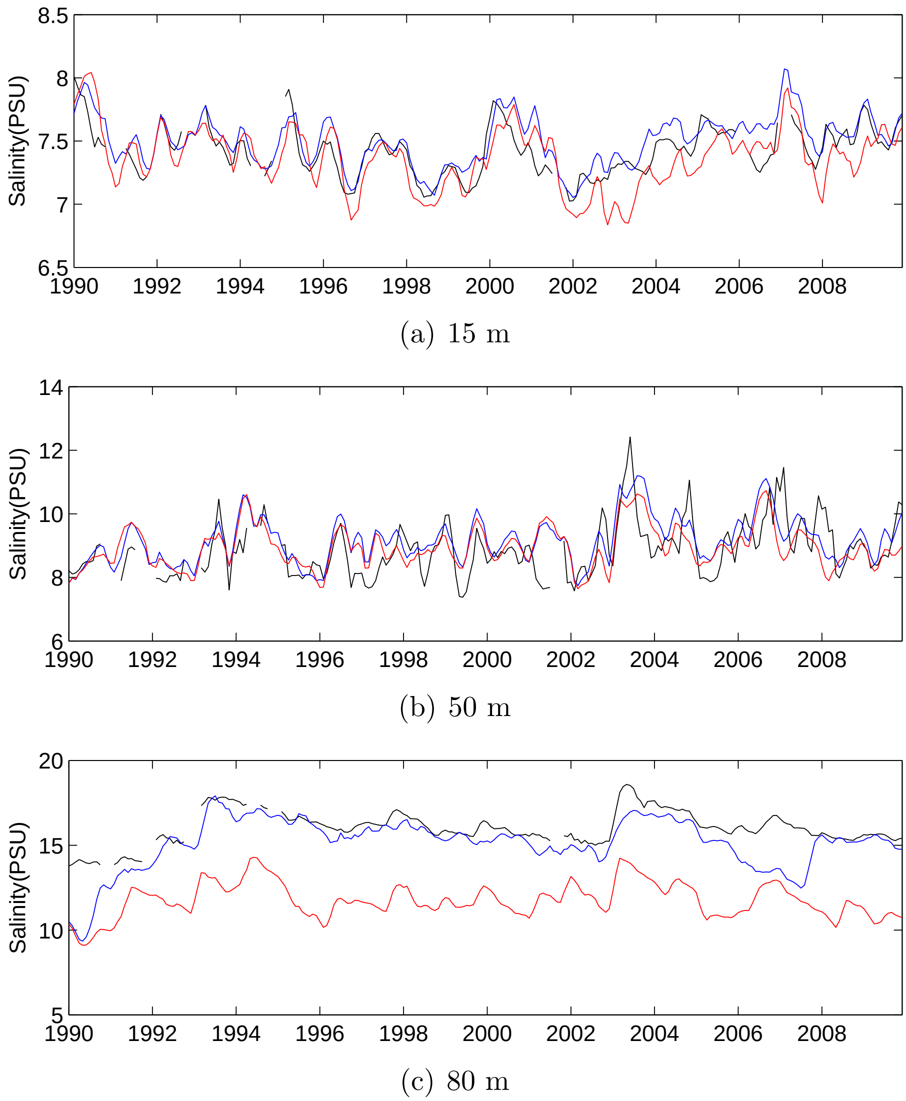
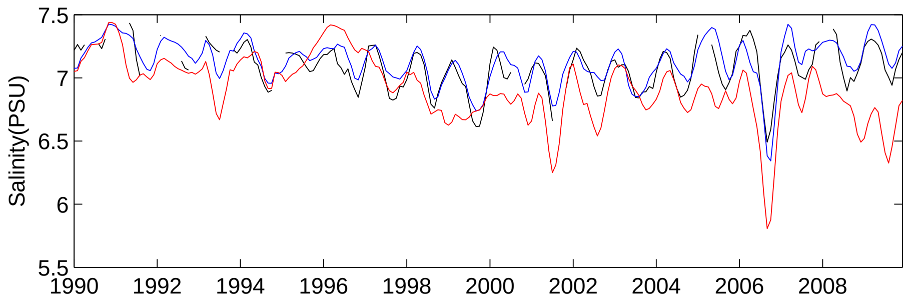


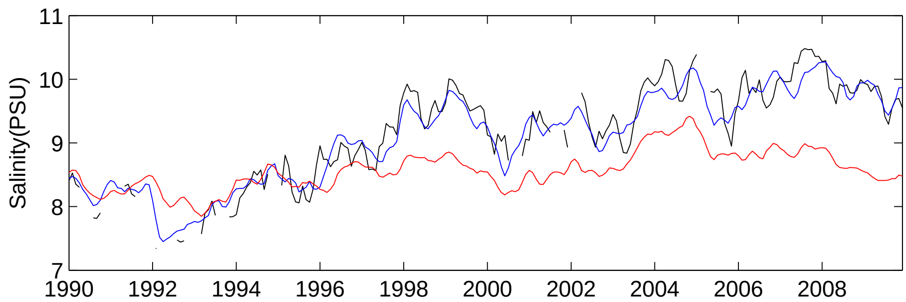
Fig. 7. The time series of salinity at 55.15° N, 15.92° E for the depth of **(a)** 15 m, **(b)** 50 m, and **(c)** 80 m. The red is the free run, the blue is the reanalysis and the black is for observations.

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.

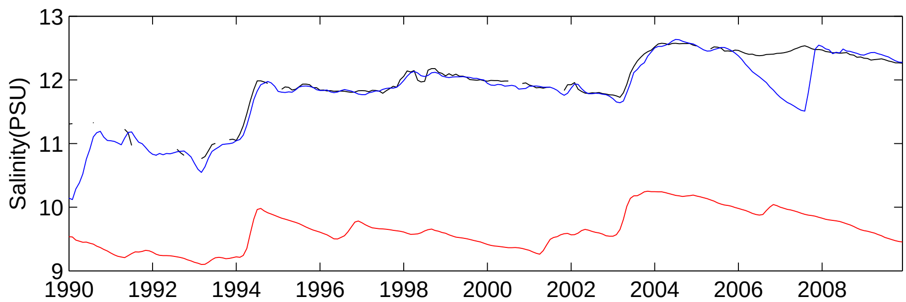
The time series of salinity at Gotland Deep station (57.15° N, 19.92° E) is shown in Fig. 8 for the upper, intermediate and bottom layer. At 15 m depth, salinity of the free run is typically improved by the assimilation (Fig. 8a). The mean RMSE is considerably decreased from 0.31 psu to 0.13 psu while the correlation coefficient is increased from 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 is 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 observations 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 the 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 demonstrated from the salinity at the depth of 175 m (Fig. 8c). The observations show a pronounced increasing trend from 1990 to 2009. The salinity reaches 12.5 psu from 2004 to 2009, indicating strong saline water intrusion. Without the assimilation, bottom saline water in the free run is gradually diluted due to



(a) 15 m



(b) 80 m



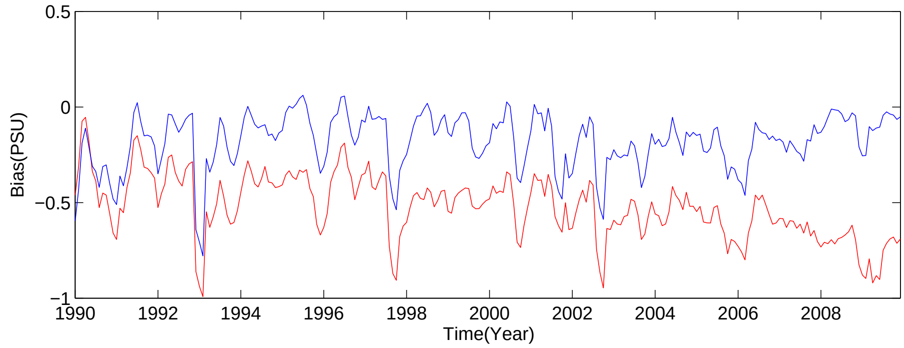
(c) 175 m

Fig. 8. The time series of salinity at 57.15° N, 19.92° E for the depth of **(a)** 15 m, **(b)** 80 m, and **(c)** 175 m. The red is the free run, the blue is reanalysis and the black is for observations.

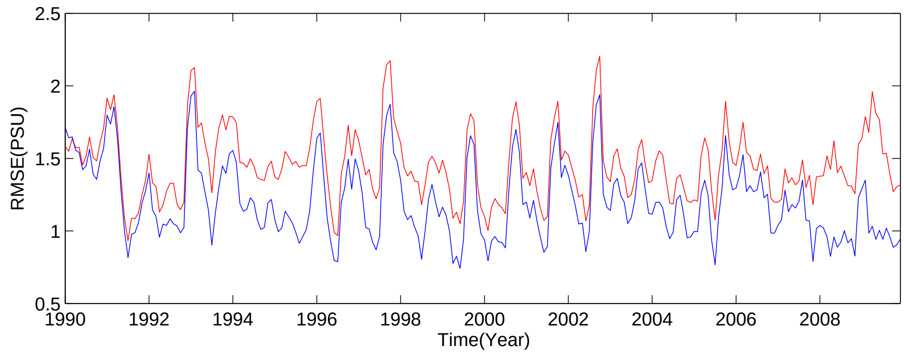
the strong vertical mixing of the model, which also affects the simulation of inflow events. The salinity is about 2 psu lower than the observations. The effect of the assimilation could be sustained for a long time because of the steady water masses in this region. Once the state of the bottom water is changed, it won't be fully replaced until another major inflow intrudes. The reanalysis 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.

4.2.2 Salinity profile verification using all data

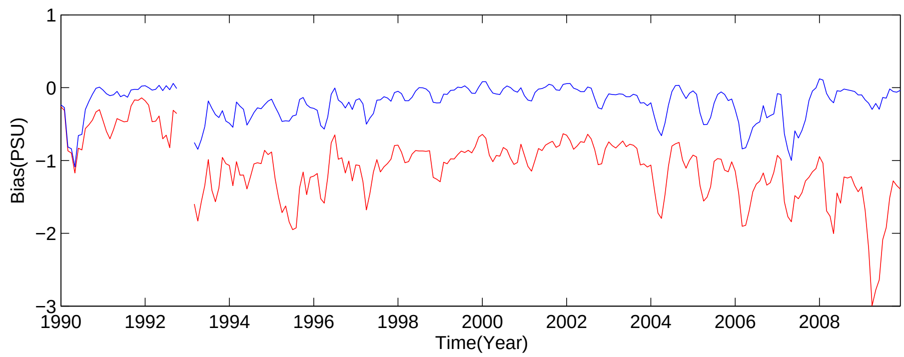
Total RMSE and bias of the salinity is compared between the reanalysis and the free run. The verification process is similar to the temperature in Sect. 4.1.3. In Fig. 9, the modeled salinity is about 0.5 psu lower than the observations in the Baltic Sea. In particular, the bias is more prominent below 60 m (about −1.07 psu) in the central Baltic Sea where salinity is largely influenced by the simulation of inflow from the Bornholm basin to 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 is significantly reduced from −1.07 to −0.21 psu in the central Baltic Sea (Fig. 9c). Similar to the bias, the RMSE is also substantially reduced in the reanalysis. For example,



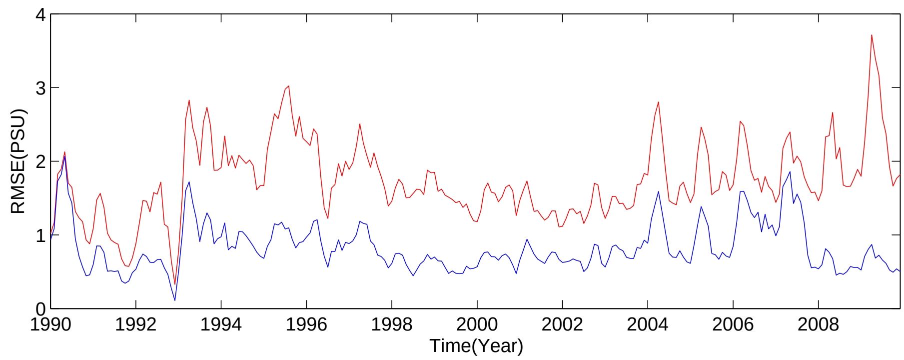
(a) total mean bias



(b) total mean RMSE

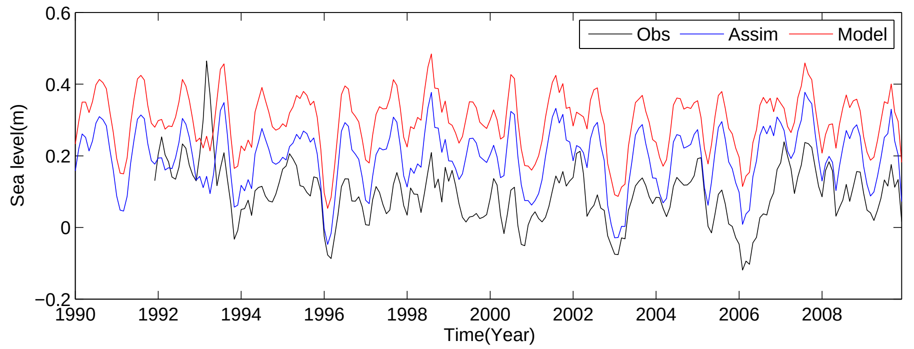


(c) mean bias below 60 m

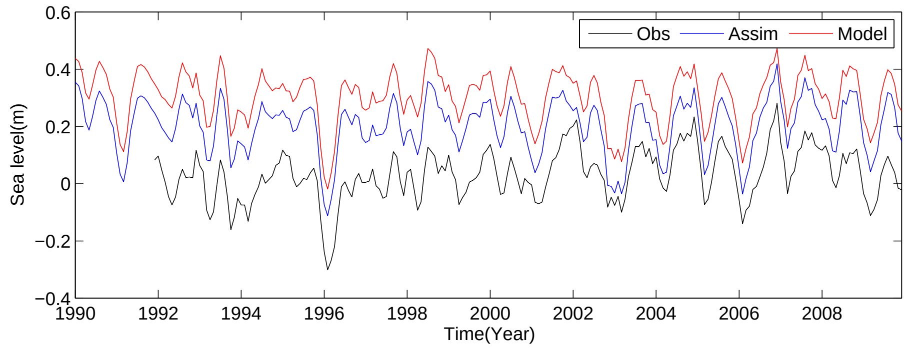


(d) mean RMSE below 60 m

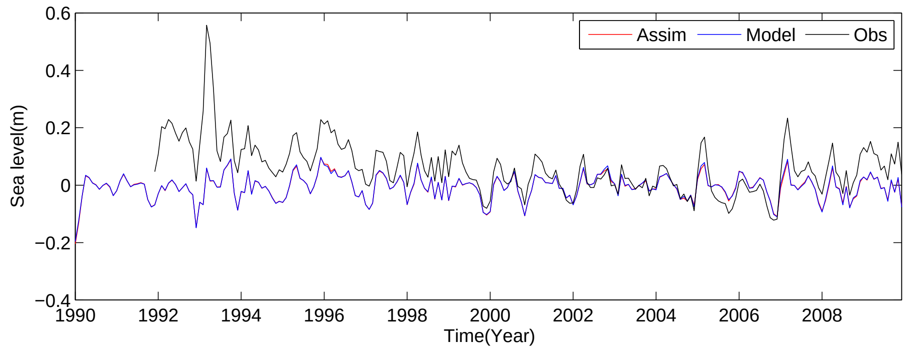
Fig. 9. The mean RMSE and bias of salinity calculated with monthly mean data from 1990 to 2009: **(a)** total mean bias, **(b)** total mean RMSE, **(c)** mean bias below 60 m, and **(d)** mean RMSE below 60 m. The red is the free run and the blue is the reanalysis.



(a) Gadser



(b) Hornbaek



(c) Diff between Gadser and Hornbaek

Fig. 10. The time series of sea level at Gedser (55.15° N, 15.92° E), Hornbæk (55.15° N, 15.92° E), and **(c)** the difference between **(a)** and **(b)**. The red is the free run, the blue is the reanalysis and the black is for observations.

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 is 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 satellite born altimeter data. However, the validation with altimeter data has severe limitations in small semi-enclosed seas like the Baltic Sea due to the limited accuracy near the coast and their low spatial resolution. Comparatively, the observed sea level from tide gauge stations has the advantage in the coastal region. In this study, the sea level from the 20-year reanalysis is compared to independent tide gauge data at 14 stations. RMSE and correlation coefficients are calculated with the data on the monthly basis (Table 1).

Table 1. The correlation coefficients, bias (in m) and RMSD (in m) 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.

	Position (degrees)	Reanalysis			Free run		
		Corr. coeff.	RMSD	Bias	Corr. coeff.	RMSD	Bias
Aarhus	56.15° N, 10.22° E	0.785	0.0668	0.1044	0.7453	0.0692	0.2069
Frederikshavn	57.43° N, 10.57° E	0.827	0.0641	0.1569	0.8033	0.0661	0.2621
Slipshavn	55.28° N, 10.83° E	0.783	0.0605	0.1084	0.7501	0.0611	0.2100
Korsor	55.33° N, 11.13° E	0.7255	0.0691	0.0922	0.7124	0.0667	0.1934
Hornbæk	56.10° N, 12.47° E	0.8776	0.0581	0.1712	0.8588	0.0608	0.2728
Rodby	54.65° N, 11.35° E	0.5268	0.1014	0.0644	0.5367	0.0989	0.1655
Gedser	54.57° N, 11.93° E	0.6794	0.0869	0.1035	0.6766	0.0854	0.2045
Tejn	55.25° N, 14.83° E	0.8775	0.0656	0.2353	0.8756	0.0649	0.3349
Kalix	65.68° N, 23.13° E	0.9153	0.0858	0.3847	0.9159	0.0856	0.4916
Klagshamn	55.52° N, 12.75° E	0.8626	0.0578	0.2231	0.8358	0.0618	0.3241
Kungsholmsfort	56.08° N, 15.54° E	0.9001	0.0609	0.2700	0.8844	0.0644	0.3716
Kungsvik	58.78° N, 11.13° E	0.9008	0.0526	0.1594	0.8848	0.0564	0.2646
Ratan	63.98° N, 20.88° E	0.9496	0.0622	0.3771	0.9480	0.0636	0.4835
Visby	57.63°N, 18.28° E	0.9378	0.0540	0.2970	0.9318	0.0559	0.3971

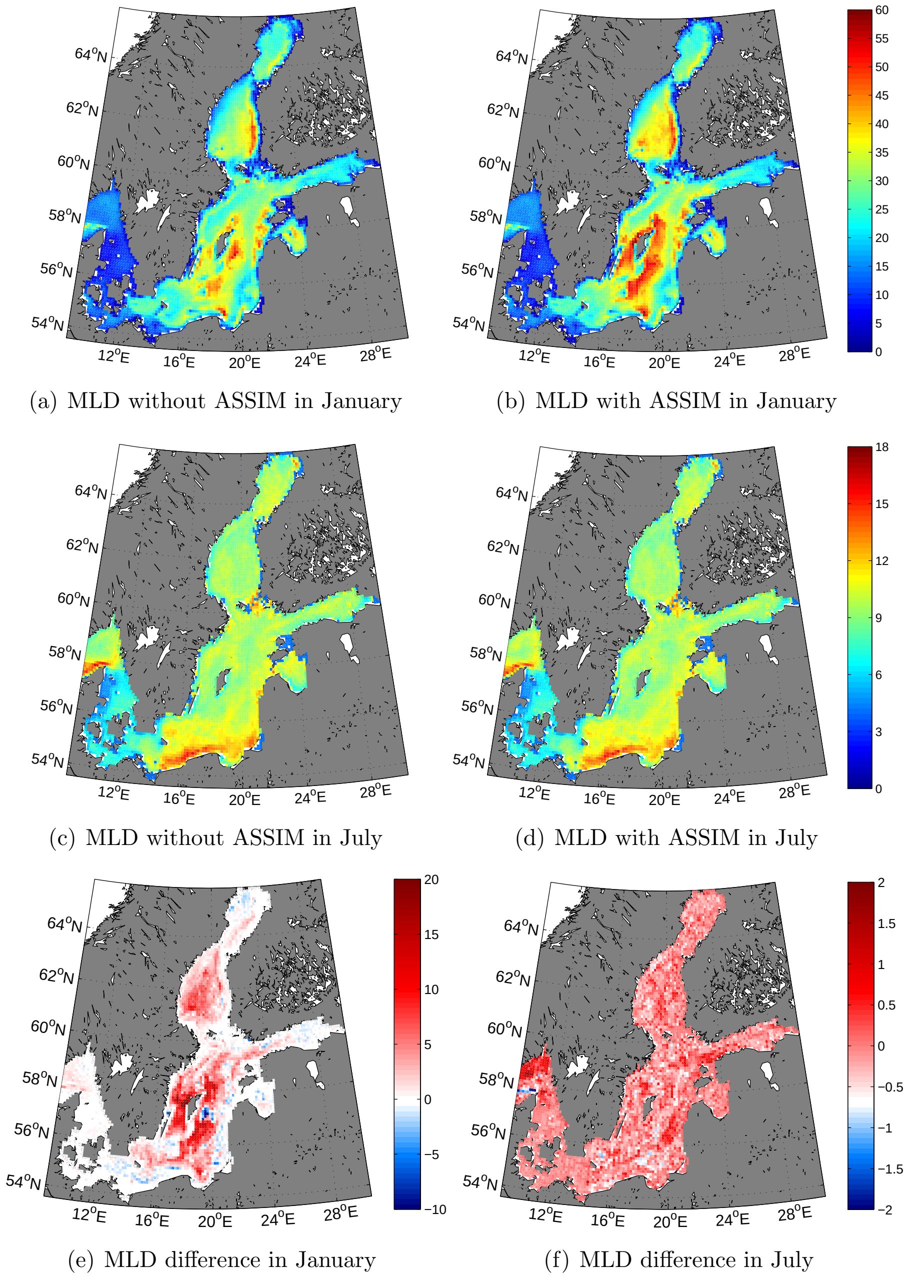
Since no sea level data are assimilated, the comparison is completely independent.

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 by nesting model system (She et al., 2007). Compared with tide gauge, the correlation coefficients at 9 stations are all larger than 0.8. At Rodby and Gedser, the coefficients are 0.52 and 0.67, respectively. These two stations are located near the Darss Sill where the sub-grid scale feature of narrow transport cannot be fully resolved even in a high resolution nested model. In general, it is encouraging that the reanalysis is better correlated with the tide gauge data than the free run by 2–5 %. In addition, the mean bias of sea level is substantially reduced by about 0.1 m for all stations, indicating the impact of T/S assimilation. In fact, assimilation of temperature is equivalent to 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. However, we find that the redistributed density field mainly contributed to reducing the mean bias of the model. In Table 1, the RMSD is also 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. From Table 1, the changes in RMSD are less than 1 cm for most stations. It suggests that the assimilation of sparse T/S profiles behaves 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 inflow in the bottom layer. Time series of sea level at Gedser and Hornbæk are presented in Fig. 10. In the free run, sea level is generally higher than the tide gauge data. Sea level in the reanalysis is decreased after the assimilation and closer to observations. As shown in Table 1, the improvements are 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 that 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 shows very minor changes between the free run and reanalysis. The strong transport in 1993 is not captured in both experiments. The variations in the transport are well produced but the magnitude is underestimated. The assimilation of T/S seems not effective to improve the barotropic transport. This is because the density changes of water masses, which are induced by the T/S assimilation, act primarily on the baroclinic transport through the Danish transition zone.

4.4 Mixed layer depth (MLD)

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 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



(a) MLD without ASSIM in January (b) MLD with ASSIM in January

(c) MLD without ASSIM in July (d) MLD with ASSIM in July

(e) MLD difference in January (f) MLD difference in July

Fig. 11. The climatological mean mixed layer depth (MLD) (unit: m) calculated from the free run and reanalysis for 20-year period.

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 depth are temperature and sigma-t (density) changes 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 depths from both experiments are presented in Fig. 11 for winter (January) and summer (July). In the Baltic Sea, the primary force for driving turbulent mixing in the mixed layer is wind-driven current. Two features could be found: first, the mixed layer depth is typically larger in winter than in summer; second, assimilating T/S profiles deepens the MLD by up to 20 m in winter and about 2 m 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 the thickening of mixed layer. The mixed layer continues to thicken and become thickest in late winter. Therefore, the mean mixed layer depth differs by 20 m between 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).

Why do larger changes occur in the MLD of winter after the assimilation than the summer? If the free run does not produce the adequately accurate MLD in summer, it must be that the controlling effect of meteorological forcing is too strong to alter via the assimilation. Forcing itself is unlikely the main cause as the reanalysis winds are quite accurate. In summer, the mixed layer is strongly linked to the surface Ekman flow. The modeled upper layer thus depends primarily 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 assimilation. Another important reason is the gradually increasing heating effect, 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 several meters near the surface 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 also weak in shallow coastal waters 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 the 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 clear 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 helps to substantiate the results from the reanalysis in Fig. 11f. The most significant differences between the free run and the reanalysis occur in wintertime, which is also consistent with Fig. 11e. In this sense, Fig. 11e indeed shows an improvement on the MLD in the free run after the T/S assimilation. It is noted that even after assimilation, the model MLD in winter is still shallower than observations.

5 Conclusions and discussions

In this paper, a 3DVAR scheme is used to construct a retrospective analysis of temperature, salinity, and sea level in the Baltic Sea from 1990 to 2009. The goal of this reanalysis is two-fold: first, the performance of the 3DVAR scheme can be assessed in a multi-decadal integration and provide more experience for future operational applications; second, the reanalysis can provide a uniformly gridded dataset for studies such as model intercomparisons, physical processes, climate variability and other purposes in the Baltic Sea. The accuracy of the reanalysis is quantified by direct comparisons against independent sea level, temperature and salinity measurements. Particular attention is focused on the effect of assimilation on reducing the bias and RMSE of model forecast.

We begin with a comparison with time series of temperature and salinity that has 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 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 markedly improved in the reanalysis. Major inflow events such as in 1993 and 2003 are captured more accurately in the reanalysis and 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 by 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 the mean RMSE and bias of salinity reduced by 0.86 psu and 0.91 psu.

The reanalysis is further validated against sea level data at 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 found to stem mainly from the reduction of mean bias, which is about 10 cm smaller than in the free run. After the mean is subtracted from the time series of sea level, the root mean square difference (RMSD) is also shown to be slightly reduced (within 1 cm). It suggests that the assimilation of T/S profiles contributes mainly to reducing the time-mean component of systematic errors of the model. The reduction of the mean bias contributes little to improve the barotropic transport, which is maintained by the water level difference between the northern Kattegat and the Arkona Sea. Differences of sea level between Gedser and Hornbæk are used as a barotropic transport index. It appears that the assimilation acts to raise the whole water column in the Danish waters other than adjust the difference of sea level. Assimilation of T/S profiles plays a more important role in deep waters because changes in density field would redistribute the water mass and adjust the baroclinic transport.

The mean mixed layer depth is compared between the reanalysis and free run for the 20 year period. In the Baltic Sea,

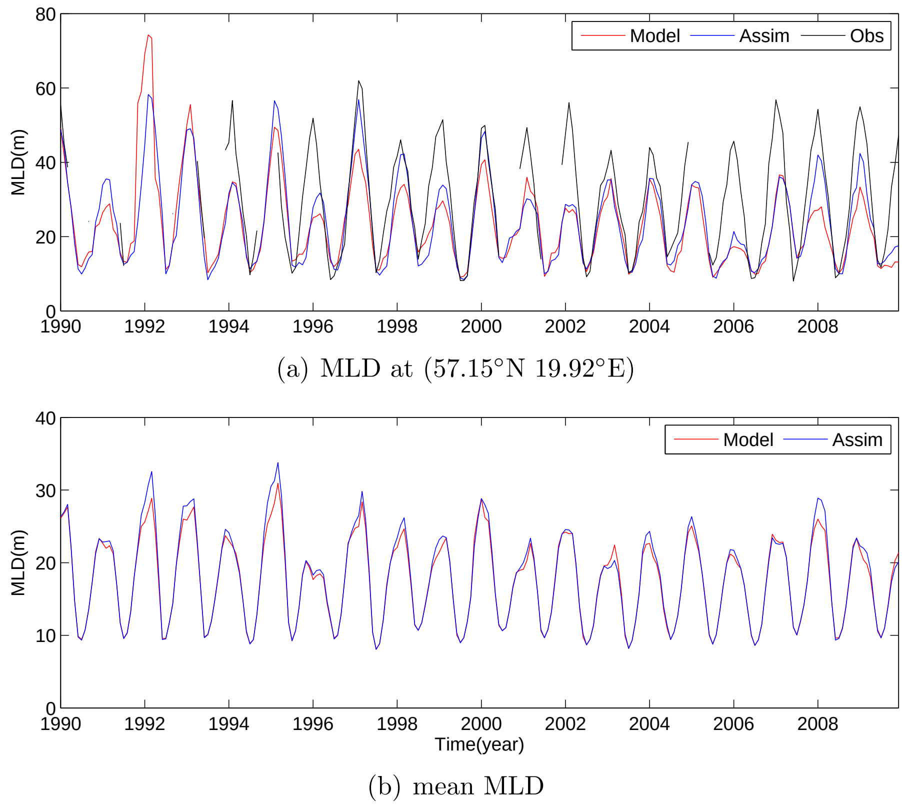


Fig. 12. The evolution of mixed layer depth (MLD) calculated from the free run and reanalysis.

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 larger in winter than in summer, differing by 20 m on average. In addition, changes in the mixed layer depth due to the assimilation appear to be minor in summertime and shallow waters. The effect of heating in summer and dominant surface forcing could be related to the relatively small effect of the assimilation. In deep waters, however, the effect of the assimilation is significant in wintertime. 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 and the assimilation helps to ameliorate some model deficiencies such as the simulation of saline water intrusion into the Baltic Proper. The reanalysis can be regarded as good surrogate data for process studies in the Baltic Sea. Furthermore, the long-term reanalysis helps to identify problems in the 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 in the 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 model. Second, significant improvement is found in the intermediate and deep layers. This is related to the longer time scale in these layers. Spatially varying 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 underestimated in winter. The underestimation in the Gotland Deep station is still about 10–40 m. Fouth, assimilation of the T/S profiles improves markedly mean sea level by 10 cm but not the variability of the sea level. Finally, the results might be less reliable in the regions with seasonal ice cover such as the Gulf of Finland and Gulf of Bothnia because only the thermodynamics of ice is included in the model. This will be improved by implementing a new ice model into the HBM. Furthermore, satellite data play a complementary role to the subsurface in situ observations and will be assimilated into the model in the future.

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