

Study of the multi-decadal evolution of the Black Sea hydrodynamics and biogeochemistry using mathematical modelling

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Front cover illustration : Pierre Alechinsky, The Black Sea, 1988-1990

Summary

This thesis addresses the biogeochemical cycles in the Black Sea (BS) during the shifting environmental context that affected the BS during the last decades of the 20th century. The study is based on sophisticated data analysis tools and on the development and implementation of a coupled 3D biogeochemical model on the BS domain.

The long term variability of the BS hydrodynamical structure was first examined on the basis of in-situ profiles (1950-2012), satellite imagery (1985-2000) and 3D modelling (1960-2000). Profiles of temperature and salinity were used to derive vertical characteristics of the BS structure: the mixed layer depth and the cold content of the Cold Intermediate Layer.

To untangle the spatial and temporal trends from this heterogeneous dataset, a general methodology was proposed and embedded in the data analysis software DIVA. The detrended climatologies and long-term time series provided by this approach were used to assess statistical relationships with local atmospheric conditions.

Satellite data (sea surface temperature and altimetry) and model results were then analyzed to relate observable surface dynamics to internal hydrodynamic properties. The main multivariate modes of variability of the BS hydrodynamic structure were highlighted on the basis of Empirical Orthogonal Function analysis. Their temporal evolution was explained by the occurrences of specific atmospheric patterns, identified on the basis of neural algorithm analysis and related to the phases of well known teleconnection systems (i.e. the North Atlantic and East Asia/West Russia oscillations).

To study the dynamics of eutrophication in the shallow Black Sea NorthWestern Shelf (BS-NWS), a benthic model component was developed that considers the environmental control on diagenetic processes and the bottom shear stress restriction on organic matter deposition. The model accurately reproduced the seasonal and spatial variability depicted by in-situ estimates of benthic nutrients and oxygen fluxes in the BS-NWS.

Outputs were used to review the role of the benthic component in BS biogeochemical cycles. The multi-decadal simulations, enabled by the low computational requirements of the benthic-pelagic coupling approach, revealed an inertial component in the dynamics of eutrophication resulting from the accumulation of organic matter during the years of important nutrient loads. This refined resolution of the BS-NWS biogeochemistry allowed us to study the phenomenon of seasonal hypoxia, which is believed to have played a part in the sudden collapse of the fisheries stocks in the late 80s.

An index H , combining the spatial and temporal extension of the seasonal hypoxic event, was proposed to quantify the annual intensity of hypoxia as a pressure on benthic communities. We have shown that hypoxia was first triggered in the late 70s by high nitrogen loads, and sustained by sedimentary organic matter accumulation after a rapid reduction of these loads in the 90s. After 2000, warmer summers again led to a increase of the H -index, by entraining hypoxic events of smaller spatial extension but increased duration. A practical relationship distinguishing the impacts of eutrophication and climatic drivers was proposed to assess the effect of their projected values on the future intensity of hypoxia.

Résumé

Cette étude concerne les cycles biogéochimiques en Mer Noire dans le contexte de transition environnementale qui a affecté la Mer Noire au cours des dernières décennies. L'étude se base sur l'analyse statistique et sur le développement et la mise en œuvre d'un modèle biogéochimique couplé. La variabilité à long terme de la structure hydrodynamique est d'abord examinée sur base de profils *in situ* (1950-2012), d'imagerie satellitaire (1985-2000) et de modélisation 3D (1960-2000).

Des propriétés verticales de la Mer Noire sont calculées à partir de profils de température et de salinité: la profondeur de la couche de mélange et la teneur en froid de la couche intermédiaire froide. Afin de distinguer les tendances spatiales et temporelles à partir de cet ensemble de données hétérogène, une méthodologie générale intégrée dans le logiciel DIVA est proposée. Les climatologies spatiales, corrigées du biais issu de la distribution temporelle des données, et les séries temporelles à long terme fournies par cette approche sont utilisés pour évaluer les relations statistiques entre ces grandeurs et les conditions atmosphériques locales. Les données satellitaires (température de surface et altimétrie) sont ensuite analysées conjointement aux résultats du modèle afin de lier les observations de surface aux propriétés hydrodynamiques internes. Les principaux modes de variabilité de la structure hydrodynamique sont mis en évidence sous forme de fonctions orthogonales empiriques. Leur évolution temporelle est alors expliquée par l'occurrence de schémas atmosphériques particuliers, identifiés par un algorithme neuronal. L'occurrence de ces anomalies atmosphériques récurrentes est liée aux phases des systèmes de téléconnection bien documentées (l'oscillation Atlantique Nord et l'oscillation Est-Asie/Ouest-Russie).

Pour étudier la dynamique de l'eutrophisation sur le plateau nord-ouest de la Mer Noire, un module benthique a été développé qui prend en considération la variabilité des processus diagénétiques et l'érosion des sédiments sous l'action des vagues et des courants. Le modèle reproduit fidèlement les variabilités saisonnière et spatiale des estimations *in situ* des flux de nutriments et d'oxygène à l'interface eau/sédiments. Les sorties du modèle sont utilisées pour réévaluer le rôle du domaine benthique dans les cycles biogéochimiques en Mer Noire. Les simulations multi-décennales, rendues possible par le faible coût en calcul du module de couplage benthique-pélagique, révèlent une composante inertielle dans la dynamique de l'eutrophisation, résultant de l'accumulation de matière organique au cours des années d'importantes décharges de nutriments.

Ce raffinement de la biogéochimie sur le plateau nord ouest de la Mer Noire nous permet d'étudier le phénomène d'hypoxie saisonnière, affectant cette région depuis la fin des années 70. Un indice H, combinant l'extension spatiale et temporelle de l'évènement hypoxique, est proposé pour quantifier l'intensité annuelle de l'hypoxie en tant que pression sur les communautés benthiques. Nous montrons que l'hypoxie fut initiée à la fin des années 70 par des décharges élevées d'azote, et soutenue dans les années 90 par l'accumulation de matière organique sédimentaire après une réduction rapide de l'apport en nutriment. Au delà de l'année 2000, des étés plus chauds ont conduit à une nouvelle augmentation de l'index H, entraînant des événements hypoxiques de moindre extension spatiale, mais de plus longue durée. Une relation pratique distinguant les effets de l'eutrophisation et des facteurs climatiques sur l'hypoxie est proposée afin d'évaluer l'effet de leurs évolutions estimées sur l'intensité de l'hypoxie pour les années à venir.

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Chapter 1

Introduction



The Sea at Odessa, Constantin Flondor, 2002

This chapter introduces the general objectives and philosophy of this thesis. It presents the Black Sea environment and the context of the strong alterations that affected this ecosystem during the last decades. The final section details the structure of the thesis.

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1 Foreword

Covering 71% of the globe, the world ocean is a main component of the Earth System and plays a major role in the regulation of climate and in the biogeochemical cycling of the basic elements of life. Oceans have nurtured the first emerging life forms and it is from the oceans that photosynthetic agents have oxygenated the atmosphere, enhancing the growth of life on the land surfaces. The marine environment also accompanied the development of the human society since its first steps, providing first food and transportation means and more recently awe-inspiring and recreational landscapes.

Currently, oceans accounts for 60% of the total economic value of the biosphere ([Costanza et al., 1997](#)), among which 60% is attributed to coastal and shelf systems ([Costanza, 1999](#)). Coastal environments, including estuaries, coastal wetlands, beds of sea grasses and algae, coral reefs and continental shelves only cover 6.3% of the world surface, but concentrate

such a density of biogeochemical transformations and complex ecosystems that they account in total for 43% of the estimated value of the world's ecosystem services. At the interface between the terrestrial and the oceanic domains, the coastal zone receives disproportionately high carbon and nutrients loads, and is estimated to host 52% of global organic matter mineralization ([Thrush and Dayton, 2002](#))

The ecological functions of coastal ecosystems and their delivery of goods and services benefiting mankind are performed in major part by their biotic components. Complex life forms have emerged thanks to the relative stability of marine environments maintained by complex equilibriums of physical, chemical and biological factors.

The fast development of human society and the traditional perception of the oceans as a boundless and open-access reserve of resources led to the emergence of pressures on every component of these equilibriums (e.g. climate change, eutrophication, overfishing). Nowadays, the limits of marine ecosystems become apparent and these environmental pressures threaten their stability and their ability to deliver goods and services to mankind and to ensure their basic ecological functions.

Coastal areas are particularly vulnerable regions because they concentrate more than half of the world population, are directly influenced by human activities and are subject to heavy pollution and over-exploitation of natural resources. Therefore, numerous research projects at global and European level concern the coastal environment (IGBP (International Geosphere-Biosphere Program), IOC (Intergovernmental Oceanographic Commission), IOCCP (International Ocean Carbon Coordination Project), IMBER (Integrated Marine Biogeochemistry and Ecosystem Research Project, ELOISE (European Land Ocean interaction Studies) and LOICZ (Land–Ocean Interactions in the coastal Zone)).

Due to logistic restrictions, the scientific study of the marine environment emerged after that of the terrestrial domains. In recent time however, impressive technological developments have produced an abundance of information on the oceanic systems. Quasi-synoptic pictures of the ocean surfaces are provided by satellites, allowing precise estimates of surface temperature and elevation, pigmented materials (including photosynthetic planktons) and, in a near future, salinity. Subsurface oceanic data, first probed through costly oceanographic cruises, can now be obtained by autonomous devices (e.g. gliders, ARGO floats) providing quasi-synchronic tridimensional pictures of the sea. While the latter mainly concerns the physical aspects, more and more optical and chemical sensors are added to these devices to provide informations on the biogeochemical aspects.

This increasing capacity to “picture the sea” reveals the important variability of the physical and biogeochemical variables used to describe the oceans, both in time and in space and across a large range of scales. Far from erratic, this variability reflects the existence of processes covering a wide range of spatial and temporal scales that control the temporal evolution of these variables ([Steele, 1985](#)). This heterogeneity is enhanced in coastal systems because the land domain imposes a physical boundary to the marine domain, and its influence generates strong gradients (for instance through river discharges or contrasting meteorological conditions).

The marine realm is thus ruled by physical, chemical and biological processes, interconnected and influencing one another across a wide range of scales ([Mann and Lazier,](#)

2006). The integration of these various driving forces in a comprehensive understanding of the marine systems dynamics inevitably requires to resort to mathematical modelling.

Models consist in idealized conceptual representations of real dynamics. Their relevance to address specific scientific questions must first be addressed in the design of the models, i.e. they should resolve the scales of the main interactions relevant to the issue of concern and then their ability to reproduce realistic dynamics has to be proved by an established validation procedure.

While dimensionally reduced models (box-models, 1D or 2D models) have been developed first because they require less computational resources, it clearly appears now that explaining and resolving the high variability depicted by the observation of marine ecosystems requires time dependent 3D models describing the transport and dispersion of biogeochemically active materials and their numerous interactions.

Once validated, models can be used to complement the fragmentary picture of marine systems provided by observation platforms and to decipher the underlying internal dynamics. Also, foreseen environmental challenges (e.g. climate change, global population growth) assign to the marine modelling community the responsibility of providing predictive models with established skills in order, precisely, to estimate to what extent the functional role of marine ecosystems is endangered by these growing environmental pressures.

While mathematical formulations appear adequate when describing well established physical processes driving fluid hydrodynamics, the use of such formulations for describing chemical and biologically mediated processes is less straightforward. Despite intense development in the recent decades, biogeochemical modelling still requires dedicated efforts. Some issues need further attention to refine the integration of processes occurring at the boundaries of the marine domain : air-sea exchanges, coastal interactions and processes at the water-sediments interface. Also, model-data integration should be extended beyond wide averages of bulk properties to optimize the exploitation of the wealth of information provided by observing platforms (Doney, 1999; Arhonditsis and Brett, 2004).

Because of its simple morphology and of the dramatic environmental shifts of the last decades, the Black Sea constitutes an ideal case study to develop biogeochemical models and to assess the adequacy of specific mathematical formulations for biogeochemical processes and to develop methodologies to infer from the results of 3D models practical knowledge supporting a sound management of coastal ecosystems.

2 The Black Sea

At the meeting point between European and Asian continents the Black Sea is a bridge between different cultures and therefore presents a high historical interest (King, 2005) and critical socio-economic stakes. The Black Sea is also the largest anoxic basin in the world and constitutes, as such, a unique marine environment.

The only connection between the Black Sea and the global ocean operates through the Turkish strait system (Bosphorus, Sea of Marmara and Dardanelles), the Mediterranean

and, finally, the strait of Gibraltar. The Bosphorus strait is approximately 31 km long, 0.7-3.5 km wide and about 39-100 m deep, so the Black Sea can be considered as a quasi-enclosed basin. The Kerch Strait in the northern Black Sea connects it to the Sea of Azov. In addition to this horizontal confinement, large riverine inputs maintain a strong vertical stratification which prevents exchanges between the active surface layer ($\sim 0-180$ m) and deep stagnant waters ($\sim 180-2000$ m). As a consequence anoxia, i.e. the absence of oxygen, is permanent in the deep layers of the Black Sea. These high riverine inputs characterize the Black Sea as an estuarine basin, similar for instance to the Baltic Sea. Due to these geomorphologic and hydrodynamic traits, the active part of the Black Sea, i.e. the surface oxygenated layer where most of the biogeochemical dynamics occur and which sustains most of the marine goods and services, represents only 13% of its total volume. The restricted volume of the active part of the Black Sea causes rapid and basin-wide responses to external stressors, and therefore sets a high sensitivity of the Black Sea ecosystem to external pressures.

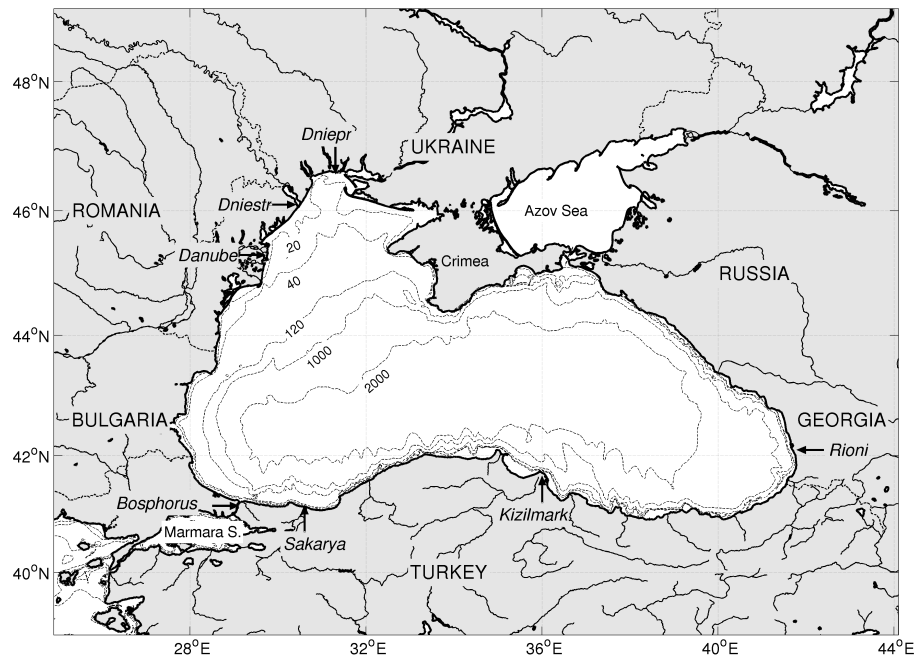


Figure 1.1: Map of the Black Sea domain : Main river entrances, bordering countries and bathymetry.

2.1 Morphology of the Black Sea basin

The Black Sea has a total volume of $5.3 \cdot 10^5$ km³, a total area of $4.2 \cdot 10^5$ km² and extends between the longitudes 28°E and 42°E and the latitudes 41°N and 47°N.

The orography around the Black Sea domain accounts for the presence of mountains in surrounding land areas: Balkans on its West side, high Caucasus ridges in the east and

Pontean mountainsides in the southern coast (Turkey). Flat lands are only found on its northern coast.

The drainage area of the Black sea, i.e. the land surface from which riverine flows to the Black Sea, is 5.21 times larger than the sea surface (Ludwig et al., 2009) and extends over almost a third of Europe and Anatolia. This is very high in comparison, for instance, with other parts of the Mediterranean Sea where this ratio typically spans from 0.4 to 2 (Ludwig et al., 2009). The resulting high riverine discharge, relatively to the the Black Sea volume, is a main characteristic of the Black Sea. This influences both its hydrodynamical structure, through freshwater inputs, and its biogeochemical structure through nutrients and sediment loads.

The bathymetry of the Black Sea (Fig. 1.1) depicts two contrasting subregions. The large and shallow northwestern shelf (NWS) covers approximatively a fifth of the Black Sea domain. It spans between Bulgaria, Romania and Ukraine and is bounded by a sudden increase in the sea bed slope after 120 m depths. The central “open basin” is bordered by Turkey, Georgia, Russia and Ukraine, and reaches a maximum depth of 2245 m. The Azov Sea is especially shallow, with a maximum depth of 14 m.

The shelf break is very sharp along the Anatolian and Russian coast and is only softened west of the Crimean peninsula and in front of the Kerch Strait. The continental shelf extends on more than 190 km in the NWS area and on less than 20 km around the southern and eastern coast of the open basin.

2.2 Atmospheric conditions

The Black Sea region is located at the edge of sub-tropical latitudes and temperate climatic zones and is influenced by the Azores and Siberia centers of high pressures and by the atmospheric patterns over Europe and Asia (Staneva and Stanev, 1998). Their relative influences combine differently over seasons and years and are influenced by the orography. That leads to abrupt and significant changes of the weather conditions (Cherneva et al., 2008).

Air temperature depicts important spatial variations, particularly during winter when the horizontal gradients are about twice their value in summer. The penetration of cold air masses from the north, facilitated by flat lands, may trigger negative temperature in winter and it is not uncommon to encounter ice in the northern coastal waters during the cold season. In some exceptional years, ice chunks issued from central Europe and carried by the Danube river have even reached the Bosphorus.

Winds are generally cyclonic. Northern and northeastern winds prevail in the NWS and come with the cold air masses. Western winds are more common along the Caucasian coast, their occurrence mostly depending on the activity of the Azores anticyclone (Staneva and Stanev, 1998; Cherneva et al., 2008). The cyclonic wind circulation generally intensifies in winter (Korotaev et al., 2003).

The importance of orography in constraining local atmospheric conditions highlights the importance of local and fine resolution atmospheric models to provide reliable forcings for modelling purposes. A clear influence of orography exerts for instance on the spatial

distribution of precipitations (Staneva and Stanev, 1998).

Teleconnection patterns are often invoked to account for the interannual variability of weather conditions (e.g. Krichak et al., 2002; Oguz et al., 2006; Kazmin and Zatsepin, 2007). They refer to large-scale (hemisphere) coherent modes of variation in the distribution of atmospheric masses. These teleconnection patterns have been increasingly used in the scientific literature since they have potentials to explain large scale correlations in the variations of weather conditions, oceanic conditions and consequent ecosystem changes (Hurrell and Deser, 2010).

The north Atlantic Oscillation (NAO) has been found to have a strong impact on the Mediterranean weather (e.g. Hurrell and Deser, 2010) and on the Black Sea hydrodynamics (e.g. Stanev and Peneva, 2002; Ginzburg et al., 2004; Oguz et al., 2006). The east Atlantic/west Russia (EA/WR) pattern (alternatively called the North-Sea/Caspian pattern (Kutiel and Benaroch, 2002)) has been found to be better associated to the Black Sea sea surface temperature (SST) during some years (Oguz et al., 2006), due to its impact on the meridional wind component over the Black Sea region. The El Niño southern Oscillation (ENSO) was found to promote in the Black Sea the occurrence of extreme (i.e. minima and maxima) SST values (Ginzburg et al., 2004).

2.3 Circulation

The circulation system has been explored on the basis of hydrographic surveys (e.g. Oguz et al., 1993; Oguz and Besiktepe, 1999), altimeter satellite data (e.g. Korotaev et al., 2003), model studies (Stanev, 1990; Stanev and Beckers, 1999; Staneva et al., 2001; Beckers et al., 2002; Korotaev et al., 2006) and autonomous observing platforms (Poulain et al., 2005; Korotaev et al., 2006).

The Black Sea circulation is dominated by a basin-wide cyclonic current (Fig. 1.2), referred to as the Rim current, which flows along the abrupt continental slope and is driven by a dominance of cyclonic surface winds and coastal freshwater inputs (Stanev, 1990; Oguz et al., 1996). Rim current speed can reach 0.5–1 m/s in the surface layer (Oguz and Besiktepe, 1999; Poulain et al., 2005) and about 0.1–0.2 m/s in deeper layers (150–300 m) (Oguz and Besiktepe, 1999). Drifter experiments have seen some drifters complete the entire basin loop within 90–180 days (Poulain et al., 2005). Because of the enhanced vorticity and intensity of winds during winter, the Rim current is intensified in winter and attenuated in summer, with a clear maximum value in March (Poulain et al., 2005). During autumn, it may break down in small scale cyclonic gyres (Stanev and Staneva, 2000; Staneva et al., 2001; Korotaev et al., 2003).

The rim current is subdivided in its interior into two main gyres (Western and Eastern gyres), involving a series of cyclonic eddies interacting with each other and with the meanders and filaments issued from the Rim current.

A narrow band separates the Rim current from the coast which is characterized by a series of anti-cyclonic eddies, in particular along the Anatolian coast. Lateral exchanges between the coastal and central region of the basin are mediated by this mesoscale activity forming on the outer boundary of the Rim current (Staneva et al., 2001; Korotaev et al.,

2003; Zatsepin et al., 2003). Given that the Rossby radius which provides a typical length scale for eddies is on the order of 20-30 km in the Black Sea, such processes can easily provide the means for meridional transport across the basin (Oguz et al., 2004). Because this meso-scale activity is related to the intensity of the Rim current, the strong influence of winds patterns on the intensity of the Rim current (Oguz and Besiktepe, 1999), at seasonal and interannual scale, establishes a control of climatic stressors on the lateral exchanges between the coastal and central region of the Black Sea.

Seasonal quasi-permanent anticyclonic eddies of larger extent also forms on the periphery of the Rim current, mostly in summer (the Bosphorus, Sakarya, Sinop, Kizilirmak, Batumi, Sukhumi, Caucasus, Kerch, Crimea, Sevastopol, Danube, Constantza, and Kaliakra anticyclonic eddies described by Staneva et al. (2001); Korotaev et al. (2003); Oguz et al. (2004) and depicted on Fig. 1.2).

Circulation on the NWS is driven by the freshwater discharge (dominated by the Danube), wind stress and interaction with the Rim current at the shelf break. Most of the year, an anticyclonic circulation dominates in the northern part of the NWS. The Danube plume shows a marked seasonality consisting of the alternate dominance of two pathways. One follows the anticyclonic circulation along the Ukrainian coast, and is dominant from May to November, while the other follows the Romanian and Bulgarian coast and dominates from December to April (Beckers et al., 2002).

A strong front is created where the NWS anticyclonic circulation meets the Rim current, characterized by important salinity and chlorophyll gradients (Oguz et al., 2002). This front is unstable and produces a number of meanders and filaments which support cross-shelf exchanges between the NWS and the interior regions (Shapiro et al., 2010).

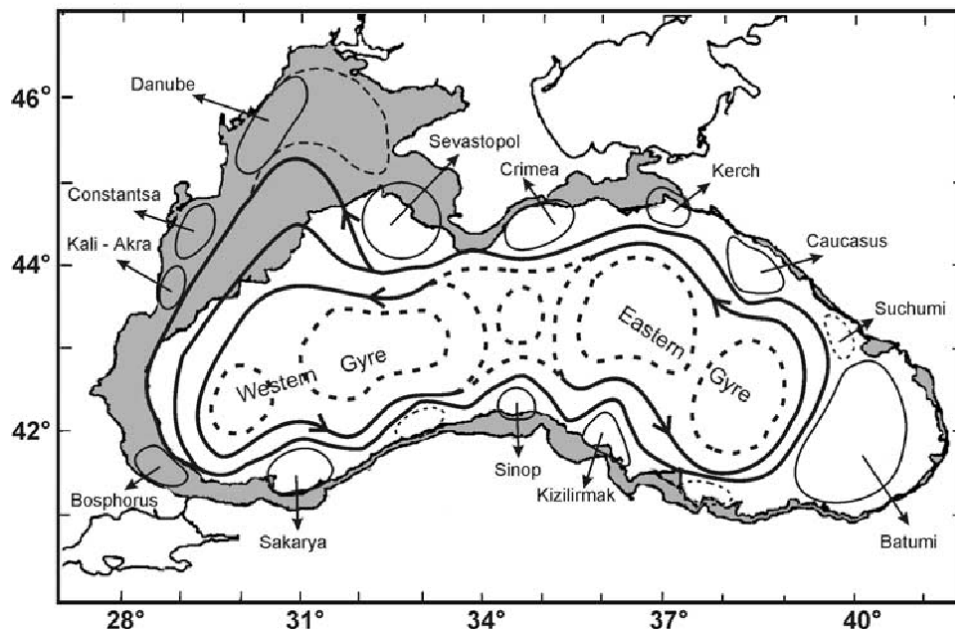


Figure 1.2: Main features of the Black Sea surface circulation inferred from satellite altimetry (reproduced from Korotaev et al. (2003)).

2.4 Water flows and salt budgets

The main exchanges between the principal water masses of the Black Sea are depicted on Figure 1.3. The salt budget is driven by the important freshwater discharges from rivers, the exchange through the Bosphorus strait and evaporation/precipitation budget over the Black Sea surface.

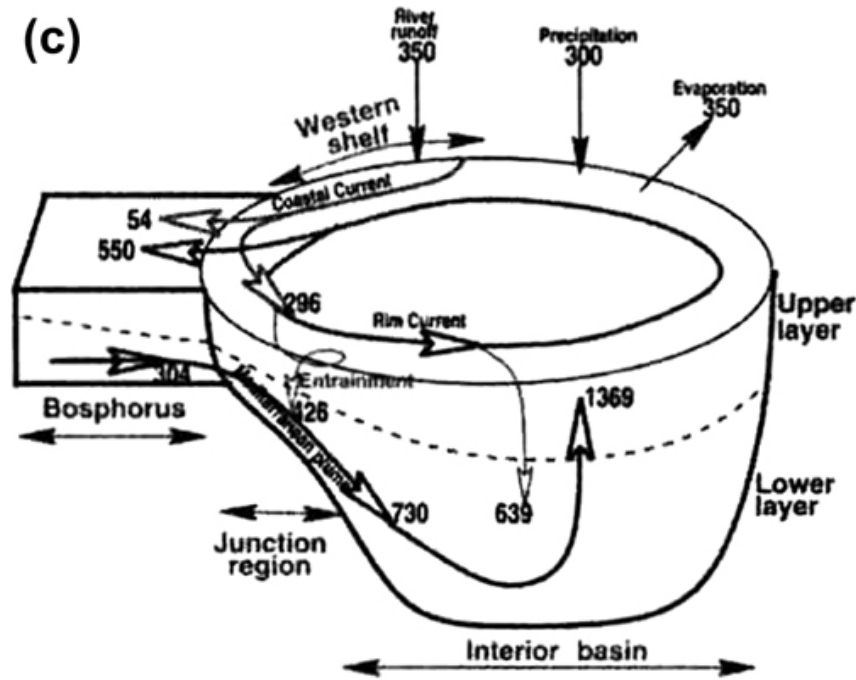


Figure 1.3: Main water flows amongst the different regions of the Black Sea and through the Bosphorus [km^3/yr] (reproduced from *Oguz et al. (2004)*).

The average annual riverine flow ($\sim 350 \text{ km}^3/\text{yr}$) is equivalent to a layer of 80 cm over the entire Black Sea surface ($4.3 \times 10^5 \text{ km}^2$). About 70% of this discharge is delivered on the NWS ($\sim 270 \text{ km}^3/\text{yr}$, from Danube, Dniepr, Dniestr and Bug river), and 55% from the Danube alone.

Annual evaporation rates exceed precipitations, which results in a net removal of $50 \text{ km}^3/\text{yr}$ on the account of air-sea exchanges (*Öszoý and Ünlüata, 1997; Kara et al., 2008*). The remaining $300 \text{ km}^3/\text{yr}$ corresponds to the net export of water through the Bosphorus strait, which balances the water volume budget.

Average Bosphorus exchanges account simultaneously for an effective outflow of water and an effective inflow of salt. This is the consequence of the layered nature of Bosphorus exchanges : the barotropic export is composed of a surface outflow of $605 \text{ km}^3/\text{yr}$ toward the Marmara sea, with the 17.9 p.s.u. salinity signature of the Black Sea surface waters, and a bottom inflow of $305 \text{ km}^3/\text{yr}$ of Marmarean deep waters (i.e previously issued from the Mediterranean sea) with a salinity signature of 35.5 p.s.u. (*Öszoý and Ünlüata, 1997*).

Those dense waters entering the Black Sea through the Bosphorus result in the so-called Bosphorus plume. Constrained by local topography, this plume sinks along the bottom, partially mixing with surrounding waters and entraining surface waters to deeper layers, with a ratio of $\sim 3\text{-}4$ to one, hence playing a key role in the ventilation of the intermediate

layers of the Black Sea (Murray et al., 1991; Stanev et al., 1997; Ivanov and Samodurov, 2001; Stanev et al., 2004).

2.5 Hydrodynamic structure

High surface freshwater inputs and bottom intrusion of salty Mediterranean waters both sustain the characteristic strong halocline of the Black Sea, located at a depth of ~ 150 m and persistent through the year. The halocline may be associated with salinity value of the order of 20 p.s.u and typically sets a sharp gradient in the density profile between values of $\sigma_t = 14.5$ and 16.6 kg/m^3 (Fig. 1.4).

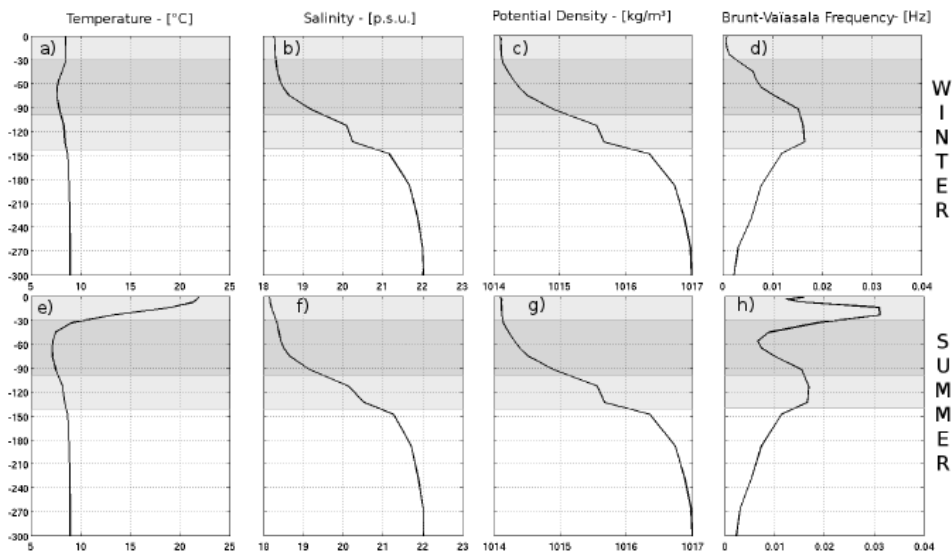


Figure 1.4: Typical temperature (a,e), salinity (b,f) and density (c,g) profiles in the open part of the Black Sea during Winter (a–d) and summer (e–h). The gray bands indicates (from up to down) the zone of summer thermocline, Cold Intermediate Layer and permanent halocline. The Brunt-Väisälä frequency highlights the region of highest vertical gradients. Note the permanence of the main halocline through the year, and the double stratification structure in summer. (Constructed on the basis of model results, see Chapter 3 for comparison with in situ data.)

This halocline sets a strong separation between surface waters, depicting a residence time of the order of the year, and intermediate and deep waters for which residence time may be counted in hundreds of years.

Below the halocline, intermediate and deep waters are characterized by almost vertically uniform properties, i.e. temperature of 9°C , salinity of 22 p.s.u and a density anomaly of $\sigma_t = 17 \text{ kg/m}^3$. A slow convective mixing induced by geothermal heating in the deep sea floor homogenizes the properties of waters below 1700 m (Murray et al., 1991).

Surface circulation influences the vertical structure through Ekman pumping and gives a dome shape to the isopycnals by lifting the halocline in the central basin, and bringing down surface waters in the periphery. As a consequence, most properties in the central Black Sea show a “radial” gradient between the basin interior and its periphery when considered at constant depth. For this reason, vertical properties are usually described by referring to the isopycnals rather than to fixed depths.

The seasonal acceleration of the Rim current is accompanied by an oscillation of the curvature of isopycnals marking the separation between the oxygenated surface waters and the anoxic deep waters, hence plays a role in the ventilation of deep waters.

As the strong permanent halocline restrains the penetration of the seasonal signal in intermediate and deep layers, the seasonal variability of atmospheric conditions and consequent surface fluxes results in a marked seasonal variability of surface properties. Sea surface temperature dynamics are closely responding to the air temperature variations (Kara et al., 2005a; Oguz et al., 2006) and their temporal dynamics is largely dominated by the seasonal fluctuations as evidenced by satellite imagery (Sur and Ilyin, 1997; Nardelli et al., 2010). Surface temperature are usually colder in the northwest and warmer in the southeast.

In wintertime, dense waters are formed where high surface cooling meets salty waters. This occurs in a band over the shelf break, west of the Crimean Peninsula, where the intense cooling typical over the NWS meets water densified by mixing at the shelf break (waters on the northernmost shelf are too fresh to form dense waters), and in the central basin, where outcropping isopycnals expose dense water to the surface cooling (Staneva and Stanev, 2002; Stanev et al., 2003). The convective sinking of these dense and cold waters is limited at intermediate levels by the permanent halocline.

Warming in spring establishes a seasonal thermocline around density levels of $\sigma_t = 14 - 14.5$. The mixed layer depth in that period is rather uniform with values usually less than 15 m. When the thermocline is formed, the dense waters generated in winter remain contained between the permanent halocline and the seasonal thermocline and form the Cold Intermediate Layer (CIL).

The CIL dynamics present a certain inertia in its sensitivity to interannual atmospheric anomalies (Piotukh et al., 2011), as (1) the whole CIL is not renewed every year and (2) the CIL of one year prepares the surface water for the next year CIL formation (Stanev et al., 2003). As a result, CIL dynamics is sensitive to lasting climatic anomalies, i.e. “regime shift”, rather than to rapid oscillations of the atmospheric conditions. The CIL acts as an additional barrier separating surface from deep waters. The CIL formation process, partly involving water issued from the NWS, has implications in the exchange of nutrients and materials between the NWS and open sea regions and in the ventilation of intermediate layers (Stanev et al., 2003).

2.6 Biogeochemical structure

The Black Sea biogeochemistry is determined by nutrients inputs from the rivers, atmospheric deposits and by the permanent vertical stratification.

The NWS region is generally eutrophic due to the important nutrients discharges from the rivers.

Nutrients and planktons in the NWS show a strong heterogeneity. This variability is controlled by the hydrodynamics of the river plumes and the various levels of light penetration affected by suspended minerals and colored dissolved organic matter from the rivers (Ragueneau et al., 2002). Nutrients ratios also change considerably spatially

and temporally (Ragueneau et al., 2002; Oguz, 2008). While Danube waters indicate a phosphate limitation, offshore measurements indicate that this situation is not persistent over the whole shelf nor throughout the year. The reason for this is to be found in the contrasting role of the sediments layer regarding phosphate and nitrogen dynamics.

The NWS region sustains a benthic ecosystem whose relative importance is enhanced by the large spatial extension of the NWS region. The ecological functions of this benthic ecosystem encompass photosynthetic injection of oxygen by macrophytes, processing of detritus and filter functions of bivalves beds, trophic base of benthophagous fishes (Zaitsev, 1997), nutrients recycling, and nutrients and carbon removal by burial in the sediments (Wijsman et al., 1999; Friedrich et al., 2002; Grégoire and Friedrich, 2004).

In the interior basin, surface mixed waters are oligotrophic for most of the year, except for occasional lateral incursions from coastal regions and wet precipitations (Oguz, 2008)

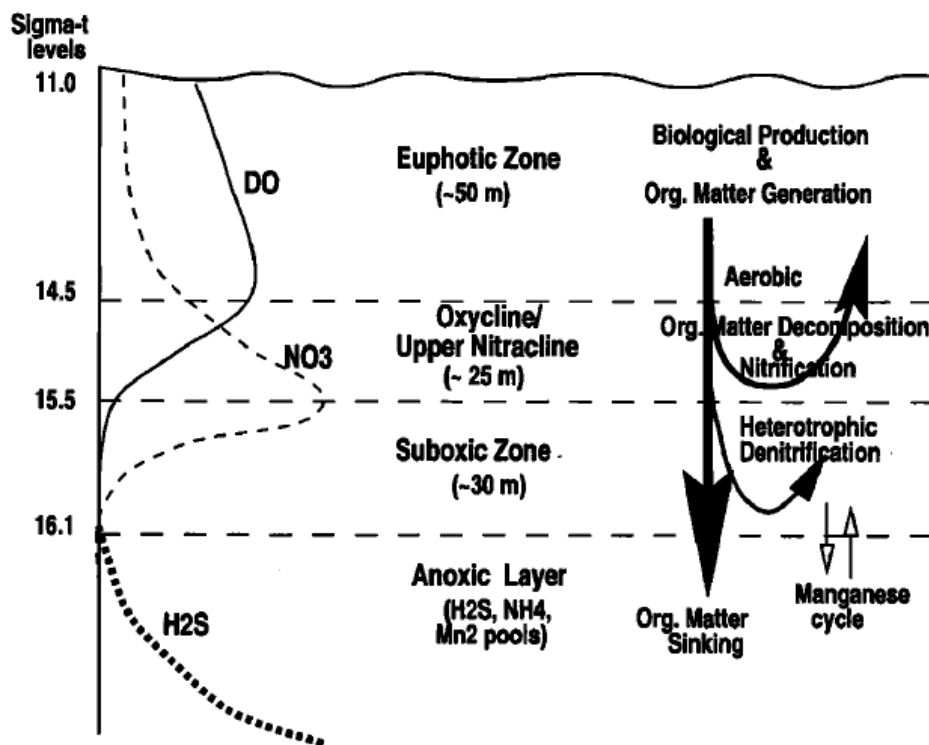


Figure 1.5: The different layers of the biogeochemical structure in the open part of the Black Sea.

The vertical biogeochemical structure of the open Black Sea water column consists (Fig. 1.5) of a well oxygenated surface layer (from the surface to the thermocline or upper boundary of the CIL layer), an oxycline where the oxygen concentration sharply decreases (between the summer thermocline and the permanent halocline), a suboxic layer characterized by very low concentrations of O_2 ($< 10 \text{ mmol/m}^3$) and H_2S ($< 0.005 \text{ mmol/m}^3$) without overlap (Murray et al., 1995), and a sulfidic layer (from below the halocline to the bottom) which constitutes large pools of H_2S and NH_4^+ .

The photic surface layer concentrates most active biological processes (e.g. nutrients uptake, plankton grazing). It is characterized by high oxygen concentrations and seasonally varying nutrients and organic material concentrations.

Below the seasonal thermocline and in the deeper part of the euphotic zone, nutrients concentrations increase due to their recycling through intense bacterial activity as well as continuous supply from the nutricline (Oguz, 2008). About 90% of sinking particles are remineralized in the euphotic zone and the subsequent lower part of the oxygenated zone, and only a small fraction sinks to the deeper anoxic layers (Karl and Knauer, 1991). Nitrates accumulated in the light-shaded zone of the lower oxycline form the so called nitracline (Fig. 1.5), which supports subsurface phytoplankton production.

Below the oxycline, that is when oxygen is depleted, mineralization of organic matter proceeds from denitrification, i.e. the process by which bacteria use nitrate and nitrite (or nitric and nitrous oxide) as the electron acceptor instead of the oxygen used in aerobic mineralization. This explains the sharp decrease in the nitrate profile which forms the lower part of the nitracline.

During winter, nutrients stocks in the euphotic zone are renewed from these nutricline depths through upwelling, vertical diffusion and seasonal wind and buoyancy-induced entrainment processes.

The boundary between the suboxic and anoxic layers involves a series of complicated redox processes (Yakushev et al., 2006). In particular, anammox reactions, in which bacteria oxidize nitrite with ammonium and finally convert it in dinitrogen, are a strong sink for the upward diffusing ammonium (Kuypers et al., 2003). As dinitrogen, also formed during denitrification, is not directly assimilated by surface phytoplankton and finally escapes to the atmosphere in gaseous form, these reactions play a major part in the cycling of nitrogen in anoxic basin such as the Black Sea (McCarthy et al., 2007). While in situ studies evidence the occurrence of dinitrogen fixation in the oxygenated layer of the Black Sea, its contribution to nitrogen budgets and the structure and mechanisms of its variability remains unclear (McCarthy et al., 2007; Fuchsman et al., 2008).

The vertical structure of phosphate concentrations derives from similar processes in the surface layer (uptake in the euphotic zone and then remineralization in the lower part of the oxygenated layer), but is complicated in the suboxic zone by the chemical interactions between phosphate, iron and manganese (Codispoti et al., 1991; Yakushev et al., 2006).

As dissolved oxygen and nitrate concentrations vanish, dissolved manganese, ammonium and hydrogen sulfide concentrations increase. Deep pools of ammonium, sulfide and manganese have been accumulating during the last 5000 years as a result of organic matter decomposition after the Black Sea was converted into a two-layer stratified system (Oguz, 2008).

The vertical extension of the suboxic transition zone is due to the fact that different processes control its upper and lower boundary. The upper boundary, defined by the disappearance of oxygen is controlled by the sinking flux of organic particles and their mineralization. The lower boundary, defined by the appearance of hydrogen sulphide depends on the lateral intrusion of oxygenated waters entrained by the convective sinking of the Bosphorus plume (Konovalov and Murray, 2001; Konovalov et al., 2006).

The dynamics of the Bosphorus plume, dependent on drivers external to the Black Sea, triggers a number of mineralisation and redox reactions (e.g. anammox, sulphide oxidation (Jørgensen et al., 1991), nitrification and denitrification) and therefore has

significant implications in the basin-wide biogeochemical budgets.

2.7 Environmental decline

Increases of the air and river-borne nutrients discharge during the developing years of the Soviet Union led to a sensible rise of nutrients concentrations and changes in the molar ratios in the coastal water from the 1960's.

These nutrients loads increased until 1990, reaching as much as 800 kt/yr of total inorganic nitrogen, 32 kt/yr of phosphate and 1500 kt/yr of silicate delivered annually by the Danube river alone (Cociasu et al., 1996). As a result, a major part of the Black Sea, particularly its northwestern shelf region, became critically eutrophic (Zaitsev, 1997; Lancelot et al., 2002).

The first consequences of this eutrophication consisted in severe shifts in the total biomass, seasonal blooms timing and composition of the phytoplanktonic communities (Bodeanu, 2002; Yunev et al., 2007), with consequences on zooplankton communities and upward across the food web. Diatoms, the most abundant group prior to the 1970s, were replaced by predominant blooms of dinoflagellates and coccolithophores (Moncheva et al., 2001). This shift was supported by the decreasing SI/N ratio of Danube waters after its damming in 1972 (Lancelot et al., 2002). However, measurements of nutrients and diatoms taken in the mid 90s offshore of the Danube delta did not reveal limiting levels of silicate (Ragueneau et al., 2002), indicating again that general assumptions do not hold easily in the NWS.

The phytoplankton biomass in the northwestern shelf area increased from 1 g/m² in the 1960s to 19 g/m² in the 1970s and 30 g/m² in the 1980s (Zaitsev, 1997). This enhanced phytoplankton biomass led to a decrease of water transparency, most sensible in the NWS but also in open waters (Fig. 1.6). On the shelf, the shading of the phyto-benthic community induced a drastic shredding of the characteristic sea grass population (*Zostera*, *Cystoseira*, *Phyllophora*) with further impact of their supported biocenosis (Kostylev et al., 2010, and references therein), reflected by a dramatic decrease of biodiversity (Zaitsev, 1997).

One of the most spectacular effect of eutrophication was the appearance of systematic seasonal hypoxia in the northern part of the NWS, first witnessed during the 70s, that induced mass benthic and fish mortalities (Zaitsev, 1997). While it was reported that the hypoxia issues vanished with the reduction of riverine nutrients discharge after 1992 (Mee, 2006), other studies indicate only a slight decrease in hypoxia and account for hypoxia occurrences until the year 2000 (last year considered in this study, UkrSCES (2002)). The case of hypoxia is discussed more extensively in Chapter 7.

The effects of eutrophication on the environmental structure and functioning of the Black Sea system were strongly enhanced by the combined occurrence of other anthropogenic stressors, mainly overfishing and alien species introduction. The individual roles of these different stressors are difficult to assess empirically as they occur simultaneously and in synergy.

Overfishing (from the 1960's) first led to the decrease of large piscivorous fishes (Za-

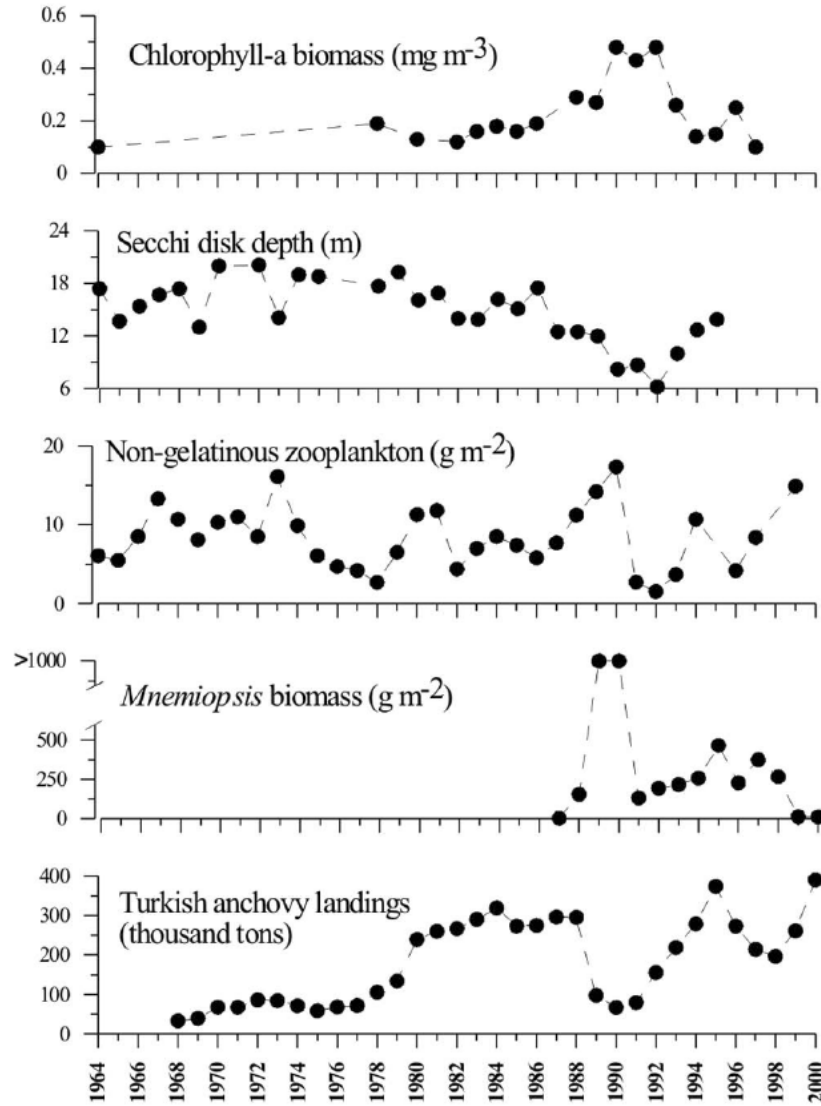


Figure 1.6: Long-term variability of (a) chlorophyll concentration (Surface value between May-September), (b) Secchi disk depth (annual mean), (c) non-gelatinous mesozooplankton biomass, (d) *Mnemiopsis leidyi* biomass (summer catches), (e) Turkish anchovy landings, (reproduced from (Oguz et al., 2004)).

itsev, 1997). This perturbation of the food web led to an increase of zooplanktivorous fishes and gelatinous species (*Noctiluca scintillans*, *Aurelia aurita*, *Pleurobrachia rhodopsis* and *Mnemiopsis leidyi*) with cascading effects on the planktonic communities (Daskalov, 2002) which combined to that of eutrophication and contributed to the decrease in light penetration (Daskalov, 2002).

In addition, erosion of the ecosystem resilience caused by overfishing (Gucu, 2002; Llope et al., 2011) allowed alien species to develop anomalously and to over-compete local species. The ctenophore *Mnemiopsis leidyi*, introduced accidentally in the ballast waters of cargo ships, competed over food resources with the local planktivorous fish populations (e.g. the anchovy *Engraulis encrasicolus*) and used to feed on its eggs and larvae. The drastic shrinking of the anchovies stocks that followed the outburst of *Mnemiopsis leidyi* in the late 80s (Shiganova, 1998) had a severe impact on the Black Sea fishery economies (Kideys, 2002) (Fig. 1.6).

The increased population of gelatinous carnivorous favored a quicker trophic loop, enhancing bacterial activity and organic matter decomposition by increasing the particulate and dissolved matter content in the upper part of the water column (Lancelot et al., 2002). This can be seen in evolution of the biogeochemical structure of the Black Sea by an uplifting of the suboxic transition zone from isopycnal levels of $\sigma_t = 15.9 \text{ kg/m}^3$ in the 60s to $\sigma_t = 15.6 \text{ kg/m}^3$ in the 90s and an increase in the sulfidic contents of the anoxic waters (Konovalov and Murray, 2001). A significant increase in the inventory of nitrate and a small upward motion of the nitracline was also observed (Fig. 1.7).

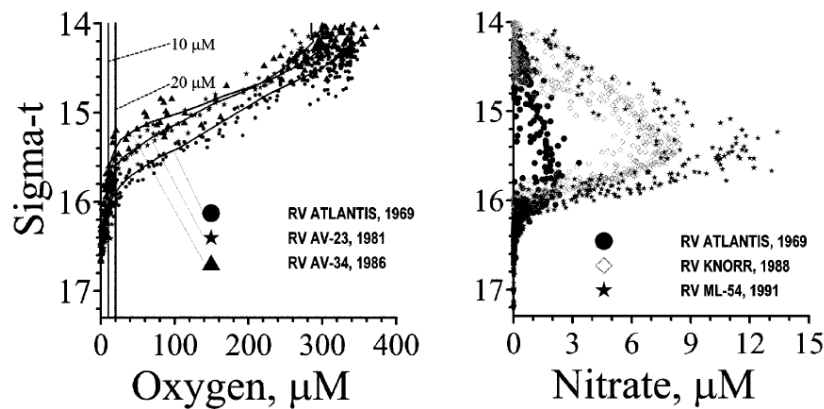


Figure 1.7: Distribution of in situ oxygen and nitrate measurements for different year (reproduced from (Konovalov and Murray, 2001)).

The sensitivity of the Black Sea ecosystem to these anthropogenic factors was also influenced by the natural oscillation of the atmospheric system (Oguz et al., 2006; Oguz and Gilbert, 2007) whether directly (e.g. temperature effect on metabolism) or indirectly by impacting on the hydrodynamical structure, hence the vertical and lateral exchanges, the residence time of water masses and the connectivity between the different region of the Black Sea. For instance the strong winters in the early 90's were associated with the decrease of the *Mnemiopsis leidyi* population below critical competing thresholds with pelagic fish groups (Kideys and Romanova, 2001). *Mnemiopsis leidyi* was finally controlled by the accidental introduction of another ctenophore *Beroe ovata* which predaes on *Mnemiopsis leidyi*. Fish stocks started to show signs of recovery first in the 1993-1995

period and more markedly at the end of the 1990's (Oguz et al., 2004)

In the late 80s and early 90s, due to the economic crisis in the former Iron Curtain countries and to several national and international programs aiming at controlling the issue of eutrophication, nutrients loads were reduced and several indicators of environmental status showed signs of recovery (Kideys, 2002) : surface chlorophyll, nutrients levels, water transparency, frequencies of harmful algae blooms and fish landings).

However, due the non-linearity of ecosystem dynamics, it is most likely that the thresholds of nutrients loads allowing the Black Sea ecosystem to fully recover to its pristine state is well below these that caused this environmental decline (Mee, 2006). Therefore, today Black Sea status should be considered as a weakened post-eutrophication state (Oguz, 2008).

3 Modelling the Black Sea

As indicated in the previous section, the Black Sea environment has suffered from a combination of various stressors. Each one of them has implications on the sensitivity of the system to others stressors and it is extremely difficult to establish a clear causal relationship between individual stressors and observed modifications of the system.

Mechanistic modelling aims at providing the tools to answer such questions.

The characteristics of the Black Sea make it an ideal object for modelling studies: simple boundaries, high sensitivity to external forcings, and presence of various specific features (e.g. strong stratification, gravity flows, localized convection zones) that allows testing numerical solutions to general oceanographic issues.

Also, many conclusions on the general state of the sea are drawn from heterogeneous and sometimes limited data sets. As variability is known to reign in the marine realm, modelling studies may refine the conclusions drawn from datasets by assessing to which extent these may have been influenced by the uneven distribution of observations.

Stanev (2005) offers an efficient review of the modelling efforts (physics) developed in the Black Sea and illustrates how these models completed observations to reach the current rich scientific understanding of Black Sea hydrodynamic mechanisms.

Amongst the most known or exploited Black Sea hydrodynamical 3D implementations one may cite the following :

- The Modular Ocean Model (MOM) is a rigid-lid, z-coordinate model first implemented by Stanev (1990). It was exploited to explore the characteristics of Black Sea horizontal and vertical circulation (Stanev, 1990), and then refined with a dedicated convection scheme to represent the ventilation of the intermediate layer (Stanev et al., 1997), the sensitivity to different sets of atmospheric forcings (Staneva and Stanev, 1998) and the process of CIL waters formation (Stanev et al., 2003). The model was later used to study the dynamics of intermediate and deep waters ventilation, exploiting the observed distribution of passive tracers of anthropogenic origins (Chlorofluorocarbons) (Stanev et al., 2004).

- The Princeton Ocean Model (POM), a σ coordinate model with free-surface implemented by (Oguz et al., 1996) was used to determine the respective role of the various drivers of surface circulation and later used for coupled biogeochemical set-up.
- The Diecast model (Staneva et al., 2001) is a z-model characterized by high-level discretization schemes and low diffusion. It allowed the authors to investigate the dynamics of meso-scale structures and their impact on coastal–interior exchanges.
- The GHER model (described in Chapter 3) uses a double- σ coordinates, free-surface, and a detailed turbulence closure scheme. The double- σ coordinates allows to overpass the common problem that arises when using z-model on steep bathymetry. This model was used to study the internal dynamics (Stanev and Beckers, 1999) and later to introduce the assets of nested models (Beckers et al., 2002).
- The HYCOM model uses hybrid vertical coordinates and has a fine horizontal resolution (3.2 km). This model was used to explore the dynamical implication of various light penetration schemes, and revealed the important role of the Black Sea natural turbidity in its vertical stratification (Kara et al., 2005a,b).
- The GETM model (Peneva and Stips, 2005) is one of the rare implementations that includes the Azov Sea in the Black Sea domain. Therefore it permitted to study the interactions between these two sub-basins.
- The Nucleus for European Modelling of the Ocean (NEMO) was implemented by Grayek et al. (2010) who resorted to the assimilation of altimeter data to explore the sea-level variability and its relationship with water cycles and winds.

Biogeochemical models have also been developed and implemented in the Black Sea, with different objectives and designs. For the open sea, 1-D studies have been realized with models of various complexities going from simple 5 state variables Fasham-like models (e.g. Oguz et al., 1996), to more complex models with several phytoplankton and zooplankton compartments (e.g. Oguz et al., 2000). In the latter version, nitrogen cycling was described through two phyto- and zooplankton groups and the microbial loop. These models were used to study how the annual distributions of phytoplankton and mesozooplankton distributions have been altered by top-down control imposed by gelatinous carnivores. Also, the model represents the impact of three gelatinous groups (*Mnemiopsis leidyi*, *Aurelia aurita*, *Noctiluca scintillans*) on the food web dynamics by diagnostically computing their grazing rates from the data.

For the northwestern shelf, in the frame of the European project EROS-21, a complex ecological model describing carbon, nitrogen, phosphorus and silicon cycling through 34 biological and chemical compartments has been developed by Lancelot et al. (2002). This model involves several phytoplankton and zooplankton groups, three groups of gelatinous organisms and a complex description of the microbial loop. The model has been applied in the Danube plume in 0 D and 1D implementations to study the consequences of the quantitative and qualitative shifts in the nutrients discharges.

At basin scale, Grégoire et al. (1998) coupled a simple 5 state-variable Fasham-like ecosystem model with a 3D hydrodynamical model with the aim of assessing the influence

of physical processes on the biogeochemical dynamics. This 3D model was then further developed and applied to study the transport of nutrients and materials from the shelf to the open sea (Grégoire and Lacroix, 2003), the cycle of nitrogen at shelf (Grégoire and Friedrich, 2004) and basin-scale (Grégoire et al., 2004).

The peculiar redox structure of the Black Sea makes it an ideal site to develop the modelling of redox processes. The redox structure was first examined with 1D model (Yakushev and Neretin, 1997) considering the interactions between oxygen, nitrogen compounds and sulfur. The model was consistently enhanced until it included manganese, iron and phosphorus cycling (Yakushev et al., 2007) and thus succeeded in describing the seasonal dynamics of the Black Sea redox structure.

The explicit inclusions of the oxic, suboxic and anoxic layers were first considered by Grégoire et al. (2008); Grégoire and Soetaert (2010) in 1D model studies designed for the open basin enabling finally the coupling between surface and deep waters dynamics.

4 Objectives

How can we characterize the long term variability of the Black Sea ecosystem and which are the specific impacts of climate and anthropogenic forcings on this variability? Which are the key processes that drive this variability? Can we provide a sound understanding of these mechanisms and integrate it to transfer a practical support for a sustainable management of its resources?

This thesis aims at answering these questions through sophisticated data analysis approaches and through the development and exploitation of a tridimensional coupled hydrodynamic and biogeochemical model. By integrating in this model previous specific efforts we intend to provide a wide picture that merges the processes ranging from the river mouths to the basin depth, acknowledging the transfer between the Black Sea body and its atmospheric and benthic interfaces. Through technical choices, we want the model to be tractable for long term simulations, suited to address the environmental shift of the past decades and to provide expectation ranges for the coming ones.

First, we want to characterize the variability of the Black Sea hydrodynamical and biogeochemical structure, in both spatial and temporal terms, to support the interpretation of trends revealed by observing systems. We put a strong emphasis on the variability of the physical characteristics, since it can explain a significant part of the variability of biogeochemical structure. Beyond the descriptive approach, we aim to explain this variability by (1) relating the various observable aspects within a multivariate description and (2) explaining the observed variability on the basis of the external forcings, which in the case of physical variables, relates to hydrological and atmospheric variability.

Second, we want to describe the main biogeochemical cycles in the Black Sea and in particular to develop a model able to reproduce the variability of the biogeochemical variables across the large environmental gradients of this domain. In particular it was quickly revealed that this could only be achieved by enforcing the description of benthic-pelagic coupling in the large and shallow NWS.

Third, we want to demonstrate the relevance of such model description by using the model to explore in more details the dynamics of the hypoxia in the NWS. The aim is to distinguish the specific impacts of its eutrophication and climate related drivers and to derive from our results practical relationships suited to support the management of this dramatic environmental affliction.

In the field of operational oceanography, models aim to reproduce or forecast the reality with the highest level of accuracy. By comparison, our approach could be characterized as “fundamental”: we aim at identifying and resolving processes rather than achieving the best matches with observations. All the simulations presented in this work are therefore achieved without any interference of observations during the simulations. Neither data assimilation neither “nudging” (i.e. the systematic relaxation of the model state toward climatological fields) are considered. This approach sometimes results in imperfect matches between modelled and observed variables, but ensures that every phenomenon seen in the model results has its origin in the model equations. In-depth validation procedures are therefore carried out to assess the model skills, i.e. to estimate in which extent the model results can be used to provide insights about the functioning of the real system, but also to characterize the error and if possible to evidence tracks for further enhancements.

5 Structure

This thesis gathers original chapters describing the model components (Chapters 3 and 5), and published chapters presenting Black Sea specific investigations (Chapters 2, 4, 6 and 7)¹.

Chapter 2 presents an application of the DIVA detrending tool on Black Sea vertical properties. We propose a general methodology allowing to untangle the spatial and temporal (both seasonal and interannual) variabilities from unevenly distributed dataset. The method is applied on mixed layer depth and CIL cold content, both vertical properties assessed from in situ profiles. The resulting trends are then exploited to relate the dynamics of these variables to atmospheric conditions. No modelling works, in the mechanistic sense used in this thesis, are considered in this chapter.

In chapter 3 we present the hydrodynamical model and its implementation in the Black Sea. Model skills are assessed using satellite and in situ observations and by comparing the variability of vertical characteristics to that reconstructed from in situ profiles in Chapter 2.

In chapter 4, the hydrodynamical model and satellite observations are used to deepen the investigations on the inter-annual variability of the Black Sea hydrodynamic features. The dynamics of distinct surface and sub-surface properties are merged into coherent multivariate modes of variations. The characterization of recurrent meteorological regimes permits to identify how the hydrodynamic structure responds to the occurrence and persistence of these regimes and allows to relate these oscillations to large scale atmospheric teleconnection patterns.

¹Chapter 6 has not been published yet

The next chapters include the biogeochemical aspects.

In chapter 5, we present the pelagic component of the biogeochemical model. Model skills are assessed against in situ measurements both for the northwestern shelf and open basin regions.

Chapter 6 details the benthic model component developed to resolve the important benthic-pelagic coupling occurring on the Black Sea northwestern shelf. Spatial and seasonal variations of the benthic-pelagic coupling system are analyzed and compared to in situ benthic fluxes estimates. A particular attention is given to the representation of sediments deposition and transport, and their impacts on the benthic contribution to nutrients and oxygen budget.

Chapter 7 finally applies the full coupled model to address the critical issue of hypoxia in the Black Sea northwestern shelf. The combined contributions of climatic and anthropogenic factors to hypoxia interannual dynamics are weighted by detailing the seasonal mechanism leading to bottom hypoxic condition. This publication also reassess the past history of hypoxia in this area, which has been imperfectly estimated due to incomplete monitoring.

The final Chapter 8 provides a brief summary and concluding remarks, and evidences a series of initiated perspectives exploiting the powerful modelling tool set up during this research.

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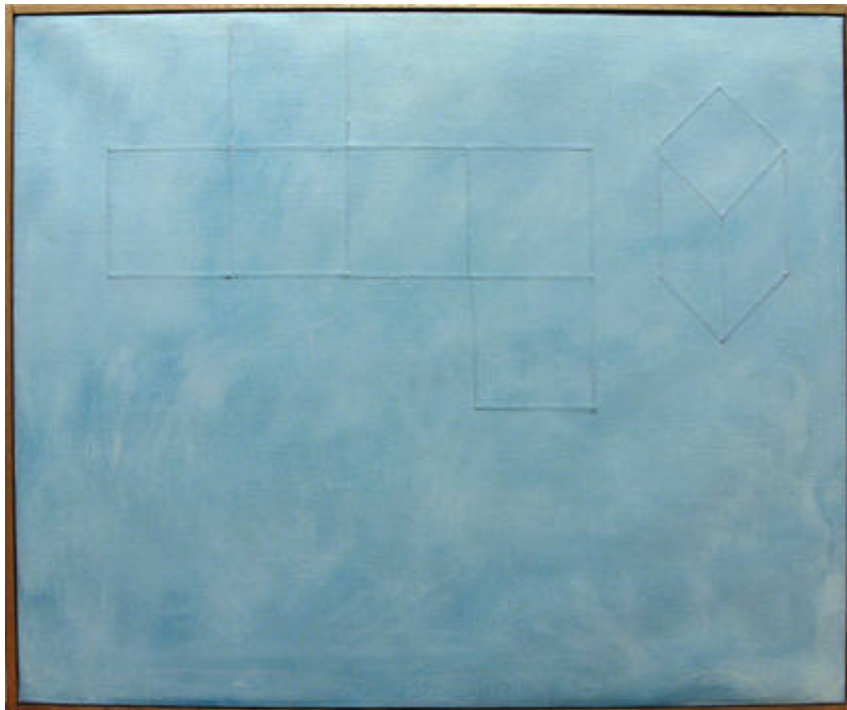
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Part I

Hydrodynamics

Chapter 2

Untangling spatial and temporal trends in the variability of the Black Sea Cold Intermediate Layer and Mixed Layer Depth using the DIVA detrending procedure.



Time and Space Series 1, Kazuo Nakamura, 1974

This chapter has been published as :

A. Capet, C. Troupin, J. Carstensen, M. Grégoire & J.-M. Beckers, 2014, Untangling spatial and temporal trends in the variability of the Black Sea Cold Intermediate Layer and Mixed Layer Depth using the DIVA detrending procedure, *Ocean Dynamics*, DOI 10.1007/s10236-013-0683-4.

The main object of this publication is to present the assets of the detrending option included in the DIVA interpolation software. An extensive application on Black Sea vertical properties reconstructed from in situ profiles evidences their interannual and seasonal variations and exploits these to derive corrected annual and monthly climatological fields. A rapid statistical analysis identifies the relationships between the identified interannual trends and atmospheric conditions.

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Abstract

Current spatial interpolation products may be biased by uneven distribution of measurements in time. This manuscript presents a detrending method that recognizes and eliminates this bias. The method estimates temporal trend components in addition to the spatial structure and has been implemented within the Data Interpolating Variational Analysis (DIVA) analysis tool. The assets of this new detrending method are illustrated by producing monthly and annual climatologies of two vertical properties of the Black Sea while recognizing their seasonal and interannual variabilities : the mixed layer depth, and the cold content of its Cold Intermediate Layer (CIL). The temporal trends, given as by-products of the method, are used to analyze the seasonal and interannual variability of these variables over the past decades (1955-2011). In particular, the CIL interannual variability is related to the cumulated winter air temperature anomalies, explaining 88% of its variation.

1 Introduction

Climatologies, i.e. average fields interpolated from in-situ data gathered over a large period, are widely used in earth sciences. However, monitoring data are typically heterogeneously distributed in time and space, leading in some cases to flawed analysis if this heterogeneity is not adequately accounted for. For instance, if the mean annual temperature field over the Northern Hemisphere is computed with all the available data, the result will overestimate the true mean temperature, since there are more measurements in summer than in winter. Similarly, the mean temperature field will be biased if data from cold and warm years are not equally represented in all regions.

To remedy this impact, which occurs when unavoidable heterogeneous distribution of data is combined with high variability, we present a detrending method ([Duchon, 1977](#)) that has been implemented in the existing Data Interpolating Variational Analysis (DIVA, [Troupin et al., 2012](#)) tool.

The cases of the Black Sea Cold Intermediate Layer (CIL) (e.g. [Stanev et al., 2003](#)) and Mixed Layer Depth (MLD) (e.g. [Kara et al., 2009](#)) are ideal examples of application since (1) the CIL (resp. MLD) exhibits an important interannual ([Oguz et al., 2006](#)) (resp. seasonal) variability and (2) sampling in the Black Sea is characterized by strongly uneven temporal coverage.

The Black Sea is an enclosed basin, characterized by a strong permanent halocline at approximately 150 m depth, which separates the surface layer, receiving substantial freshwater inputs from several large rivers discharging mainly to the northwestern Shelf, and the deep waters receiving saltwater inflows from the Mediterranean Sea through the Bosphorus. The surface layer is advected by a basin-wide cyclonic current, referred to as the *Rim Current* and further subdivided in two main gyres ([Korotaev et al., 2003](#)), which intensifies in winter and controls the curvature of the halocline (shallower in the center of the basin, deeper in the periphery).

Cold and dense waters are formed in winter, when surface cooling breaks down the

summer thermal stratification and the water column above the halocline becomes fully mixed. The convective sinking of the cold surface waters is limited by the permanent halocline, because of denser saline water below. This mechanism leads to the formation of a minimum temperature layer located between the halocline ($\sim 100\text{--}150$ m) and the summer thermocline ($\sim 20\text{--}50$ m), known as the *Cold Intermediate Layer* (CIL). [Stanev et al. \(2003\)](#) located the main regions of CIL formation: (1) West of the Crimea peninsula, where surface cooled fresh waters are mixed with underlying saltier waters; (2) In the central basin where the winter outcropping of the deep isopycnals allow the cooling to penetrate directly to the density levels of the CIL (which is not possible for the northernmost part of the northwestern shelf area where surface cooling is nevertheless stronger).

The detrending method applied in this work provides monthly climatological fields of the MLD and the CIL cold content (CCC), i.e. the temperature anomaly integrated over the CIL vertical extension (Sect. 3.1), while recognizing the impact of their seasonal and interannual variabilities on the data representativity. The trends assigned to each year by the methodology provide long-term time series used to investigate the interannual variability of MLD and CCC and their relationship to atmospheric drivers.

While [Oguz et al. \(2006\)](#); [Capet et al. \(2012\)](#) showed that the CIL follows the interannual variability of air temperature, [Stanev et al. \(2003\)](#) identified that it is not entirely renewed every year and that the remaining CIL at the end of summer prepares the winter CIL formation for the next year. Also, [Piotukh et al. \(2011\)](#) indicated the preponderant influence of winter mean (rather than annual mean) surface air temperature on the thermohaline characteristics of the cold content for the next summer. This indicates that the Black Sea hydrodynamics, and in particular regarding the CIL, present regular seasonal cycles, and that interannual variability may be perceived as year long persistent anomalies. The Rim Current, which derives mostly from the surface wind vorticity (negative curl causes strong Rim Current), is known to affect the Black Sea vertical structure but its specific impact on the CIL is difficult to appreciate directly because the occurrence of cyclonic wind patterns is correlated to that of cold air temperature ([Capet et al., 2012](#)).

The paper is organized as follows: Section 2 provides a short description of DIVA and describes the detrending procedure and its implementation within DIVA. Section 3 presents an application of the detrending methodology on the Black Sea MLD and CCC and an analysis of their temporal trends. The conclusions concerning the Black Sea and general limitations of the method are discussed in Section 4.

2 Data Detrending

2.1 The DIVA method

DIVA stands for Data-Interpolating Variational analysis. It is a method used to interpolate spatially inhomogeneously distributed data. The principle of DIVA is to construct an analyzed field φ that satisfies a set of constraints expressed in the form of a cost function over a domain Ω . Typically, in oceanography, Ω is the part of the considered domain covered by the sea. The cost function is made up of: (1) an *observation constraint*, which

penalizes the misfit between data and analysis, (2) a *smoothness constraint*, which penalizes the irregularity of the analyzed field (gradients, laplacian etc), and (3) a *behavior constraint*, which takes into account physical laws (advection, diffusion, sinks/sources).

In this paper, only the first two constraints will be considered. In the particular case where the observation constraint is much stronger than the smoothness constraint, the results of the minimization of the cost function is a spline interpolation: the analysis has to contain all the data points. Such a solution is not suitable in the case of atmosphere or ocean observations because it does not consider the noise present in the data (measurement errors, but also *representativity* errors). In other words, the estimated field should mimic the observations rather closely, although maintaining a reasonable degree of smoothness to avoid over-fitting the data.

Formulation

Let us assume that we work with data anomalies, i.e. a reference (or background) field is subtracted from the data points prior the analysis. Considering a series of N data anomalies d_i at locations (x_i, y_i) , the cost function reads, in Cartesian coordinates:

$$\begin{aligned} J[\varphi] &= \int_{\Omega} (\nabla \nabla \varphi : \nabla \nabla \varphi + \alpha_1 \nabla \varphi \cdot \nabla \varphi + \alpha_0 \varphi^2) d\Omega \\ &+ \sum_{i=1}^N \mu_i [d_i - \varphi(x_i, y_i)]^2 = J_{\text{smooth}}[\varphi] + J_{\text{obs}}[\varphi], \end{aligned} \quad (2.1)$$

where μ_i , α_0 and α_1 are coefficients related to characteristics of the dataset (Section 2.1). ∇ is the horizontal gradient operator and $\nabla \nabla \varphi : \nabla \nabla \varphi = \sum_i \sum_j (\partial^2 \varphi / \partial x_i \partial x_j) (\partial^2 \varphi / \partial x_i \partial x_j)$, the generalization of the scalar product of two vectors.

The first term of (2.1) measures the spatial variability (curvature, gradient and value) of the analyzed field and is identified as the smoothness constraint. The penalization of second derivatives is similar to the smoothing spline formulation (e.g. Wahba, 1975; Wahba and Wendelberger, 1980). The second term is a weighted sum of data-analysis misfits and is identified as the observation constraint: it tends to pull the analyzed field towards the observations. The analyzed field $\varphi(x, y)$ is obtained as the balance between observation and smoothness constraints, once the parameters have been determined. Further details about the DIVA interpolation technique can be found in Brasseur et al. (1996); Troupin et al. (2013).

Analysis Parameters

By using a non-dimensional version of (2.1), it can be easily shown (e.g. Troupin et al., 2012) that the coefficients of (2.1) are related to: (1) the relative weights w_i attributed to each observation d_i , (2) the correlation length L and (3) the signal-to-noise ratio λ , according to:

$$\alpha_0 = \frac{1}{L^4}, \quad \alpha_1 = \frac{2}{L^2}, \quad \mu_i = \frac{4\pi\lambda w_i}{L^2} \quad \text{with} \quad \sum_{i=1}^N \frac{1}{w_i} = N.$$

These relations simply show that knowing L , λ and w_i allows the determination of the analysis parameters α_0 , α_0 and μ_i of the cost function.

Some tools are implemented in DIVA in order to estimate the values of L and λ , based on the data correlations and on generalized cross validation (Brankart and Brasseur, 1996; Troupin et al., 2013).

Finite-Element Solver

The minimization of (2.1) is solved with a finite-element technique: the domain of interest Ω is covered by a mesh made up of triangular elements (see Figure 2.3a), and in each element, the solution φ_e is expanded in terms of connector values, which ensure the solution is continuously derivable (Brasseur et al., 1996), and shape functions, which serve to compute the field at any desired location.

2.2 Implementation of Detrending in DIVA

If we define one group (e.g. the year), each data point is in one and only one class C_j (e.g. 1990, 1991, ...) of this group. The data-analysis misfit term of the functional (2.1) can be rewritten by including an unknown trend value for each class ($d_{C_1}, d_{C_2}, \dots$):

$$\begin{aligned} J_{\text{obs}}[\varphi] &= \sum_{i \in C_1} \mu_i [d_i - d_{C_1} - \varphi(x_i, y_i)]^2 \\ &+ \sum_{i \in C_2} \mu_i [d_i - d_{C_2} - \varphi(x_i, y_i)]^2 + \dots \end{aligned} \quad (2.2)$$

If the function $\varphi(x, y)$ were known, minimization with respect to each of the unknowns d_{C_j} would yield

$$d_{C_1} = \frac{\sum_{i \in C_1} \mu_i [d_i - \varphi(x_i, y_i)]}{\sum_{i \in C_1} \mu_i} \quad (2.3)$$

and similarly for the other classes: the trend for each class is the weighted misfit of the class with respect to the overall analysis. Obviously, the solution φ is not known, since it is actually the result of the minimization process, but this issue is solved by iterating and starting with an analysis without detrending. Using the field φ , we calculate a first guess of the trends in each group and subtract it from the original data. Following this, a new analysis is performed, the trends are recalculated, and the iterations continue until a specified convergence criterion is fulfilled.

The procedure can be generalized with several groups of classes (e.g. year, month, time of the day, ...), in this case detrending is applied hierarchically: (1) Trends for the first group are calculated and removed from the data; (2) The second group is treated and so on; (3) Once the data have been detrended, a new DIVA analysis is performed; (4) With the new analysis, the data-analysis misfit (or residual) can be reused to improve the trend estimates. The procedure is repeated a predefined number of times, which ensures convergence in all the cases we tested.

2.3 Synthetic Example

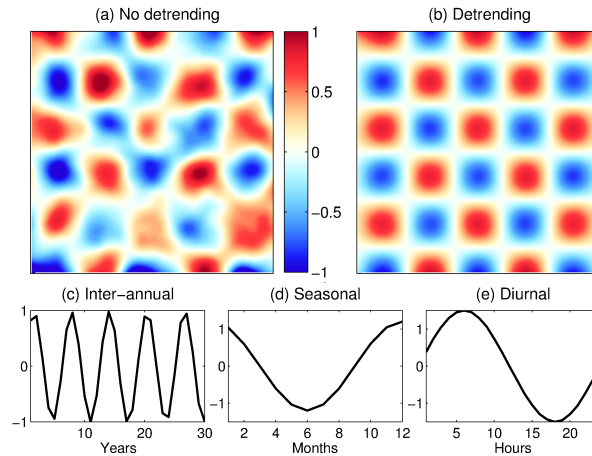


Figure 2.1: Example of a reconstruction without detrending (a), with detrending (b), and the trends obtained from the data (c)-(e), where the x-axis indicate the different classes of the three groups. The color bar is common to (a) and (b)

To illustrate how the detrending helps to reconstruct the spatial distribution of a time-varying variable, we consider the following artificial example : A variable with a fixed and known spatial distribution (a sin-cosine structure) is modulated by a seasonal cycle, a daily cycle and interannual variations. Samples are taken randomly in space and time and are then used to reconstruct the spatial distribution with DIVA. The results with and without considering detrending are compared.

In this example, the groups considered for the detrending are thus years, months and hours. The corresponding classes are the discrete values of these (e.g. 0, 1, ..., 23, for the group "hours").

Without detrending, each observation is considered an equal representative of the same static field, disregarding the temporal structure of the data, which amounts to ignore the non-synoptic character of punctual sampling and results in a flawed analyzed field, dependent on the sampling distribution (Figure 2.1a).

When considering the detrending, the periodic structure is perfectly recovered (Figure 2.1b). Note that the reconstruction is perfect in this case because the temporal trend is spatially homogeneous.

Along with the detrended spatial analysis, the tool also provides the trend identified for each group (Figure 2.1c-e) which may also be of direct scientific interest when the technique is applied to field observations, as shown in the next section.

3 Real-case application : the Black Sea Cold Intermediate Layer

3.1 Materials

Data extraction

While interpolation methods are often applied on variables that may be directly measured (e.g. sea temperature, salinity, ...), this examples addresses vertical properties derived from vertical profiles : the CIL cold content (CCC) (e.g. [Stanev et al., 2003](#)), and the mixed layer depth (MLD) ([Kara et al., 2009](#)).

Profiles of temperature and salinity are obtained from the World Ocean Database ([Boyer et al., 2009](#)) in the box 40°– 47°30'N, 27°– 42°E for the period 1955-2011.

Since the CIL has a minimal depth deeper than 50 m, analysis (interpolation and detrending) are only carried out for the deeper parts of the Black Sea (>50 m). The CIL cold content (CCC) corresponds to the relative heat deficit in the CIL and is thus expressed negatively in terms of J m^{-2} ([Piotukh et al., 2011](#)). It is computed as the vertical integral of the temperature anomaly over the vertical extension of the CIL, limited by the $T = T_0$ isotherms and a density criterion ($\rho > 1014 \text{ kg m}^{-3}$) ([Stanev et al., 2003](#)):

$$\text{CCC} = c\rho \int_{\text{CIL}} [T(z) - T_0] dz, \quad (2.4)$$

where ρ is the density and c the heat capacity. The value of CCC is set to 0 if the profile covers the usual CIL vertical extent without displaying temperatures lower than T_0 . Historically, the value $T_0 = 8^\circ\text{C}$ has often be used to define the CIL ([Blatov et al., 1984](#)). However, according to recent observations that attest the presence of the CIL layer as a physical phenomenon without temperature below 8°C , we rather use the value $T_0 = 8.35^\circ\text{C}$ recommended by [Stanev et al. \(2013\)](#). In order to allow an unbiased estimation of the CIL cold content, eligible profiles should (1) contain a minimum of 6 measurements, (2) contain an upper observation above 30 m, (3) extend to lower boundary of the CIL (or close to the bottom).

For the MLD the analysis are performed on the whole Black Sea and Sea of Marmara, while the Azov Sea was excluded from the analysis for lack of data. The MLD is defined as the depth where a density difference $\Delta\rho$ compared to the 3 m depth density reaches a threshold of 0.125 kg m^{-3} as proposed for the Black Sea by [Kara et al. \(2009\)](#). Eligible profiles for the MLD should (1) contain a minimum of 4 measurements, (2) contain an upper observation above 3 m depth, (3) present a density difference bigger than 0.125 kg m^{-3} .

Data Distribution

The monthly distribution of data is heterogeneous, with a minimum of 892 selected profiles in January and a maximum of 3131 in May. The winter-summer imbalance is evident: the July-September period has 60% more profiles than in the January-March period. The

interannual data distribution is also quite irregular with a majority (59%) of profiles between 1982 and 1995.

While the spatial coverage is sufficient for the considered analysis, selected profiles are generally more concentrated close to the coast than in the central basin and are more numerous in the western basin than in the eastern part (profile locations are shown for March in Figures 2.3 and 2.2 and for all months in the Supporting Material).

Data Weighting

In order to reduce the influence of specific missions with a large number of profiles concentrated in a small area and within a relatively short period, a different weight w_i (Section 2.1) is applied on each data point, according to

$$w_i = 1/N_i,$$

with N_i , the number of measurements within the same month and same year, and within a 0.2° radius around the i^{th} data point.

Atmospheric Predictors

Meteorological time series used to analyze the CIL interannual trend are constructed from the ERA-40 (1958–2000; 1.125° resolution) and ERA-interim (1980–2012; 0.75° resolution) reanalysis, provided by the European Center for Medium-Range Weather (ECMWF) data server. The 1958-2012 merged time series are constructed by unbiasing the distinct datasets in order to equal the distinct averages over the overlapping period (1980-2000). Based on previous studies (Oguz et al., 2006; Piotukh et al., 2011; Capet et al., 2012), the time series constructed as potential predictors concern winter (December-March) and summer (May-September) air temperature and wind curl anomalies. For a given year (e.g. 1994), T_w refers to the winter temperature of this year (December 1993 to March 1994) while T_{w-1} refers to that of the previous year (December 1992 to March 1993), and so on.

3.2 Results

Climatologies

Annual and monthly climatologies for CCC and MLD may be found in the Supporting Online Material, both as pictures and NetCDF files. These climatologies are suitable for further use (e.g in modelling studies), and benefit from the general assets of the DIVA interpolation methods (Troupin et al., 2012, 2013). For instance, previous MLD climatologies presented by Kara et al. (2009) does not account for the presence of coast during spatial interpolation, resulting in a contamination of the Black Sea field from profiles issued from the Marmara Sea. In the following, we focus on a few selected analysis to illustrate specific issues of the DIVA detrending tool.

Consistently with the current knowledge of the Black Sea circulation, the annual MLD climatology (Figure 2.2) reveals deeper mixed layer on the periphery of the central basin. Stronger mixing appears clearly all along the shelf break, from the Crimea Peninsula, where the region of convective CIL formation is well marked, to the Bosphorus entrance. On the northwestern shelf, the freshwater input maintains a shallow mixed layer in the vicinity of the river mouths.

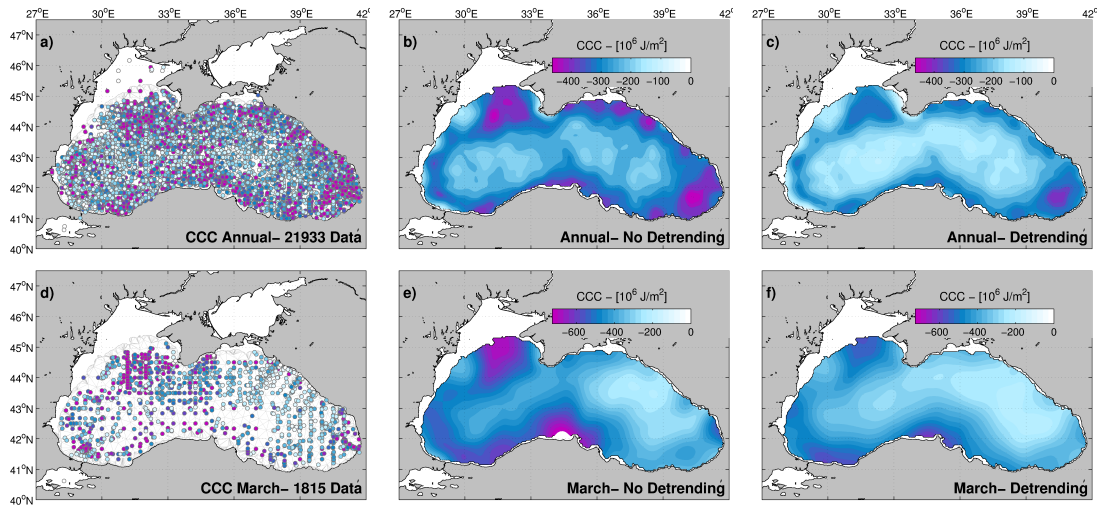


Figure 2.2: Mixed Layer Depth : (a) Values obtained from the vertical profiles and annual climatologies interpolated using DIVA (b) without and (c) with detrending. (d) Values obtained from the vertical profiles for March and monthly climatologies interpolated using DIVA (e) with and (f) without detrending.

The CCC climatologies indicates a region of persistence of the CIL layer located west of the Crimea peninsula, between the shelf slope and the Rim current. During summer, high cold content is maintained along southern peripheral region, where recurrent anticyclonic eddies between the coast and the Rim Current induce a deep halocline level (~ 110 – 140 m) which gives space for the CIL well below the warm surface waters. This is particularly visible in the south-eastern region of the strong semi-permanent Batumi eddy (e.g. Korotaev et al., 2003) located in the easternmost part of the basin. The ratio between CCC in the Rim current zone and the central part is in agreement with the ratio [1.5–2.5] given in Piotukh et al. (2011).

Effects of the Detrending on the Analysis

The magnitude of the CCC interannual variability is slightly higher than that of its seasonal variability. The majority of data has been collected during the period between 1985–1995 which was a "cold" period characterized by low air temperature and high CIL cold content (Oguz et al., 2006; Piotukh et al., 2011; Capet et al., 2012). Because of this distribution, a classic analysis without detrending gives more weight to these years, which results in a bias towards high cold content in the annual and monthly climatologies, not representative of the averaged situation for the period 1955–2011. The detrending procedure corrects this bias as illustrated by the comparison of Figures 2.3b–c and 2.3e–f, showing the annual and monthly climatology for March (see Supporting Online Material

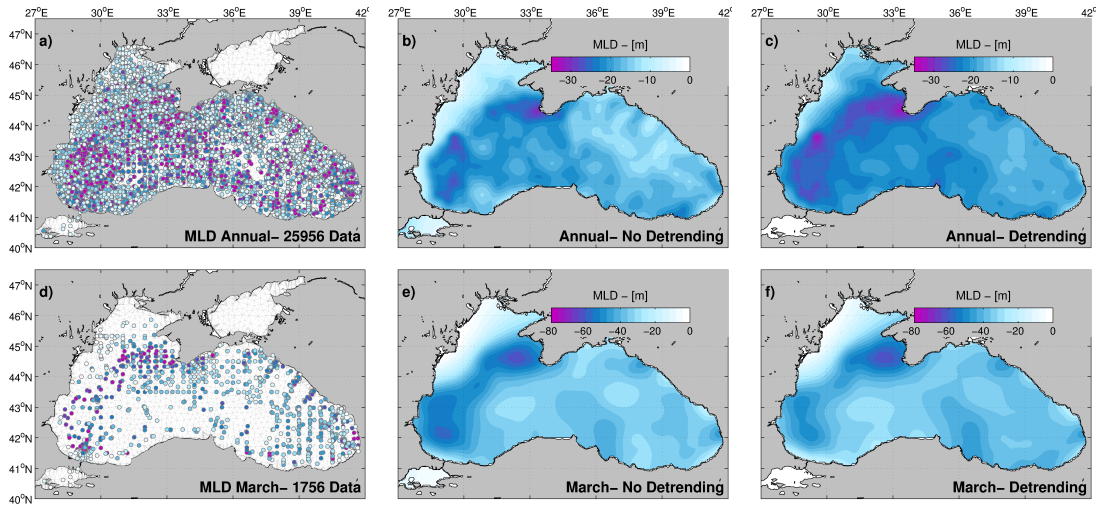


Figure 2.3: CIL Cold Content: (a) Values obtained from the vertical profiles and annual climatologies interpolated using DIVA (b) without and (c) with detrending. (d) Values obtained from the vertical profiles for March and monthly climatologies interpolated using DIVA (e) with and (f) without detrending.

for the others months) obtained with and without detrending. It is also worth mentioning that without detrending, localized CIL minima are introduced to the climatologies: these are artifacts resulting from irregular data distribution across years and are eliminated with the detrending method.

In the case of the MLD, seasonal variability is higher than interannual variability. This example thus illustrates the bias introduced this time by the uneven seasonal distribution of the original data. As more data are available in summer time, when the MLD is small, the classical analysis results in annual climatology fields biased towards small MLD values, which is corrected by the detrended analysis (Figures 2.2b-c). Because of the low interannual variability, with respect to the seasonal variability, the detrending method does not impact much on the monthly climatologies.

Interpretation of the Trends

As a by-product of the climatologies, DIVA provides the trends assigned to each month and each year. The trend corresponding to one class (e.g. a given year) corresponds to the averaged misfit of the data of this class with respect to the overall analysis. Obviously, these temporal trends still bear some representativity error due to the spatial distribution of data, but this error is minimized by the detrending procedure by comparison with the trends that would be obtained from the anomalies with respect to a basin-wide average. In order to consider realistic values rather than anomalies, the time series referred to as “trends” in the following and depicted in Figures 2.4 and 2.5 are obtained by adding the average value of the annual analysis to the trends initially provided by DIVA.

Compared to the time series constructed by simply averaging the data within each year, the present interannual trend allows a better consideration of (1) uneven spatial distribution, because they rely on the misfit with the climatological analysis rather than on the

absolute values, hence consider the spatial variability; (2) uneven seasonal distribution, because seasonal trends are identified simultaneously, during the same iterative procedure. The temporal trends derived from the analysis are therefore appropriate to study the temporal dynamics of the analyzed variable.

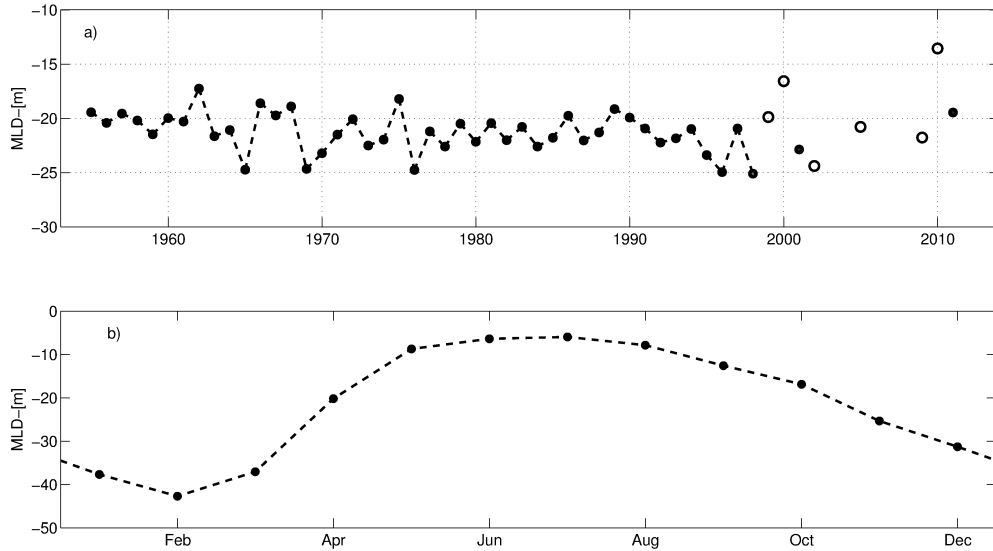


Figure 2.4: (a) Interannual variability of the mixed layer depth as identified by the DIVA de-trending tool over the period 1955-2011, (filled circles : years with more than 50 eligible profiles; empty circles: years with more than 25 and less than 50 eligible profiles). No significant relationship between the annual anomalies and atmospheric predictors may be derived. (b) Climatological seasonal cycle reconstructed by DIVA with detrending.

In the following we use the trends to compare the range of seasonal and interannual variability of CCC and MLD, and assess whether systematic relationships between the interannual trends and atmospheric conditions may be identified.

The seasonal trend is very clear in the case of MLD (Figure 2.4b), revealing the stronger mixing in February, the sharp onset of the thermocline from March to May, and the slower deepening of the mixed layer from August to February.

The seasonal trend of the CCC (Figure 2.5b) indicates the formation season from December to March, and then a first decrease until May, when surface warming erodes the upper layer of the CIL, and then another decrease starting from August when the MLD starts to deepen.

No systematic relationships between the interannual trend of MLD and the selected atmospheric predictors could be identified. This indicates that other factors influence this fast responding dynamic (e.g. wind stress). On the large scale the interannual trend of MLD (Figure 2.4a) depicts a slow deepening from the 60's to mid 90's, and presumably a shallowing afterwards, but the latter is hindered by the lack of data for the last decade. This long term tendency, also visible in the case of CCC (Figure 2.5a), is in agreement with the long term influence of North Atlantic Oscillation on the sea surface temperature (Oguz et al., 2006; Capet et al., 2012).

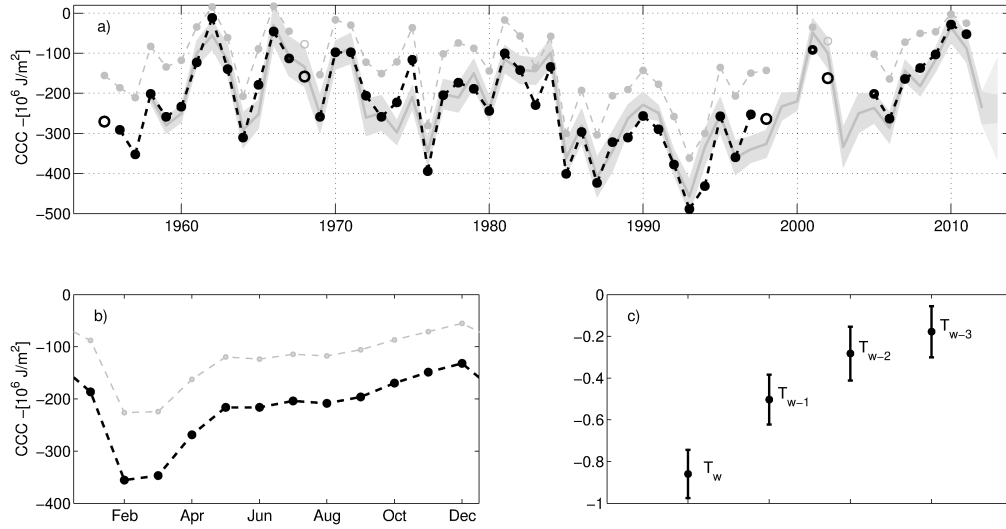


Figure 2.5: (a) Interannual variability of the CIL cold content as identified by the DIVA detrending tool over the period 1955-2011 (black circles and dotted lines) and predicted by a stepwise regression model (plain gray line, the shaded area represents the confidence bounds, $p < 0.01$) using the cumulated anomalies of winter air temperature as predictors. Only the years with more than 50 eligible profiles are considered to compute the regression coefficients (filled circles), other years containing more than 25 profiles are also indicated (empty circles). The explanatory power of past anomalies allows one to infer prediction for the 2013 CIL cold content, assuming average $\pm$ one standard deviation for the unknown T_w value in 2013. (b) climatological seasonal cycle reconstructed by DIVA with detrending (c) Standardized coefficients of the selected predictors: central value, $p < 0.05$ confidence intervals. To allow the comparison with previous works, we indicated on panels (a) and (b) the results obtained by using the historical definition $T_0 = 8^\circ \text{C}$ (gray circles and dotted lines).

The inertial dynamic of the CIL cold content results in a more coherent signal of interannual variability. In that case, a stepwise regression procedure could be used to express the signal as a response to the atmospheric predictors. We found that four years of winter temperature anomaly were significant ($p < 0.05$) in describing the CIL variability, explaining together 88% of the signal obtained from the detrending procedure (Figure 2.5a). Summer and wind curl predictors were discarded as non-significant by the stepwise regression procedure. The preponderance of winter predictors over summer predictors confirms the results of Piotukh et al. (2011). The decreasing standardized coefficients (-0.86, -0.50, -0.28 and -0.18 for T_w , T_{w-1} , T_{w-2} and T_{w-3} respectively, Figure 2.5c) reflect the decreasing influence of past winter air temperature anomalies. Using predictors from past years only ($T_{w-1}, T_{w-2}, T_{w-3}$) explains 20% of the CIL variability, thus giving a partial prediction ability, which was used to infer a prediction interval for the year 2013 by considering the range of average $\pm$ one standard deviation for T_w for the unknown 2013 winter air temperature.

4 Conclusions

A detrending tool is integrated in the DIVA spatial interpolation tool to correct climatology analysis from the bias caused by uneven temporal sampling over a period with substantial temporal variability.

DIVA is applied to the mapping of the mixed layer depth and cold content of the Black Sea CIL. These properties are derived from the vertical profiles available for the period 1955-2011. The comparison of the reconstructed fields obtained with and without detrending illustrates the ability of the method to rectify the monthly climatologies from the bias caused by a higher availability of profiles during the cold 1985-1995 period (CCC example), and the annual climatologies from the bias caused by a higher availability of profiles during the summer period (MLD example).

Moreover, the detrending procedure provides the user with the temporal trends identified to unbiased the spatial analysis. These trends may be used to analyze the temporal variability of the considered variable.

As an example, the information on the interannual variability of the cold content of the Black Sea CIL is exploited to evidence, through a stepwise regression analysis, the cumulative effect of air temperature anomaly. Considered jointly, the winter air temperature anomalies of the four past years explain significantly ($p < 0.05$) up to 88% of the CCC interannual signal. Moreover, the inertial dynamic of the CIL results in a part of explicative power from the past predictors (i.e. air temperature anomalies of the previous years), which gives a partial (20%) predictive ability concerning the CIL intensity for the year to come.

The chosen example demonstrated the effect of the most apparent representativity error: the one issued from the seasonal and interannual variability but the same method could be used for other sources of representativity errors (e.g. diurnal variability, different instruments or protocols, different databases, different observation depths, ...). In the same way that spatial analysis are corrected from uneven temporal distribution, the

temporal trends are partly corrected from the influences of spatial uneven distribution as these are reconstructed from the anomalies between data and the spatial analysis rather than from the anomalies between data and a basin-wide average (see for instance the discussion in (Piotukh et al., 2011) concerning the CCC case). In its present form, however, the detrending procedure still identifies trends which are considered as uniform over the entire spatial analysis domain. This assumption should be carefully considered for large domains where temporal variability may differ across subregions. For instance, in a domain that encompasses the Equator and mid-latitudes, the seasonal trend that will be removed is likely to be too strong for the equatorial region and too weak for temperate latitudes.

Also, the different trends (e.g seasonal, interannual) are considered to be independent and additive. While this constitutes a valid first approximation, it may be expected that seasonal variations between contrasting years differ in reality by more than a simple constant. Extensive analysis, exploiting the interannual trend to identify contrasting periods, may consider partitioned datasets to evaluate the consistency of the overall seasonal trend during these sub-periods.

The relevance of climatological analysis computed over large period affected by temporal variability is a general question, that has to be considered specifically for each application. Appropriately, the detrending tool presented in this study provides, along with the climatological product, the additional temporal information needed to address this question.

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Chapter 3

The Hydrodynamic Model: GHER3D



Ocean Love, Ronnie Landfield, 1981

This chapter provides a description of the hydrodynamical model used in this study. A summary of the model's equations is given before detailing some aspects that have required a particular attention during the set-up of the Black Sea implementation. Model skills are evaluated using satellite and in situ data, and exploiting the vertical properties reconstructed from in situ profiles in Chapter 2.

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1 The GHER model

The physical and hydrodynamical components of the coupled model are resolved by the GHER3D model, developed by the GHER group, University of Liège. The mathematical formulations and numerical characteristics of this model have been initially described in [Nihoul \(1998\)](#) and [Beckers \(1991\)](#). Since its initial development, the GHER3D general circulation model has been successfully applied to numerous oceanographic cases, e.g. in the North Sea ([Delhez, 1996](#)), the Mediterranean Sea ([Beckers, 1991](#); [Barth et al., 2005](#); [Vandenbulcke, 2007](#)) and the Black Sea ([Grégoire et al., 1998](#); [Beckers et al., 2002](#); [Grégoire and Friedrich, 2004](#); [Vandenbulcke et al., 2009](#)).

1.1 Equations

The GHER3D model solves the prognostic variables of salinity, temperature, sea surface elevation, turbulent kinetic energy and horizontal components of the velocity. The approximations of hydrostaticity (local vertical instabilities are considered to mix instantly), Boussinessq (density variations are much smaller than the average density and do not affect inertia), and β -plane (the curvature of earth is locally neglected), allows to simplify the equations of Navier Stokes to the following forms:

$$\nabla \cdot \mathbf{v} = 0 \quad (3.1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{u} + f \mathbf{e}_z \wedge \mathbf{u} = -\nabla_h q + \frac{\partial}{\partial z} \left(\tilde{\nu} \frac{\partial \mathbf{u}}{\partial z} \right) \quad (3.2)$$

$$\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T = \frac{\partial}{\partial z} \left(\tilde{\lambda} \frac{\partial T}{\partial z} \right) + \frac{1}{c_p \rho_0} \frac{\partial I}{\partial z} + \kappa_h \nabla_h^2 T \quad (3.3)$$

$$\frac{\partial S}{\partial t} + \mathbf{v} \cdot \nabla S = \frac{\partial}{\partial z} \left(\tilde{\lambda} \frac{\partial S}{\partial z} \right) + \kappa_h \nabla_h^2 T \quad (3.4)$$

$$\frac{\partial k}{\partial t} + \mathbf{v} \cdot \nabla k = \tilde{\nu} \left\| \frac{\partial \mathbf{u}}{\partial z} \right\|^2 - \tilde{\lambda} \frac{\partial b}{\partial z} - \epsilon + \frac{\partial}{\partial z} \left(\tilde{\nu} \frac{\partial k}{\partial z} \right) \quad (3.5)$$

Where f represents the Coriolis frequency, $\mathbf{v}$ is the velocity vector, whose horizontal part is noted $\mathbf{u}$, T is the temperature, S the salinity, k the turbulent kinetic energy and ϵ its dissipation. c_p is the heat capacity of the water, ρ_0 the reference density, I is the insolation (see below) and $\tilde{\nu}$ and $\tilde{\lambda}$ are the eddy viscosity and diffusivity. κ_h represents horizontal diffusivity and is introduced to ensure the numerical stability of the model.

q is the generalized pressure defined by

$$q = \frac{p}{\rho_0} + gz \quad (3.6)$$

with g the gravitational acceleration, b is the buoyancy given by the state equation

$$b = -\frac{\rho(T, S) - \rho_0}{\rho_0} g \quad (3.7)$$

and linked to the generalized pressure by

$$\frac{\partial q}{\partial z} = b \quad (3.8)$$

The resolution of vertical turbulence uses a k turbulent kinetic energy closure scheme described in Nihoul et al. (1989); Delhez et al. (1999). The evolution equation for ϵ is replaced by an algebraic equation. It requires to specify the mixing length l_n , which is assumed to depend only on the geometry of the basin (Beckers, 1991).

Horizontally, the GHER model uses Cartesian coordinates and is discretized using a conventional Arakawa C-grid, where velocities are defined at the grid cell boundaries, and the scalar variables are defined at the center of each grid cell. This immediately yields the advection and the pressure gradient terms, while requiring an averaging operation for the Coriolis term, and is thus well adapted to models with a relative high resolution.

Vertically, the model uses a double σ coordinate system. This consists in splitting the domain into two superposed regions, the limit between them being placed at the average shelf break depth (120 m in our simulations). In each of those regions, a normal σ transform is applied. The double σ transform allows to represent abrupt bathymetry breaks if they are located at the prescribed depth.

The model has a semi-implicit integration scheme which is conservative for tracers. Furthermore, it uses mode splitting, a now common practice: for computational efficiency, the barotropic time step, used to solve the vertically integrated equations, is much (60 times) smaller than the baroclinic time step. This approach is justified by the fact that the barotropic mode describes essentially fast processes, while the baroclinic modes are more representative of slow processes.

1.2 Surface Fluxes

Atmospheric fluxes of momentum (wind stresses), heat and fresh water are computed interactively at each time step, considering the state of the sea surface and the atmospheric conditions.

Atmospheric data used to force the model are issued from the ECMWF¹ Two sets are exploited :

- ERA-40 reanalysis, available during 1958-2001, on a 1.125° grid at a resolution of 6-hour.
- ERA-Interim reanalysis, available during 1980-present, on a 0.75° grid at a resolution of 6-hour.

The relevant fields encompass winds velocities at 10 m, air and dew point temperature at 2 m, sea level pressure, precipitations and cloud cover.

¹European Center for Medium-Range Weather Forecasts (<http://www.ecmwf.int/>).

Atmospheric fields are filtered in order to suppress the erroneous influence of land atmospheric conditions on the coastal grid cells (Kara et al., 2007). Terrestrial conditions are affected by orographic constraints and land albedos and therefore differ from the marine conditions. The filter consists in replacing the land point values by extrapolated oceanic values before interpolating atmospheric products from their original grid to the model grid. It allowed a significant reduction of the error of sea surface temperature in coastal areas (Kara et al., 2007).

While spatial interpolation is achieved during the model simulation using a bilinear interpolation scheme, wind components are downscaled beforehand to 0.2° by spline interpolation, which allows for a better conservation of the wind curl, hence a better representation of the Black Sea circulation features.

As atmospheric fields over the Black Sea have been extensively described in earlier studies we refer to Kara et al. (2007, 2005) for comments about the ECMWF products over the Black Sea. A detailed analysis of the recurrent weather patterns affecting the Black Sea and their relationship with large scale atmospheric teleconnection systems is presented in Chapter 4.

Momentum

The wind stress τ_w , i.e. the entraining effect of wind on surface waters, is obtained by:

$$\tau_w = C_D \rho_a \|\mathbf{u}_w\| \mathbf{u}_w \quad (3.9)$$

with ρ_a the air density, and $\mathbf{u}_a$ the wind velocity at 10 m. The drag coefficient C_D is parameterized according to Kondo (1975).

Heat

Heat fluxes sum the contributions of short and long waves radiative fluxes, sensible and latent heat fluxes. Here, these fluxes are computed interactively rather than imposed from external sources, and thus account for the actual state of the sea which prevents the inconsistencies that may result from imposed fluxes (Staneva et al., 1995).

Surface shortwave radiation Radiative heating represents the main energy input into the ocean. The important contribution of shortwave radiations to the thermal stratification of the Black Sea, hence the need of a precise insolation penetration scheme was underlined by Kara et al. (2005).

Insolation at the surface, Q_s , is obtained from the solar zenith angle, θ , and the fractional cloud cover (Rosati and Miyakoda, 1988). The absorption of light in the water column results in a volume heat source. Because of the great importance of light vertical distribution in biogeochemical applications, the light penetration scheme is further developed for the biogeochemical model. As this refinement involves state variables specific to the biogeochemical module (absorbing and diffusive materials), this detailed light absorption scheme is presented in Chapter 5. Purely hydrodynamical simulations rely on the

following simplified scheme. Solar incoming radiation is subdivided, with fixed proportions, amongst three band widths : infrared (IR), long (l) and short (s) waves, each with specific attenuation coefficients (Zielinski et al., 2002). Because this optical model assumes fixed sea water optical properties, the volumetric distribution of the surface insolation is computed only once at the beginning of the simulation.

At a depth z , the radiative flux is thus given by

$$I(z) = |Q_s| [(p_{IR}) \exp(k_{IR}z) + (1 - p_{IR}) \cdot ((p_l) \exp(k_l z) + (1 - p_l) \exp(k_s z))] \quad (3.10)$$

with $z = 0$ at the surface and negative in the water column, p_{IR} (0.54) is the fraction of infrared solar energy, and p_l (0.63) the fraction of long-wave radiation amongst the $(1 - p_{IR})$ visible part. k_{IR} (4 m^{-1}), k_l (0.23 m^{-1}) and k_s (0.09 m^{-1}) are the attenuation coefficients in the infrared, long- and short-wave solar energy respectively.

Net long-wave radiation This contribution to the heat flux is the sum of upward long-wave radiation of the ocean and downward long-wave radiation of the atmosphere. The former is generally larger than the latter, leading to a net loss from the ocean to the atmosphere. The net long-wave radiation is calculated following the scheme of Clark et al. (1974):

$$Q_b = \epsilon \sigma T_s^4 (1 - 0.8C^2) (0.39 - 0.05\sqrt{e_a}) + 4\epsilon \sigma T_s^3 (T_s - T_a) \quad (3.11)$$

where ϵ is the emissivity of the ocean, σ the Stefan-Boltzman constant, e_a the atmospheric vapor pressure in hPa and T_a the air temperature at a reference level.

Latent and sensible heat fluxes Latent heat flux is the heat transfer resulting from evaporation or condensation processes. It is equal to the rate of evaporation times the latent heat of evaporation.

$$Q_L = C_H L \rho_a \|w^*\| (q_s - q_a) \quad (3.12)$$

where ρ_a is the air density, $\|w\|$ the scaled wind velocity, L the latent heat of evaporation, q_a the specific humidity of air, and q_s the specific humidity of saturated air at sea surface temperature, T_s .

The sensible heat flux is due to the temperature difference between the air at the ocean surface and the air at the reference level. It is expressed as

$$Q_S = C_H c_{p_a} \rho_a \|w^*\| (T_s - T_a) \quad (3.13)$$

where c_{p_a} is the heat capacity of air and T_a the temperature of air.

Both sensible and latent heat fluxes depend on the turbulent exchange coefficients C_H , parameterized according to Kondo (1975).

Because we did not consider corrective terms in our simulations (“nudging”), and used the model for long simulations (several decades), it appeared necessary to scale the $\|w\|$ factor in the expression of these heat exchanges. The initial formulations (Rosati and Miyakoda, 1988) effectively rely on in-situ wind expressions, whereas the forcings used in

the model consist in spatially and temporally averaged wind speeds, significantly reducing the magnitude $\|w\|$.

While this issue has been further stressed for the exchanges of gasses at the sea surface (Chapter 7), an accurate estimation of the the scaling factor c_w to be applied to the effective wind speed $\|w^*\| = c_w \|w\|$ for different resolution of the original wind forcing $\|w^*\|$ has not been exhaustively investigated.

Rather, we compared several values of c_w and assessed the corresponding model skills in resolving the Sea Surface Temperature (SST) and the generation of the Cold Intermediate Layer (CIL) by confronting model results against observations. Given the resolution of the forcings used for this study, the value of $c_w = 1.4$ yielded the best results.

Freshwater

Mass transfers resulting from evaporation, condensation and precipitation are not considered in the model. These processes however impacts on the freshwater balance and are represented as pseudo-fluxes of salinity, prescribed in accordance with the computed latent heat fluxes.

2 Numerical Implementation in the Black Sea

The present implementation is designed to be coupled with the biological model and to be used for long term simulations (multi-decadal) and scenario projections, Also, the objective of this study is to resolve the processes driving the seasonal and interannual variability, rather than to reproduce exactly the occurrence of events of small spatial and temporal scales.

Given these objectives, the model has to be free of systematic drifts, without relying on “nudging” (relaxation terms towards *a priori* climatologies) or data assimilation as this would hamper the model reliability for scenario runs. While data assimilation could have resulted in more precise simulations for the years with a significant availability of data, we favored in general the ‘data free’ approach, designing for each study cases specific validation procedures asserting the relevance of the model for each specific application.

2.1 Domain and Bathymetry

The bathymetry, initially taken from [Smith and Sandwell \(1997\)](#), was adapted for a proper use of double σ coordinates. The major problems to face are the numerical instabilities assoicated with very thin cells, and the interpretation of horizontal gradient for adjacent cells on a very steep slope, such has the Black Sea shelf break.

In the present implementation, the limit between the upper and lower σ region is fixed at 120 m, with twenty levels in the first layer giving a average vertical resolution of 1 m in the surface, and eleven levels for the deeper waters.

The very thin cells are avoided by fixing a minimum bathymetry of 15 m, as well as a 30 m minimum difference for the first layer of the second σ zone.

Using double- σ vertical coordinates, rather than simple σ coordinates, allows to avoid major spurious horizontal gradient problems related to the strongest slopes at the shelf break (Deleersnijder and Beckers, 1992). However, errors remain wherever strong slopes are present. These cases can be characterized by checking where the depth difference between two adjacent cells strongly exceeds the average height of those cells, that is, where the proportion

$$\alpha = \frac{z(i) - z(i+1)}{\Delta z(i+1/2)} \gg 1 \quad (3.14)$$

, where $z(i)$ is the depth of a particular cell, $\Delta z(i)$ the cell's height and the indexes j and k are omitted.

The resulting spurious gradients are avoided by filtering the bathymetry. We recursively smoothed the bathymetry for the couples of points showing the greater diagnosed α , until no adjacent cells present an α upper than a given threshold, fixed to 2 in this study. This filtering leads to small modifications of the real bathymetry, but it allows to minimize the consequences of a known problem of sigma coordinates applied to steep slope areas, while ensuring volume conservation and avoiding to smooth the bathymetry where it is unnecessary.

2.2 Open Boundaries

The enclosed character of the Black Sea greatly helps to solve the issue of boundary conditions. However, a few openings remains that have to be addressed.

For simplicity and due to the difficulties to find appropriate data we have chosen not to take into account exchanges with the Azov Sea, so the Kerch strait is considered to be closed.

Rivers

The river fluxes of the six main rivers, Danube, Dniepr, Dniestr, Rioni, Kizilmark and Sakarya, are imposed on a monthly basis. Annual flows for the Black Sea main rivers and their average seasonal repartition were obtained from the SESAME European integrated project. The dataset concerns the period 1960–2000 and is constructed by combining direct fluxes measurements, precipitation data and hydrographic modelling (Ludwig et al., 2009). River flows after 2000 were reconstructed from national flow data gathered by the Black Sea Commission.

The Bosphorus

The representation of Bosphorus exchanges is a delicate issue in the set-up of a Black Sea 3D model as it is an essential component of the hydrodynamic system and is characterized by very small scales and strong gradients. The objective here is to represent at best its

implication in the Black Sea system, i.e. its role in the water and salt budgets, its role in sustaining the vertical position of the halocline and the so-called Bosphorus plume entrainment of surface water in deeper layer.

In their MOM implementation, [Staneva and Stanev \(1998\)](#) base the parametrization of Bosphorus exchanges on the conservation of the Black Sea water content. The barotropic transport at the strait is inferred from the fresh water balance, smoothed in time, while an undercurrent is computed based on the conservation of the salt content, which affects salinity but does not imply correction on momentum. The resulting plume behavior is driven by a specific convective sinking scheme detailed in [Stanev et al. \(1997\)](#), and tuned to match observation data regarding depth of penetration of the plume in the central basin. The use of z vertical coordinates implies the need of a convective sinking scheme to avoid excessive mixing associated to the sinking of the Bosphorus plume, which is less critical in terrain following vertical coordinates.

In the Black sea implementation of the HYCOM model ([Kara et al., 2005](#)), the basin is totally closed and river and Bosphorus fluxes are imposed as buoyancy fluxes at the surface, using the air-sea buoyancy framework fluxes used for the representation of evaporation/precipitation on the rest of the sea surface. The Bosphorus flow is imposed using monthly climatological values taken from [Staneva and Stanev \(1998\)](#). The resulting behavior of the Bosphorus plume is driven by the K-Profile parametrization included in the model, as no specific sinking scheme has been introduced for this Black Sea implementation. The result is a vertical buoyant plume in the vicinity of the Bosphorus Strait which sinks vertically from the surface to the bottom and then behaves as a gravity flow until depths of 100m. The author mentions the fact that this representation helps in maintaining the stratification of the Black Sea.

In their more recent study [Grayek et al. \(2010\)](#) use a more complex approach based on assimilation of surface altimetry to quantify the exchanges at the Bosphorus entrance.

The parametrization used in the present study has been chosen regarding the constraints and objectives detailed in the introduction of this section. The barotropic flux imposed at the Bosphorus Strait is computed based on the difference between the surface elevation at Bosphorus entrance with a fixed reference value, such that the Bosphorus outflow finally controls the long term stability of the average surface elevation, hence the total water content. The computed flow is not applied directly but imposed as a correction with a relaxation timescale of 1 month to enforce stability. This parametrization allows the delay needed for the seasonal excess fresh water balance due to river discharges to reach the Bosphorus entrance, and thus allows a seasonal signal to develop in the global average sea surface elevation, while ensuring total volume conservation at a longer timescale.

For the baroclinic repartition of this flux a fixed profile of horizontal velocities is imposed representing 2 flows of opposite sign : surface outgoing flow and bottom incoming thinner incoming flow. A vertically homogeneous bias is added to this velocity profile, thus shifting the balance between the amount of incoming and out coming water, to match the imposed barotropic transport.

The salinity $S_{B,in}$ imposed to the entering waters is then computed in order to ensure

a conservation of the basin total salt content,

$$S_{B,in} \cdot Q_{B,in} + F_{B,out} \cdot Q_{B,out} + P = 0, \quad (3.15)$$

where the incoming Bosphorus flow $Q_{B,in}$, the outgoing flux of salt $F_{B,out}$, and the salt pseudo-flux P due to precipitation and evaporation overall the basin's surface are diagnosed at each time step.

The fact that the Black Sea altimetry and the volume mean salt content does not show significant trends for the last hundred years (Staneva and Stanev, 1998) justifies the decision to base this parameterization on the conservation of total volume and total salt content. This representation maintains the average level of the halocline for multi-decadal simulations, but is flexible enough to allow for inter-annual variations.

3 Skill assessment

The model skills in reproducing the Black Sea hydrodynamics are assessed by confronting the model results to satellite and in situ data. In order to account for the uneven distribution of in situ observations, and the impact it could bear on averaged values, the model results are considered where and when observations are available. The model correspondences to in situ observations are obtained by spatial interpolation of the corresponding weekly average.

The objective of these validation procedures is not only to quantify the model's skills but also to provide some qualitative description of the main error sources. The skills of both low and high resolution implementations are discussed hereafter.

3.1 Target Diagrams

An extensive literature exists on the qualification and quantification of models errors (e.g. Allen et al., 2007; Stow et al., 2009). Graphical summary representation, such as proposed by Taylor (2001), provides a uniform and integrative approach by allowing to overview several metrics in a glimpse. In the following we opted for target diagrams (Jolliff et al., 2009), which distinguish the contribution of the average bias (B), and the Centered Root Mean Square Difference ($CRMSD$), to the Root Mean Square Difference ($RMSD$) by exploiting the relationship $RMSD^2 = B^2 + CRMSD^2$, with

$$B = \bar{m} - \bar{o} \quad (3.16)$$

$$RMSD = \sqrt{\frac{1}{N} \sum_{n=1}^n [m_n - o_n]^2} \quad (3.17)$$

$$CRMSD = \sqrt{\frac{1}{N} \sum_{n=1}^n [(m_n - \bar{m}) - (o_n - \bar{o})]^2 \cdot \text{sign}(\sigma_m - \sigma_o)} \quad (3.18)$$

where m_n are the model correspondences to the observations o_n . $\bar{x}$ represents the average $\frac{1}{N} \sum_{n=1}^n x$, and N is the number of observations.

In order to provide comparable metrics for different variables, these are normalized by the standard deviation of the observations, $\sigma_o = \sqrt{\frac{1}{N} \sum_{n=1}^n [o_n - \bar{o}]^2}$. We thus consider the normalized values $B^* = \frac{B}{\sigma_o}$, $RMSD^* = \frac{RMSD}{\sigma_o}$ and $CRMSED^* = \sqrt{1 + \sigma^{*2} - 2\sigma^* R} \cdot \text{sign}(\sigma_m - \sigma_o)$, with $\sigma^* = \frac{\sigma_m}{\sigma_o}$.

$RMSD^*$ is then equivalent to the model efficiency (Jolliff et al., 2009), for which a value greater than 1 indicates that, in terms of prevision, an average of the observations performs better than the model. The sign given to $CRMSED$ and $CRMSED^*$ indicates whether the variability around average is over-estimated ($CRMSED > 0$) or under-estimated ($CRMSED < 0$) by the model.

3.2 Satellite Sea surface temperature

Chapter 4 provides the details on the satellite surface temperature datasets. It includes a detailed assessment of the model skill in reproducing the interannual variability of sea surface temperature, isolated by removing from the interannual series climatological daily fields. Here we use this reconstructed climatological cycle to characterize the model skill in resolving the seasonal variability of SST.

First we address the question: How well does the model resolve the spatial pattern of SST, and how does this change along the season? To answer this question, we compute the target diagram statistics on each daily field.

In order to have a stable reference, the metrics are normalized by the spatial standard deviation, averaged in time, assessed from the reconstructed daily satellite climatologies : $\sigma_{O,spat.} = \frac{1}{N_Y} \sum_{d \in Y} \sigma_{O,spat.}(d) = 0.77^\circ\text{C}$, where Y represents every Julian day of the year, and N_Y the number of its elements.

The normalized target diagrams on Fig. 3.1 a,b shows $CRMSED^*$ values that are always smaller than 1, indicating an good performance in reproducing the spatial pattern, and systematically positive, indicating larger departures from the average value in the model than in the satellite data or, in other terms, that the model depicts stronger gradients.

In summer, $RMSD^*$ is higher than one due to a negative bias, larger than the average $\sigma_{O,spatial}$ in absolute value. The unnormalized target diagram (Fig. 3.1 c,d) provide a quantification of this bias which reach a maximum underestimation of -1.25°C (resp. -1.13°C) in summer in the high (resp. low) resolution case. This figure compares the RMSD between model and satellite data with the RMSD obtained between satellite products and in situ observations ($= 0.65^\circ\text{C}$, Nardelli et al. (2010)).

The next question is: How does the model resolve the seasonal cycle, and does this change spatially? To answer this question the statistics are computed for each grid cell (model results are interpolated on the satellite products grid) and normalized using the temporal standard deviation, averaged spatially: $\sigma_{O,temp.} = \frac{1}{N_X} \sum_{\vec{x} \in X} \sigma_{O,temp.}(\vec{x}) = 6^\circ\text{C}$, where X is the spatial domain.

The seasonal variations are pretty well resolved basin-wide (given the large seasonal

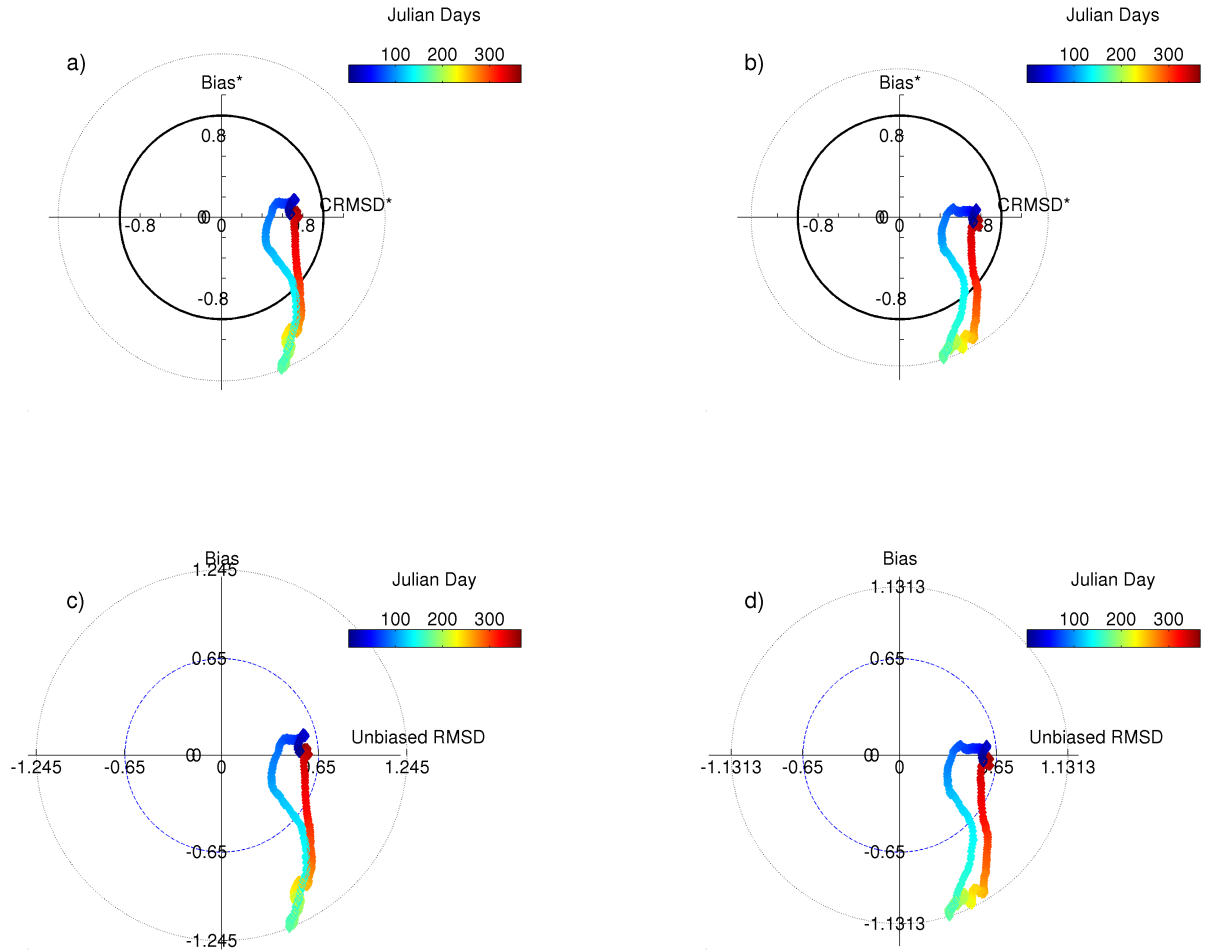


Figure 3.1: Target diagram indicating the model skill to resolve the spatial variability of SST. (a) Normalized diagram for the high resolution model, (b) normalized diagram for the low resolution model, (c) unnormalized diagram for the high resolution model, (d) unnormalized diagram for the low resolution model.

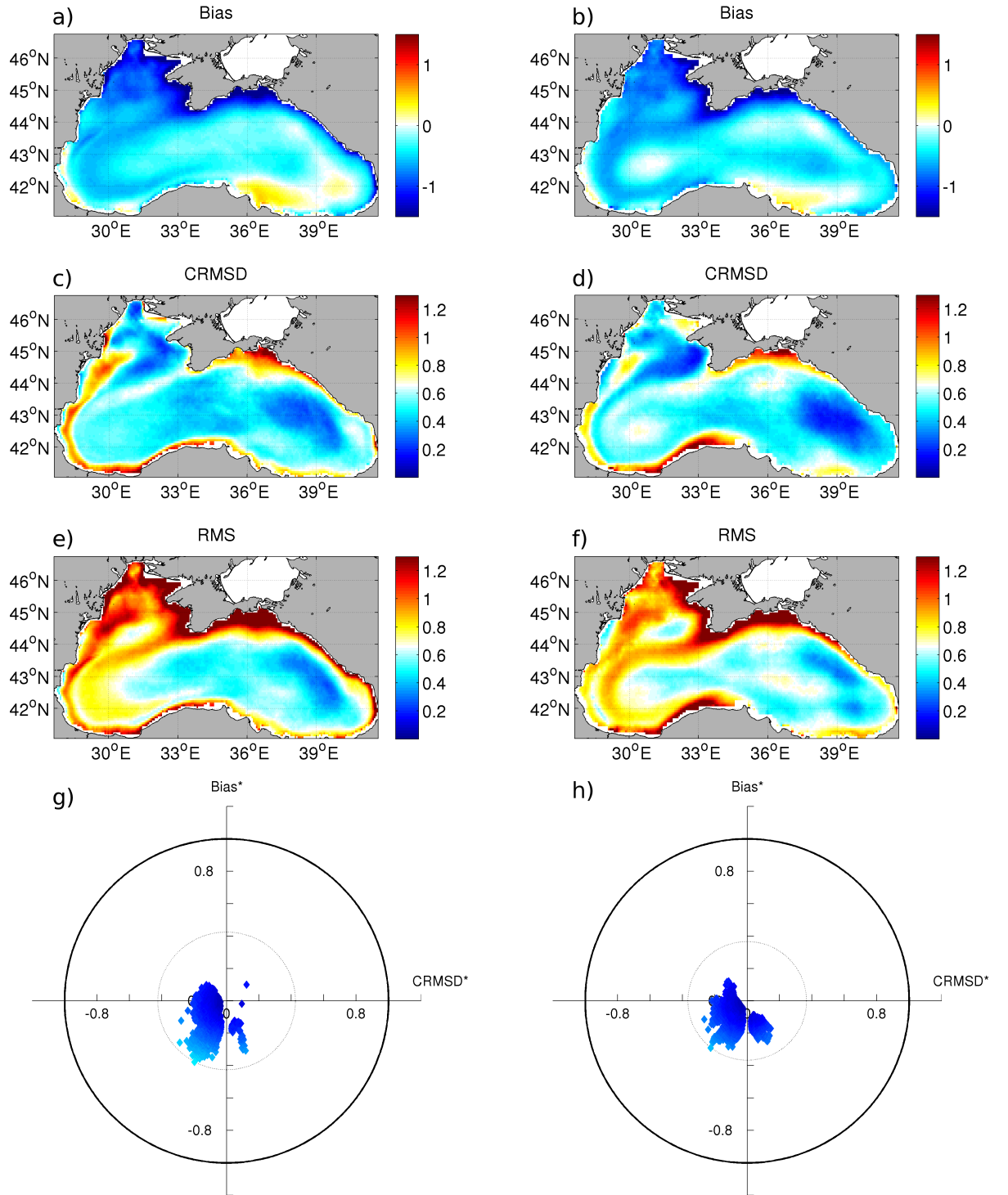


Figure 3.2: Spatial distribution of the seasonal model skills for SST. (a) Average bias, (c) Centered Root Mean Square Difference, (e) Root Mean Square Difference, (g) Normalized target diagram for the fine resolution model. (b), (d), (f), (h): Idem for the low resolution model.

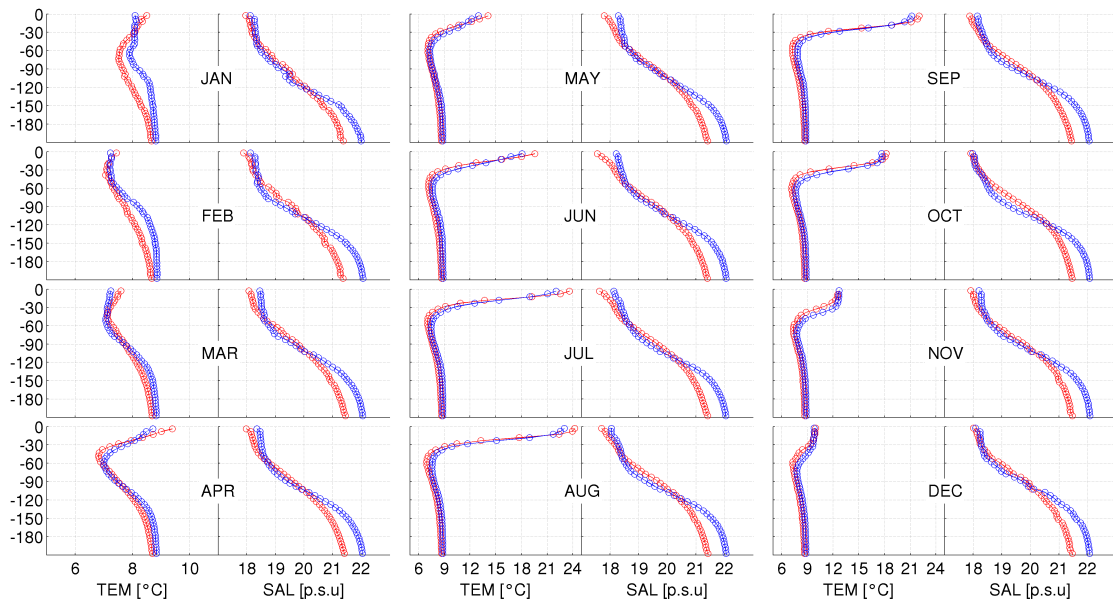


Figure 3.3: Monthly vertical profiles of temperature and salinity in the central basin reconstructed from observations (red) and results from the coarse model (blue).

range). The RMSD (Fig. 3.2) is impacted by an important bias along the northern coast, supposedly revealing some persisting inconsistencies in the atmospheric forcings, and from large CRMSD indicating some temporal mismatch (1) along the southern branch of the Danube plume, that flows along Romanian and Bulgarian coast, and (2) in front of the Kerch strait, that links the Black Sea to the Sea of Azov.

3.3 In situ temperature and salinity

The salinity and temperature data gathered in Chapter 2 are used to reconstruct the vertical profiles in the open basin (Fig. 3.3) and NWS (Fig. 3.4) in order to illustrate the model skills regarding vertical structures.

Visual appreciations of these graphics picture a "pretty good agreement" between model and observations. Specific features such as the depths of thermocline, CIL layers and halocline are resolved accurately, both for the NWS and open basin regions. Seasonal variations of the temperature profiles are consistent both in the surface and subsurface layers (see for instance the CIL reformation on Fig. 3.3). Some mixing issues are however indicated by small discrepancies between the salinity profiles, most marked in the case of the winter months on the northwestern shelf.

3.4 Reconstructed vertical properties

As the physical model is intended to be used for coupled implementations an objective focus is set on key processes of the hydrodynamical-biogeochemical coupling.

We therefore use the vertical properties reconstructed from in situ observations in Chap-

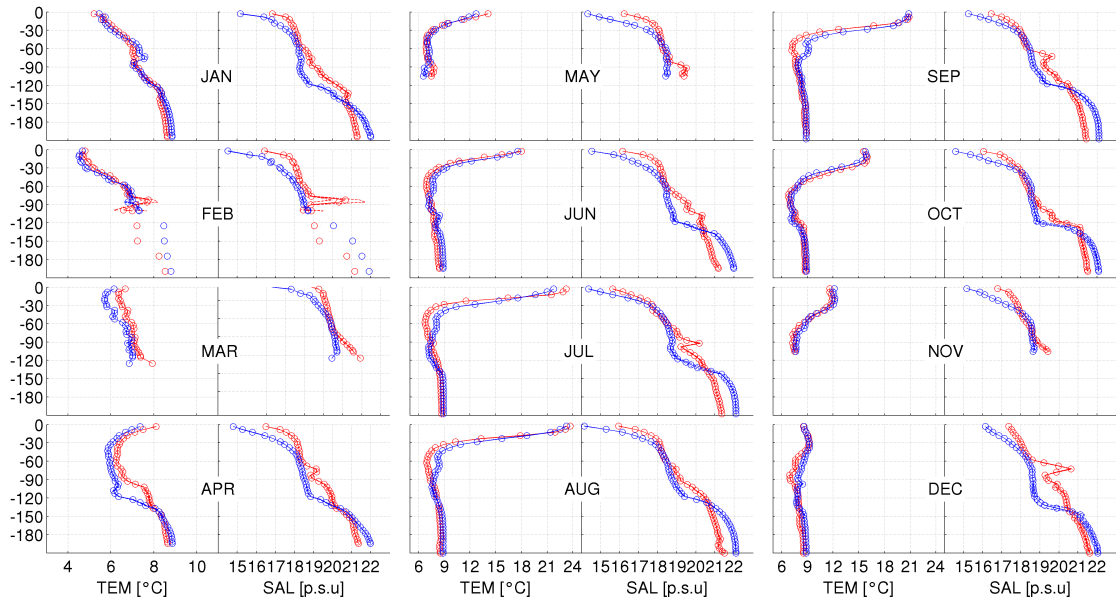


Figure 3.4: Monthly vertical profiles of temperature and salinity in the NWS reconstructed from observations (red) and results from the coarse model (blue).

ter 2, and follow the same methodology to reconstruct these properties from the model results.

The seasonal (resp. interannual) temporal variability is addressed by comparing the medians of data contained in each monthly (resp. annual) bin. Target diagrams in Fig. 3.5, 3.6, 3.8, picture the models skills normalized using the temporal standard deviation of the monthly (resp. annual) medians of observations.

Spatial variability is addressed by comparing the monthly climatologies obtained in Chapter 2 to those issued from the model simulations. Again, the reference deviation is taken as the average of the spatial standard deviations observed for each month.

Mixed layer depth

Mixing occurs earlier on the shelf than in the open basin (Fig. 3.5, 3.6).

Despite a small overestimation by the model, the seasonal variability is well resolved for the shelf part. In the open basin, even if the correlation is good, a marked overestimation in January-February-March affects the overall seasonal skill.

Inversely, the skill to represent the interannual variability appears higher in the open basin than in the NWS region.

The linear relationship that appears between B and $CRMSD$ on Fig. 3.7 reflects that the stronger bias is locally confined and not distributed basin-wide: strong bias at this location causes a larger spatial gradient, and consequently, a larger summed squared distance between each pixel and the spatial average.

Visual comparison of the climatologies (Fig. 3.7) locates this overestimation in the

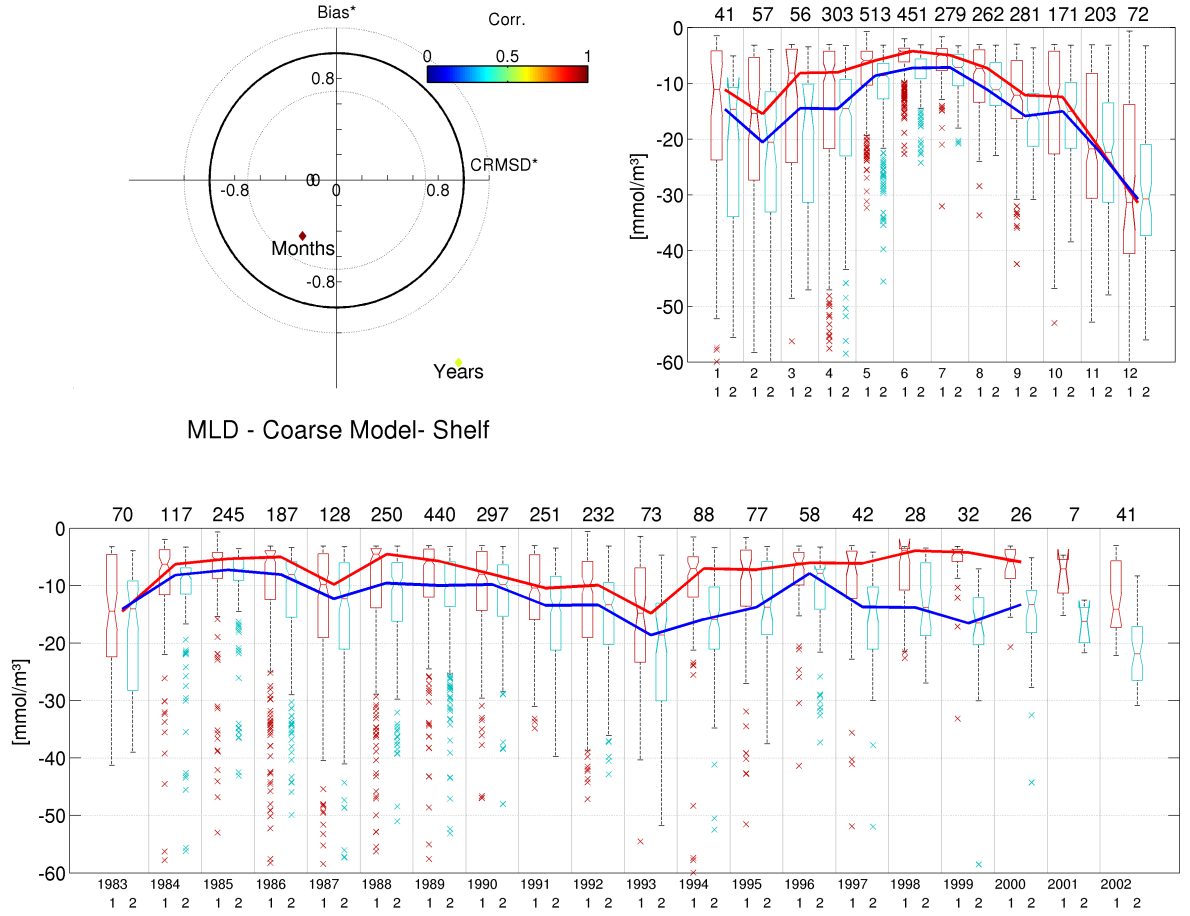


Figure 3.5: Mixed Layer depth: Temporal model skills for the NWS region. (a) Normalized target diagram. (b) Monthly variability from model (blue) and observation (red), number above the panel indicates the number of observations for each month. (c) Monthly variability from model (blue) and observation (red). Numbers above the panels (b) and (c) indicates the number of observations for each month.

periphery of the central basin. Despite the quantitative discrepancies, the location of extrema is qualitatively reproduced, i.e. the larger mixed layer depth along the NWS break, in particular West of the Crimea peninsula.

CIL cold content

Figure 3.8 and 3.9 indicates an overestimation of the summer erosion of the CIL layer, balanced by a strong formation process. As a result of this balance the interannual variability is fairly well reproduced, while depicting a persistent underestimation.

Spatially (Fig. 3.9), the area of CIL formation appears well located, while some mismatching dynamic of the Batumi eddy (1.1) prevents the early spreading of the CIL in the south-eastern part of the basin. The faster erosion of the CIL in the Bosphorus plume location in June is well reproduced by the model.

Interestingly, a bulk of CIL cold content persisting between the shelf break and the Rim

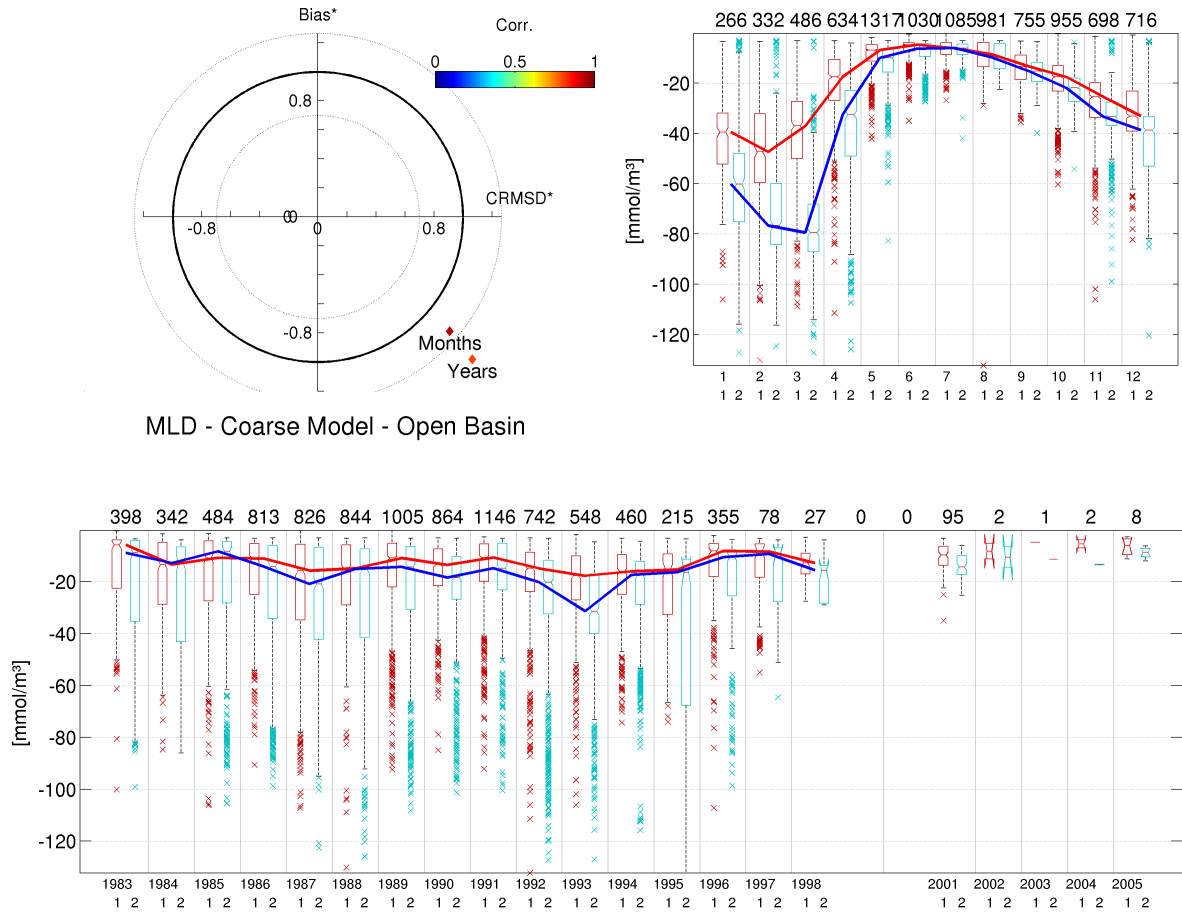


Figure 3.6: Mixed Layer depth: Temporal model skills for the open basin region. (a) Normalized target diagram. (b) Monthly variability from model (blue) and observation (red), number above the panel indicates the number of observations for each month. (c) Monthly variability from model (blue) and observation (red). Numbers above the panels (b) and (c) indicates the number of observations for each month.

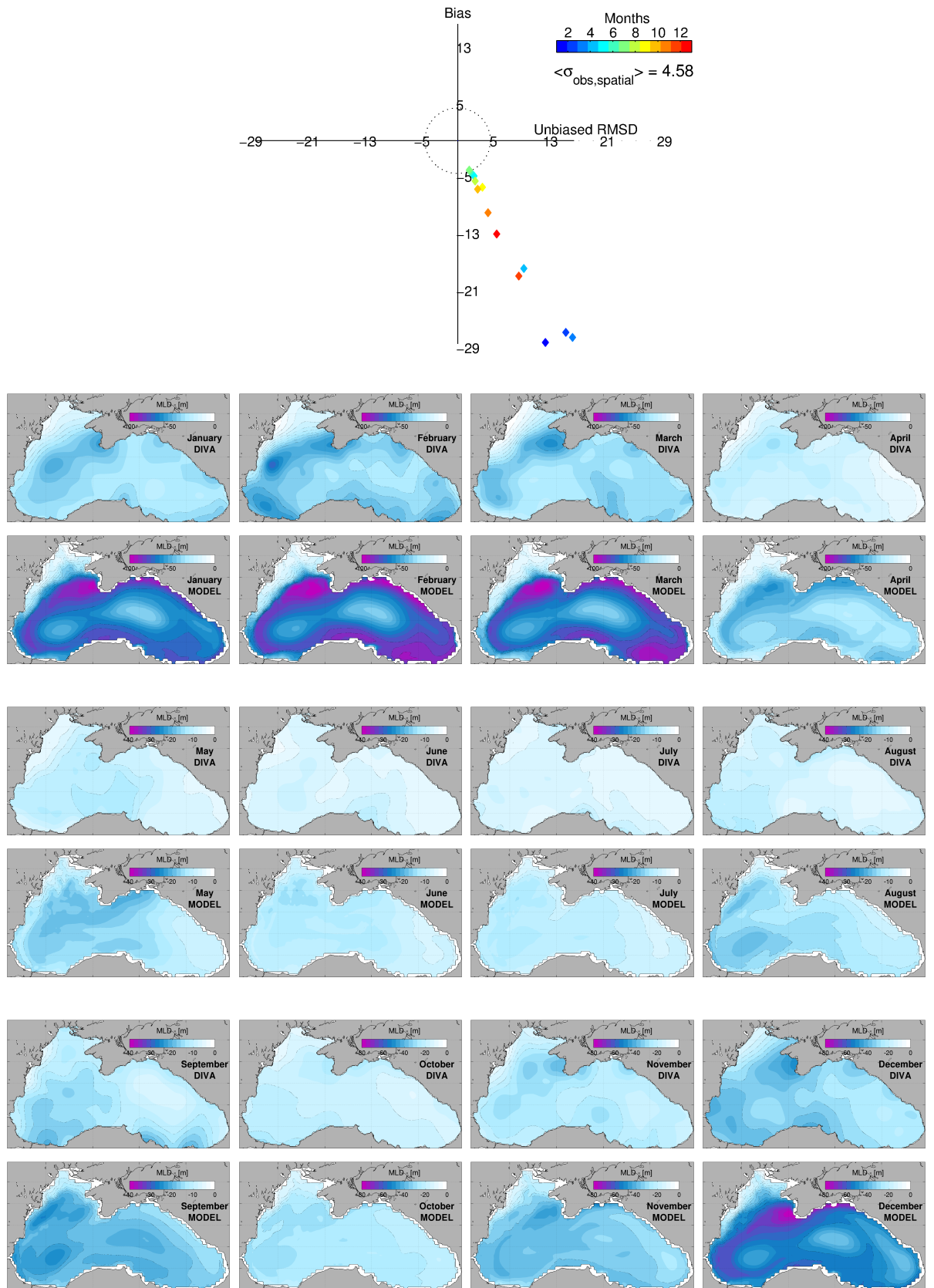


Figure 3.7: (Top) Target diagram representing the spatial skill for each month : Mixed layer depth. (Lower Panels) Monthly climatologies obtained from (DIVA) Chapter 2 and (MODEL) coarse grid model simulations.

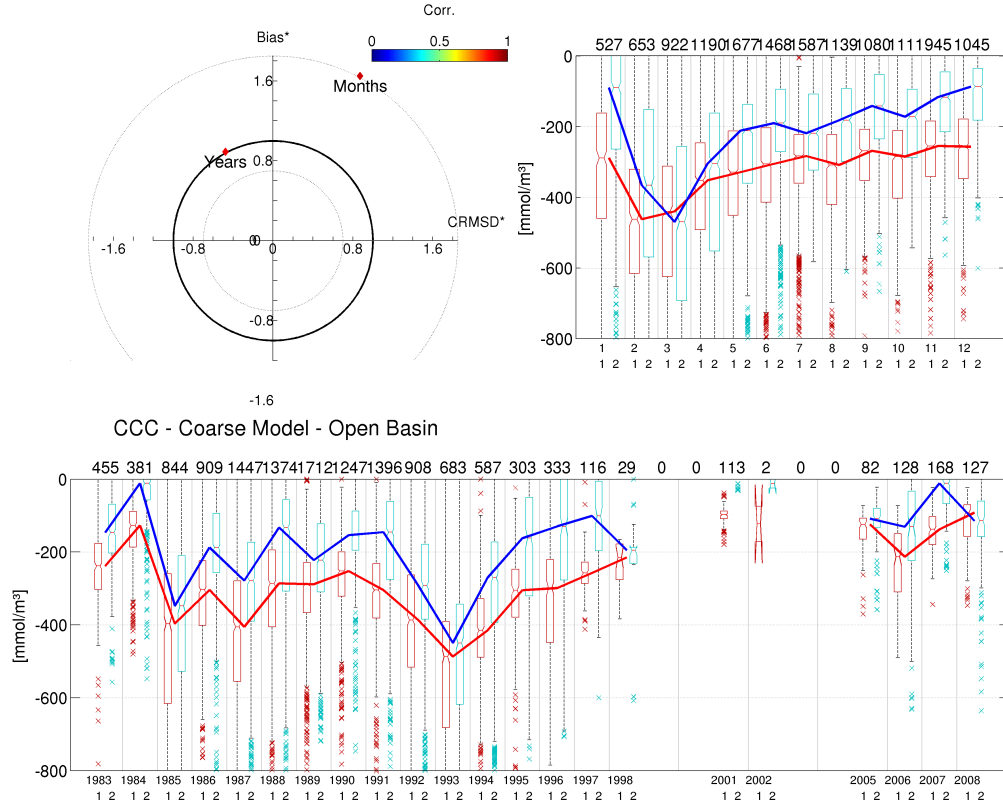


Figure 3.8: CIL cold content: Temporal model skills for the open basin region. (a) Normalized target diagram. (b) Monthly variability from model (blue) and observation (red), number above the panel indicates the number of observations for each month. (c) Monthly variability from model (blue) and observation (red). Numbers above the panels (b) and (c) indicates the number of observations for each month.

current west of the Crimean Peninsula can be seen both from the observations and model results.

3.5 Summary and discussion

In a whole, it can be summarized that the dynamics of SST is fairly well reproduced, with the exception of a maximal 1°C global underestimation in summer, mostly affecting the north coast and northwestern shelf, a flawed representation of the southern branch of the Danube plume and local mismatches around the Kerch strait arising from the ignorance of exchanges with the Azov Sea.

The resolution of Danube southern plume is strongly affected by the spatial resolution of the wind forcings and may be weakened by our open boundary set-up: all the Danube inflow is induced in the model at one location while, in reality, the Danube river splits in three tributaries (the Chilia, Sulina and St Georges branches, from north to south).

Interestingly, it appears that the overall performance is not enhanced by finer model

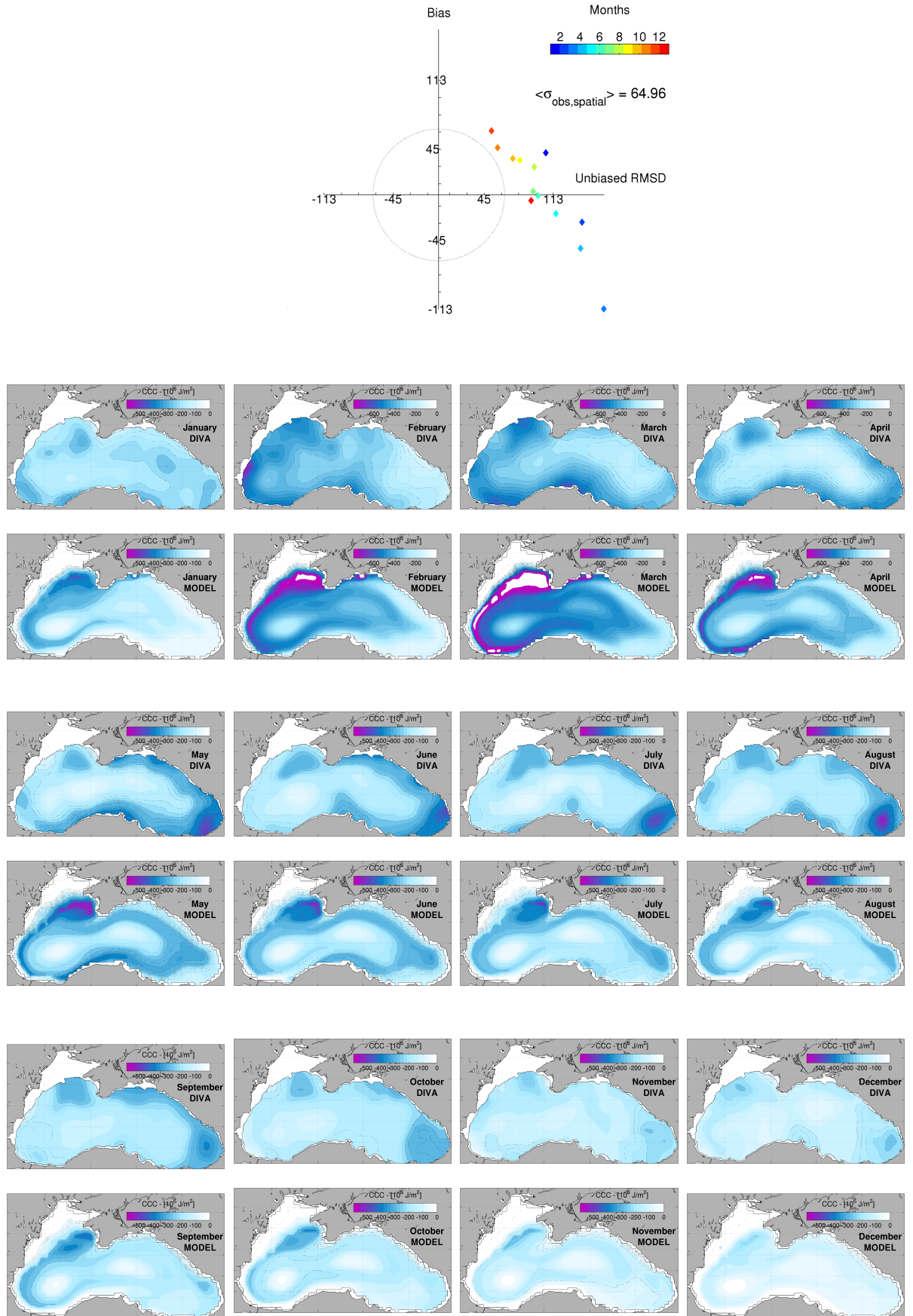


Figure 3.9: (Top) Target diagram representing the spatial skill for each month : CIL Cold content. (Lower Panels) Monthly climatologies obtained from (DIVA) Chapter 2 and (MODEL) coarse grid model simulations.

resolution. This points towards a specific error in some processes non-directly related to the model resolution. It should be noted that the spatial resolution of the satellite products (0.0625°) is coarser than the fine resolution model.

The persistence of spatial gradient in the bias may indicate an underestimation of the horizontal transport that could be linked to a global underestimation of the Rim current, or to the underestimation of meso-scale induced lateral diffusion. An underestimated Rim current intensity would also explain the lack of CIL cold content accumulation in the southeastern basin.

The visual comparison of vertical profiles of salinity pictures a slight over-mixing both on the shelf and in the basin interior.

The flawed resolution of the mixed layer depth's interannual variability in the NWS could have an origin in the restricted spatial resolution of wind forcings, which is relatively worse on the shelf given the shelf's smaller extension. Alternatively, it may be that the interannual variability of the riverine discharge, which again impacts more on the NWS than in the open basin, is not well caught by our forcing data.

It appears from the previous analysis that the lack of a convective sinking scheme results in that the CIL water formation process entrains more mixing in the model than observed. This may also explain the underestimation of the surface temperature in the areas of CIL formation.

Notwithstanding the mentioned inconsistencies and the fact that spatial incoherence affect the model's skills, it can be said that, in essence, the model presents a fair aptitude to reproduce the hydrodynamical mechanisms of the Black Sea.

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Chapter 4

Interannual variability of Black Sea's hydrodynamics and connection to atmospheric patterns



The 2nd Day of the Creation, M.C. Escher, 1925

This chapter is published as :

Capet, A., Barth, A., Beckers, J. M., & Marilaure, G., 2012, Interannual variability of Black Sea's hydrodynamics and connection to atmospheric patterns. *Deep Sea Research Part II: Topical Studies in Oceanography*, 77, 128-142.

It proposes both an original characterization of atmospheric variability, and an in-depth analysis of the multivariate hydrodynamic modes of oscillation in response to these patterns.

For consistency, only the ERA-40 atmospheric forcing set has been considered (1960-2000). To restart the same experience with the ERA-interim sets (1980-present), would be greatly informative though, because of the intense warming that may be observed during the last years (1995-present).

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Abstract

The long term variability (1962-2000) of the Black Sea physical processes (e.g. temperature, main circulation, cold intermediate layer, sea level) and its relation to atmospheric conditions and large scale climate patterns are investigated using an eddy-resolving tridimensional model in combination with statistical tools (e.g Empirical Orthogonal Functions, Self Organizing Maps). First, the ability of the model to represent the interannual dynamics of the system is assessed by comparing the modeled and satellite sea surface temperature (SST) and sea level anomaly (SLA) decomposed into their dominant Empirical Orthogonal Functions (EOFs). The correlation between the spatial and temporal EOFs modes derived from model and satellite is usually satisfactory and this gives some confidence in using the model as a tool to investigate not only the SST and SLA dynamics but also the dynamics of connected variables.

Then, the long term variability (1962-2000) of the Black Sea hydrodynamics is assessed by decomposing into their dominant EOFs modeled SST, SLA and selected key hydrodynamical variables associated to the main circulation and vertical structure of the water column. Significant correlations between the EOFs associated to these variables are investigated in order to link the variability of surface fields and the internal dynamics of the system.

In particular, the intensity of the general cyclonic circulation (the Rim current) is shown to impact strongly on (1) the mean sea level, (2) the SST response to air temperature (AT), (3) the formation of the cold intermediate layer, (4) the meridional repartition of the SST anomaly and (5) the exchanges of heat between the north-western shelf and the open basin.

In order to appraise the variability of atmospheric conditions over the Black Sea during 1962-2000 and their role in driving the hydrodynamics, a self-organizing maps technique is used in order to identify spatial recurrent patterns of atmospheric fields (ie. AT, wind stress and curl).

The impact on these patterns of large scale climatic variability over the north Atlantic, the Eurasia and Pacific Ocean (estimated by respectively the north Atlantic oscillation (NAO), the east Atlantic/west Russia oscillation (EA/WR) and the El Niño southern oscillation (ENSO) indexes) is assessed. Distinct time scales of influence of the large scale teleconnection patterns on the AT are identified : EA/WR drives the short scale (1-5 years) variations of SST, while the long term (>5 year) trends of the NAO drive the long term SST trends.

The drastic changes that have occurred in the Black Sea deep sea ecosystem at the end of the 80's are connected to an intensification of the general circulation which has promoted an export of riverine materials from the eutrophicated north-western shelf to the deep sea.

Finally, in the last two decades, we find an increased duration of persistent atmospheric anomalies regime that have the potentials to drive the system away from its average state as occurred in the late 80s. If persistent in the future, such long lasting atmospheric anomalies may have a significant impact on the ecosystem functioning.

1 Introduction

The important river discharge characterizing the almost enclosed Black Sea, combined with the import of salty Mediterranean waters through the Bosphorus, result in a strong permanent halocline which restricts the “active part“ to upper $\sim 150\text{m}$. This confinement makes the Black Sea surface layer particularly sensitive to changing environmental conditions.

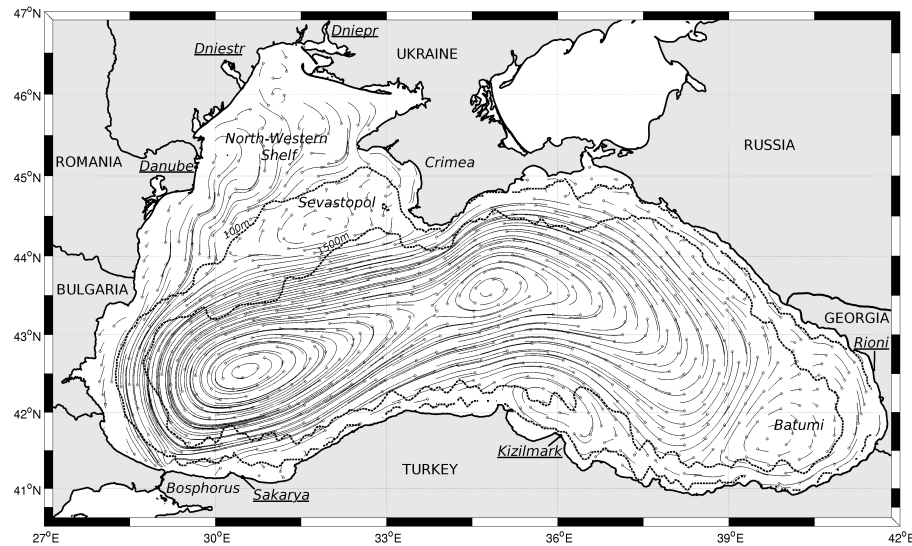


Figure 4.1: The Black Sea surface circulation, as simulated by the model used in this study, in May (climatological 1962-2000). The 6 main rivers considered in the model are underlined, the 100 and 1500 m depth contours are depicted in dotted line. During May, the Batumi and Sevastopol anticyclonic gyres, which are important structures of the Black Sea circulation (as discussed in the text) are well visible.

The north-western part of the Black Sea (i.e. the north-western shelf denoted in the following as the NWS) consists of an almost 200-km wide shelf representing about 13% of the total area and receiving the fresh water inputs of the Danube, Dnestr and Dniepr rivers (the Danube being by far the most important river bringing about 75% of the total river input into the whole sea). The surface circulation consists of a persistent cyclonic coastal current referred as the Rim current (Figure 4.1). Between this main current and the coast, a number of seasonal anticyclonic eddies develop. The Batumi eddy in the extreme East of the basin and the Sevastopol eddy situated above the NWS slope, West of the Crimea peninsula are the most permanent mesoscale structures of the Black Sea (Staneva et al., 2001; Korotaev et al., 2003). The permanent halocline is dome-shape, due to the geostrophic dynamics associated with the Rim current. This curvature is enhanced in winter by the intensification of the Rim current. In summer, a seasonal thermocline creates a double pycnocline structure which allows the existence of the cold intermediate layer (CIL), a layer of minimal temperature situated between the halocline and the thermocline and defined by the 8°C isosurfaces. Two important regions of formation coexist for the dense and cold waters constituting the CIL (CIW). The first one, accounting for $\sim 42\%$ (Stanev et al., 2003) of the annual CIW production, is a small area West of the Crimea peninsula, where the strong winter cooling is accompanied by the possibility of mixing

with underlying salty waters (the latter is not true for the northernmost NWS area where surface cooling is however more important). The second area, in the northern part of the central basin, accounts for $\sim 28\%$ (Stanev et al., 2003) of the annual CIW production. Surface cooling in this area is not as important as on the NWS, but the outcropping of the deep isopycnals, associated with the winter intensification of the Rim current, allow the cooling to penetrate directly to the density levels of the CIL.

The Black Sea region is located at the edge of various atmospheric systems and their relative influences combine differently over the seasons and over the years, leading to abrupt and significant changes of the weather conditions (Cherneva et al., 2008). Teleconnection patterns are often invoked to account for these different weather conditions (e.g. Krichak et al., 2002; Oguz et al., 2006; Kazmin and Zatsepin, 2007). They refer to large-scale (hemisphere) coherent modes of variation in the distribution of atmospheric masses. These have been growingly used in the scientific literature, since they have potentials to explain large scale correlations in the variations of weather conditions, oceanic conditions and consequent ecosystem changes (e.g. Niemann et al., 1999). Although the north Atlantic Oscillation (NAO) has been found to have a strong impact on the Mediterranean weather (e.g. Hurrell and Deser, 2010), and on the Black Sea hydrodynamics (e.g. Stanev and Peneva, 2002; Ginzburg et al., 2004; Oguz et al., 2006) the east Atlantic/west Russia (EA/WR) pattern (alternatively called the North-Sea/Caspian pattern (Kutiel and Benaroch, 2002)) has been found to be better associated to the Black Sea sea surface temperature (SST) during some years (Oguz et al., 2006). The El Niño southern Oscillation (ENSO) was found by Ginzburg et al. (2004) to promote in the Black Sea the occurrence of extreme (i.e. minima and maxima) SST values.

Through the last decades, the Black Sea ecosystem, and particularly its NWS has been the scene of drastic changes (e.g. eutrophication, collapse of fish stock, alien species invasion) with important consequences for the surrounding economies (Zaitsev, 1997; Langmead et al., 2009). It clearly appears that only the combination of human pressures (overfishing, riverine pollution, alien species introduction, ...) with natural decadal modulation of the hydrodynamic structure allows to explain these severe ecosystem shifts (Oguz and Gilbert, 2007; Llope et al., 2011).

The main aims of this paper can be summarized as follows: (1) to assess and understand the variability of the Black Sea physical conditions at interannual and decadal scales and in particular, to connect the variability of surface fields (i.e. SST, sea level anomaly (SLA)) with the internal dynamics of the system, (2) to estimate the impact of atmospheric conditions over the Black Sea on the dynamics of the system, (3) to link the variability of atmospheric fields with large scale climate variability, (4) to examine the existence of a trends in SST during the period 1962-2000 and the effect of global warming in general, (5) to connect the variability of the Black Sea physical environment to the drastic changes in the ecosystem that mainly occurred at the end of the 80's.

More specifically, a 3D hydrodynamical model is used to provide at high resolution (5km) and at basin scale synoptic physical variables (temperature, salinity, velocity, sea surface height (SSH), Energy). The ability of the model to simulate the interannual variability of the Black Sea hydrodynamics is first assessed by comparing the SST and SLA provided by the model and by satellite. The 4 dominant EOFs of modeled and satellite SST and SLA are compared by estimating the correlation between the spatial

and temporal EOFs. As shown in this study, this level of validation allows assessing the performances of the model in representing surface fields but also the internal dynamics of the system. Then, long term simulations are performed in order to assess the variability of the Black Sea hydrodynamics at interannual and decadal scales. The variability of SST, SLA, CIL cold content, Rim current intensity, vertical mixing is estimated through a EOFs decomposition of these variables. Corresponding variabilities from different variables are identified by correlation analysis between their dominant EOFs. This allows to connect processes and to understand the internal dynamics of the system.

We identify recurrent typical patterns of atmospheric conditions over the Black Sea area over the period 1962-2000 and we assess the impact on these patterns of large scale climatic variability associated with the atmospheric systems over the north Atlantic, the Eurasia and Pacific Ocean (estimated by respectively the NAO, EAWR and ENSO indexes).

The innovative aspects of the work can be summarized as follows. (1) In previous studies, the assessment of the long term variability of the Black sea physical properties is assessed using either satellite data (e.g. [Stanev and Peneva, 2002](#); [Ginzburg et al., 2004](#); [Nardelli et al., 2010](#); [Grayek et al., 2010](#)) or in-situ data (e.g. [Oguz et al., 2006](#); [Oguz and Gilbert, 2007](#)). Both approaches have its own limitations: satellite SST are only available since 1985 while in situ observations have a limited spatial coverage and are not ideal to take into account the spatial variability of the system which is very important especially in the NWS region. Here, the model represents the spatial variability of the system at high resolution (5km). (2) This study quantifies the correlations between the variability of several physical processes and this allows to gain an enhanced and integrated understanding of the Black Sea internal dynamics at interannual and decadal scales as well as its connection with atmospheric conditions over the Black Sea. (3) Most of the time the spatial structure of atmospheric fields is ignored and the impact of climate indexes is usually not quantified appropriately but rather is estimated based on the similarity of variability of basin scale average fields and climate indices. Here, a SOM analysis of atmospheric conditions provides recurrent spatial patterns of air temperature (AT), wind stress and curl. Keeping the spatial information allows further understanding than provided by the study of basin average values ([Kazmin and Zatsepin, 2007](#)). The impact of large scale climate conditions on atmospheric patterns is assessed through a statistical test. (4) The deterministic model presented in this study is run without any data assimilation and can then be used for scenarios studies.

The paper is organized as follows. The model is briefly described in section 2. Section 3 describes and compares the modeled and satellite derived SST and SLA main modes of variability (EOFs) and assesses the ability of the model to correctly reproduce the different levels of variability of these surface variables. Section 4 analyzes over the period 1962-2000 the main modes of variability of the simulated fields decomposed into their dominant EOFs. Correlations between the temporal EOFs associated to different variables are investigated in order to propose a physical meaning to the different EOFs modes. This allows to link the dynamics of surface properties with the internal functioning of the system. Section 5 is devoted to the analysis of atmospheric conditions and identifies recurrent regimes of AT and wind circulation anomalies. General relationships with teleconnection indexes are depicted in this section. Results from the previous sections are discussed in section 6 and in particular, the question of a potential impact of

climate change is addressed. Conclusions and perspectives are given in section 7.

2 The 3D model

The GHER3D general circulation model has been successfully applied to explore the general circulation of the North Sea (Delhez, 1996), the Mediterranean Sea (Beckers, 1991; Barth et al., 2005) and the Black Sea (Grégoire et al., 1998; Beckers et al., 2002; Grégoire and Friedrich, 2004; Vandenbulcke et al., 2009).

For the present implementation, the model is run on a regular Arakawa-C grid of resolution $\Delta x = \Delta y = 0.045^\circ$ (5×4 km), using the terrain following double-sigma vertical coordinates system (Beckers, 1991). The open boundaries are restricted to the Bosphorus and the 6 main rivers : Danube, Dniepr, Dniestr, Rioni, Kizilmark and Sakarya. Annual values of the river flows are provided by Ludwig et al. (2009), as well as climatological seasonal repartitions used to construct the monthly river forcing. The parameterization of the Bosphorus is set up to ensure the representation of the two-layer exchange, needed to sustain the halocline, while ensuring long term conservation of total salt content and total water content.

Atmospheric data used to force the model are issued from the ECMWF¹ ERA40 reanalysis, available during 1960-2001, on a 1.125° grid, using 2m AT and dew point temperature, 10 m winds, sea level pressure and precipitations. Winds components are downscaled to 0.2 by spline interpolation, which allows a better conservation of the wind curl. All atmospheric fields are filtered in order to suppress the erroneous influence of land points on the coastal sea conditions (Kara et al., 2007). The wind stresses, the heat fluxes and the pseudo fluxes of salt associated to evaporation and precipitation are computed interactively considering the state of the model surface layer. The model is run without any relaxation term or data assimilation.

Analyzes of the integrated kinetic energy content (not shown) indicates that 2 years of spin-up are needed to recover from the climatological initial conditions. Results, saved as weekly averages, are thus considered over the 39 years period from 1962 to 2000.

3 Satellite products and model validation

In this section, we describe the satellite SST and SLA data sets used to assess the ability of the model to simulate the interannual variability of the Black Sea. With this aim, modeled and satellite SST and SLA are decomposed into their dominant EOFs and these EOFs are compared (8.2).

This comparison constitutes a rigorous and demanding assessment of the model performances in representing the successive orders of variability of the Black Sea hydrodynamics. The validation effort goes beyond a classic comparison of surface observable values since, as shown in the following, the various modes of variability of SST and SLA (estimated

¹European Center for Medium-Range Weather Forecasts (<http://www.ecmwf.int/>).

from the EOFs analysis) are significantly correlated to the internal dynamics of the system (e.g. CIL properties, mixing, circulation).

3.1 Sea surface temperature

SST fields measured by Advanced Very High Resolution Radiometer (AVHRR) are provided by NOAA² and are processed by Nardelli et al. (2010). For comparison issues, weekly averages are computed from the daily satellite products while the model results are binned on the corresponding 1/16 grid.

The seasonal cycle represents almost 99% of SST variability, and largely overpasses the interannual variability (Nardelli et al., 2010). This study focuses on the interannual variability of the system and therefore, the validation exercise needs to assess the ability of the model to simulate processes at this scale. A typical seasonal cycle is extracted from model and satellite data as explained in 8.1 and the EOFs are computed on the obtained anomalies.

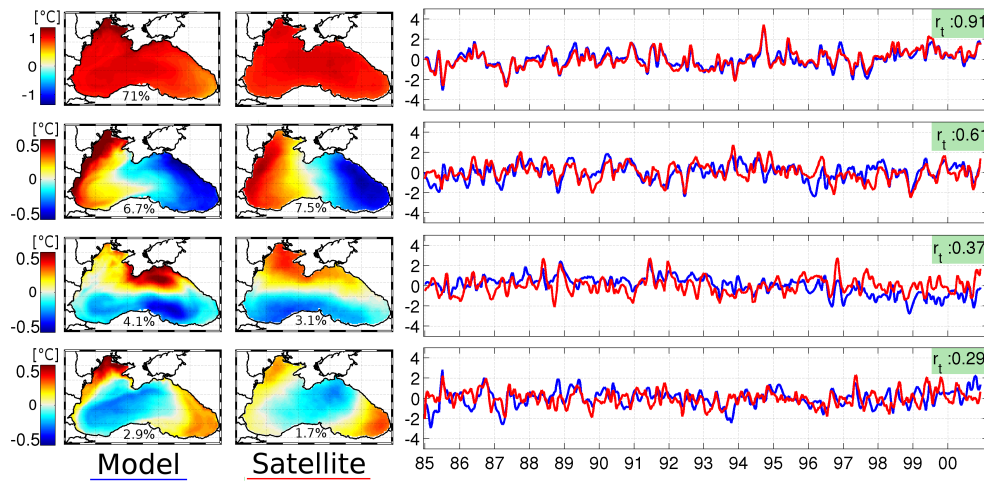


Figure 4.2: From top to bottom, the first EOFs of the SST anomalies (1985-2000) sorted by decreasing order of explained variability. From left to right: the spatial structure of the model EOF, the spatial structure of the satellite EOF and the associated temporal amplitudes (blue for model, red for satellite). The percentages of variability accounted for by the modes are indicated in the right corners of the spatial maps, while green boxes give the spatial (r_s , on the left panels) and temporal (r_t , on the right panels) Pearson correlation coefficients between the model and the satellite products.

Figure 4.2 shows that, both in the model results and in the satellite data, the four dominant EOFs account together for $\sim 85\%$ of the SST anomalies variability.

The first mode explains more than 70% of the variability and corresponds to a basin scale increase/decrease of the SST anomaly (the spatial pattern has the same sign over the basin). The associated temporal EOFs are highly correlated ($r_t = 0.91$). The lower spatial correlation ($r_s = 0.52$) can be explained by the underestimation by the model of the variability in the Batumi area. Due to the low spatial variability of this first mode,

²National Atmospheric and Oceanic Administration (<http://www.noaa.gov/>).

the spatial correlation coefficient is more sensitive to small differences in variabilities in the modeled and satellite data set. It should be noted that this distinct SST variability in the Batumi region does not appear anymore when the EOFs are computed over the period 1962-2000 (see section 4, Figure 4.4) which suggests that it is specific to the 1985-2000 period.

The second and third modes explain respectively 6-7 and 3-4 % of the variability and correspond to respectively the modulations of the zonal and meridional gradient of the SST anomaly. Modeled and satellite EOFs are well correlated in space and time.

The fourth mode explains less than 3% of the variability and while the modeled and satellite spatial patterns are well correlated, the temporal modes are weakly correlated indicating that this level of detail lies at the limit of model capability.

3.2 Sea level anomaly

The SLA images are processed and distributed by the AVISO program³. These anomalies are computed with respect to the Mean Dynamical Topography (MDT)(CNES, 2011). As the MDT field is not directly available for the Black Sea, average SSH over the 1993-1999 period is taken as a proxy, and is subtracted from the modeled SSH to produce the model SLA which are then binned on the AVISO 1/8 grid for comparison.

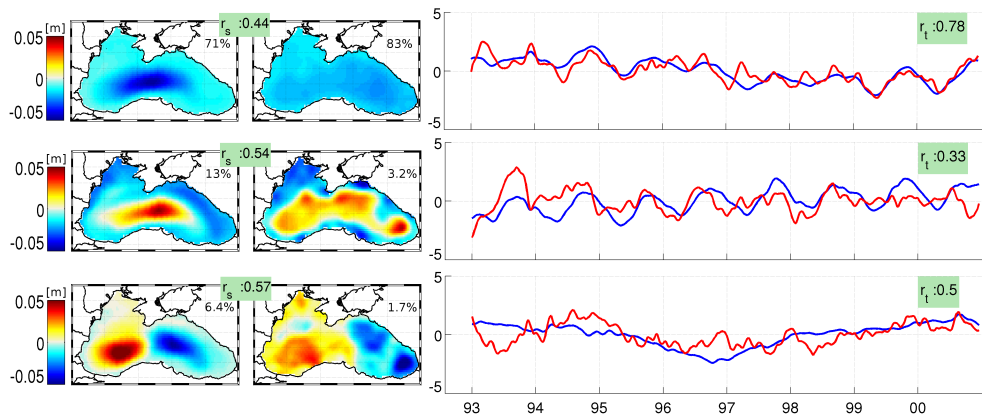


Figure 4.3: From top to bottom, the first EOFs of the SLA (1993-2000) sorted by decreasing order of explained variability. From left to right : the spatial structure of the model EOF, the spatial structure of the satellite EOF and the associated temporal amplitudes (blue for model, red for satellite). The percentage of variability accounted for by the modes are indicated in the right corner of the spatial maps, while green boxes give the spatial (r_s , on the left panels) and temporal (r_t , on the right panels) correlations between model and satellite products.

In the case of SLA, interannual and seasonal variations present similar amplitudes. Furthermore, the seasonal cycle does not correspond to one EOF (as for SST) but rather is dispatched among the first two EOFs as also found by Grayek et al. (2010). This prevents the clear identification of a climatological seasonal cycle over the period 1993-2000. Therefore, the EOF decomposition of modeled and satellite SLA over 1993-2000 is

³Archiving, Validation, and Interpretation of Satellite Oceanographic data (<http://www.aviso.oceanobs.com/index.php?id=1394>).

realized on the SLA rather than on the anomalies compared to a typical seasonal cycle as for SST (Figure 4.3).

The first three modes of modeled and satellite SLA explain more than 88% of the SLA variability. For the first mode which accounts for 71% and 83% of the SLA variability in the model and the satellite data, respectively, the spatial pattern is homogeneous in sign and corresponds to a basin-wide rising or lowering of the sea surface with a maximum intensity in the center of the basin.

This enhanced curvature is more pronounced in model results but has also been evidenced by [Grayek et al. \(2010\)](#), using the SLA produced by AVISO over a larger period (1993-2006).

The second EOF presents a spatial structure characterized by an opposed variability between the coastal areas and the deep basin and is therefore associated to the variability of the curvature of the sea surface. The third EOF accounts for a difference in the zonal repartition of water masses, as detailed in ([Grayek et al., 2010](#)).

For these two modes the model and satellite spatial EOFs are significantly correlated ($r_s > 0.5$) but, as in the case of SST, the satellite SLA presents a distinct variability in the Batumi area.

The general lower variability in the modeled compared to the satellite SLA (compare the modeled and satellite temporal EOFs shown in Figure 4.3) can be explained by the absence of steric effects ([Grayek et al., 2010](#)) and of a volumetric impacts of precipitation and evaporation ⁴ in the model. These two processes may add noise to the SLA response to circulation features. However, the correlation coefficients between modeled and satellite SLA are significant except in the case of the second mode ($r_t = 0.33$)

4 Long term model analysis

In this section the long term variability of the Black Sea hydrodynamics is analyzed using model results from a simulation over the 1962-2000 period. SST and SLA variabilities are connected to the internal dynamics by addressing a selection of key properties for the Black Sea : the mixed layer depth (MLD) ([Kara et al., 2009](#)), the cold intermediate layer cold content (CCC) ([Staneva and Stanev, 2002](#)) and the mean kinetic energy (MKE), as representative of the intensity of surface currents (please refer to 8.3 for details about the computation of these quantities).

The EOFs of each of these variables (including SST and SLA) are computed separately, after subtraction of their respective seasonal cycle and after applying a low pass filter (1-year moving average) on the anomalies. In this way, the responses to rapid variations of the Black Sea weather are filtered out and only anomalies with a time scale of one year or larger are considered.

Then, we estimate the Spearman rank correlation between the dominant EOFs of SST and SLA and those of the selected hydrodynamical variables. As this paper investigates

⁴Precipitation and evaporation are represented through pseudo fluxes of salinity rather than through volumetric variations.

the temporal variability, correlations are estimated between the temporal EOFs modes and variables that are correlated ($r > 0.5, p < 0.05$) are presented in Figures 4.4, 4.5 and 4.6.

This section describes the modes and the correlations between them. For briefness, each EOF is referred by the acronym of the corresponding variable followed by the rank of the EOF (e.g. MLD-1 is the first mode of mixing layer depth). In section 6, we physically interpret the different modes of variability of the physical variables and try to connect them to atmospheric variables.

SST-1 (Figure 4.4) is best linked with MLD-1 ($r = 0.67$) and CCC-1 ($r = 0.6$). Although the spatial patterns of these three modes differ, they all are homogeneous in sign and thus consist in synchronous basin-wide anomalies. It means that to a basin wide increase (resp. decrease) of the SST corresponds a decrease (resp. increase) of the MLD (counted in meter negatively from the surface), and a decrease (resp. increase) of the CCC (low CCC corresponds to a higher temperature in the CIL or to a smaller CIL volume).

More specifically, SST-1 is rather homogeneous with an enhanced variability on the shallow NWS. MLD-1 and CCC-1 exhibit a spatial structure similar to the typical pattern of distribution of MLD: deeper on the periphery, in particular above the shelf slope West of Crimea and shallower in the central basin where a permanent rising of the halocline occurs. For these two variables, the region between the shelf slope and the Rim current presents an enhanced variability where a deepening of the MLD corresponds to an increase of the CCC.

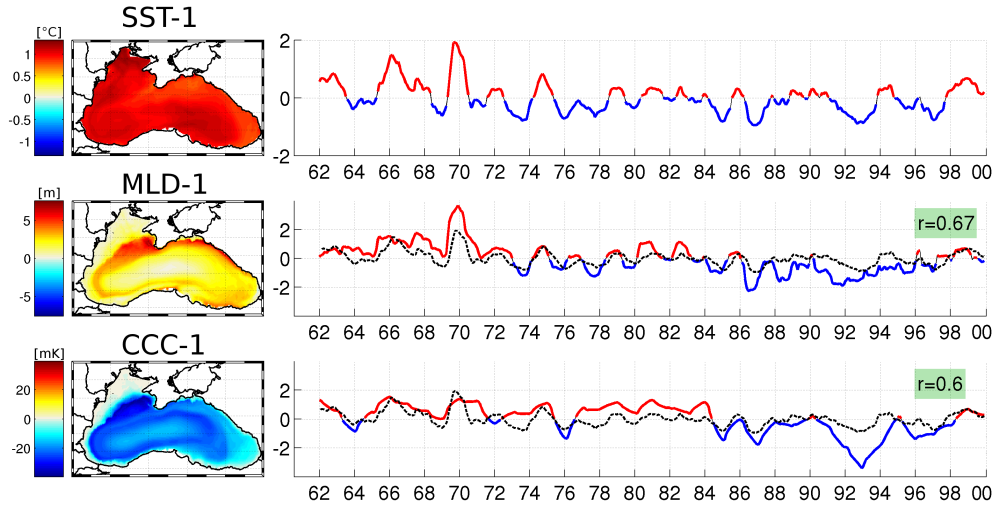


Figure 4.4: The first EOF of SST (SST-1) (top), MLD-1 (middle) and CCC-1 (bottom). Left: spatial components of the EOFs. Right: temporal components of the EOFs, with evidenced positive (red) and negative (blue) phases and with the Spearman rank correlation coefficient (green boxes) estimated with SST-1 (SST-1 reproduced in dotted lines).

SST-2 only shows significant correlation with CCC-2 ($r = 0.54$). The spatial pattern of SST-2 exhibits an East/West front with temperature anomalies of opposite sign in the western and eastern basin. The interface is modulated by the influence of the Rim current. The spatial distribution of CCC-2 (Figure 4.5) evidences anomalies of opposite sign in the two main regions of CIL formation described in the introduction and identifies their area of influence.

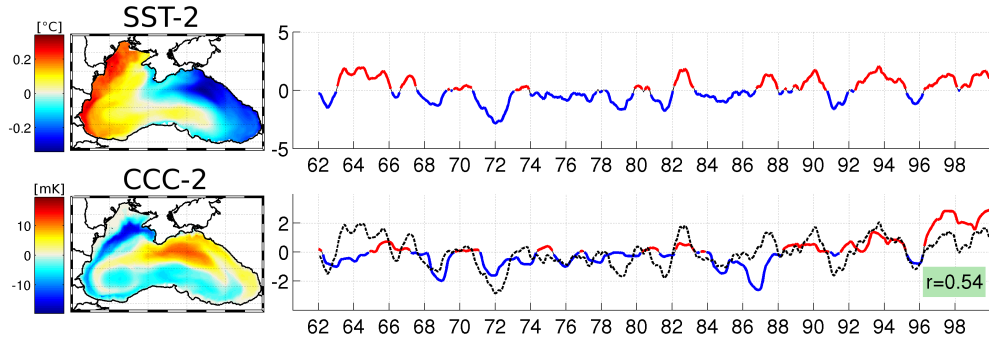


Figure 4.5: Second EOF of SST (SST-2, on the top) and CCC-2 (bottom). Left: spatial components of the EOFs. Right: temporal components of the EOFs, with evidenced positive (red) and negative (blue) phases and with the Spearman rank correlation coefficient (green boxes) estimated with SST-2 (SST-2 reproduced in dotted lines).

Figure 4.6 presents the EOFs correlated with SLA-1. The strongest correlation occurs with MKE-1 ($r = 0.94$), which is a proxy of the Rim current (as evidenced by its spatial pattern). The next best related EOFs are MLD-1 ($r = 0.67$), CCC-1 ($r = 0.61$) and SST-3 ($r = 0.53$).

5 Atmospheric conditions

In this section, we analyze the variability of atmospheric conditions affecting the Black Sea region. Characteristic meteorological regimes are identified and related to the large-scale teleconnection patterns. Results of this section are used in section 4 in order to highlight the role of atmospheric conditions in driving the hydrodynamical modes identified in section 4.

5.1 Identification of recurrent atmospheric patterns

Coherently with the analysis of hydrodynamical variables, a typical seasonal cycle is first subtracted from the atmospheric data used to force the model (see section 2 and 8.1), and then the obtained anomalies are smoothed by a 1-year moving average.

Monthly averaged anomalies of AT, zonal and meridional wind speed and the wind curl are then jointly integrated in the Self Organizing Map (SOM) analysis (8.4), in order to identify recurrent spatial patterns of coincident anomalies of these various fields.

The six typical spatial patterns identified by the SOM analysis are presented in figure 4.7 showing the winds components and the AT associated to each pattern. Additionally, and in order to familiarize the reader with the SOM concept, figure 4.8 presents for each month (from 1962-2000) the anomalies of the wind components and indicates to which recurrent patterns (shown in Figure 4.7) these anomalies are mapped by the SOM procedure.

Pattern 5 is characterized by the highest positive temperature anomalies and by southern winds (Figure 4.7) which are more often from the west as indicated by the position

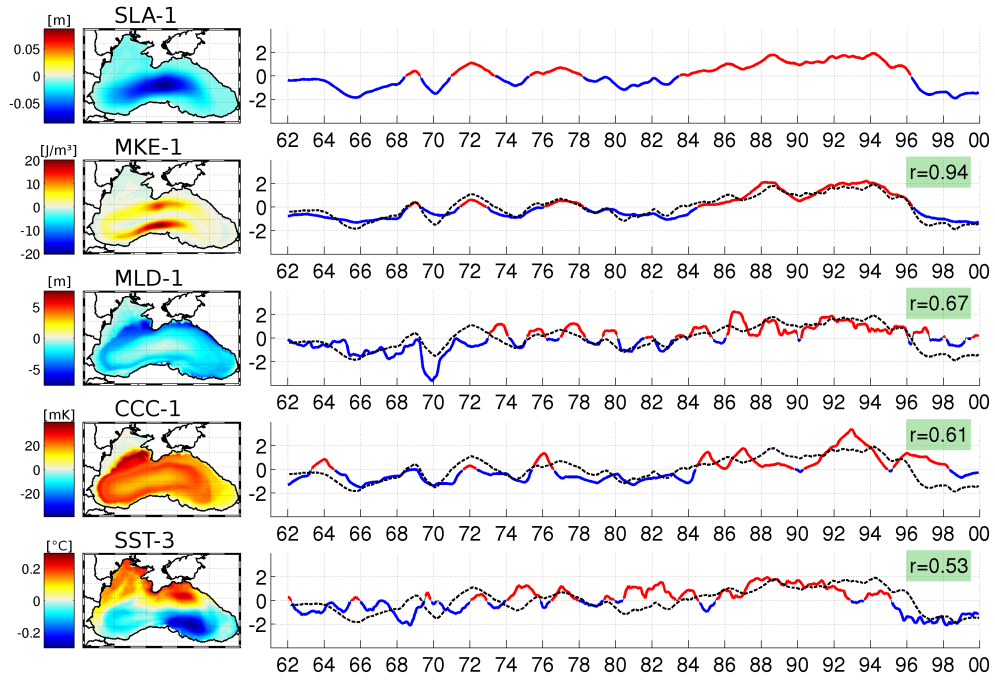


Figure 4.6: Top to bottom: First EOF of SLA (SLA-1), MKE (MKE-1), MLD (MLD-1), CCC (CCC-1), and third EOF of SST (SST-3). Left: spatial components of the EOFs. Right: temporal components of the EOFs, with evidenced positive (red) and negative (blue) phases and with the Spearman rank correlation coefficient (green boxes) estimated with SLA-1 (SLA-1 reproduced in dotted lines).

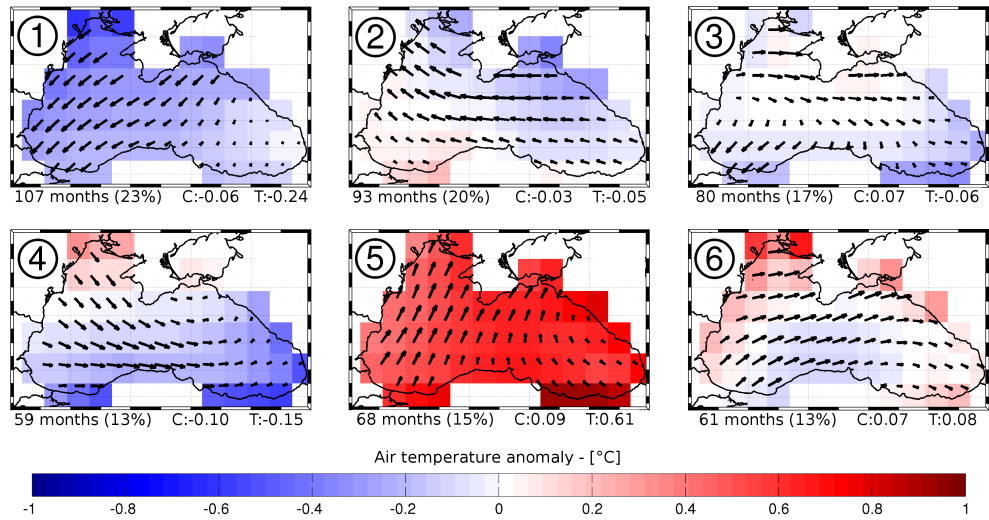


Figure 4.7: Typical patterns of the meteorological anomalies as identified by the SOM analysis for the period 1962-2000 (the encircled number on each panel labels the pattern for further references in the paper). At the bottom of each panel are indicated the number and percentage of months mapped toward this pattern, as well as the corresponding basin averaged wind curl (C , [s⁻¹]) and AT (T , [°C]) anomalies.

of pattern 5 in figure 4.8 which is slightly shifted on the right axis corresponding to westerlies.

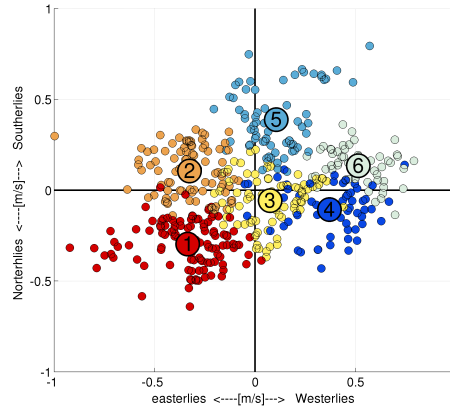


Figure 4.8: Monthly anomalies of meridional and zonal winds components (small circles, basin scale average values for all the months between 1962-2000). The larger circles locate the pattern identified by the SOM analysis. One color is associated to each pattern and the months mapped toward a given pattern have the same color.

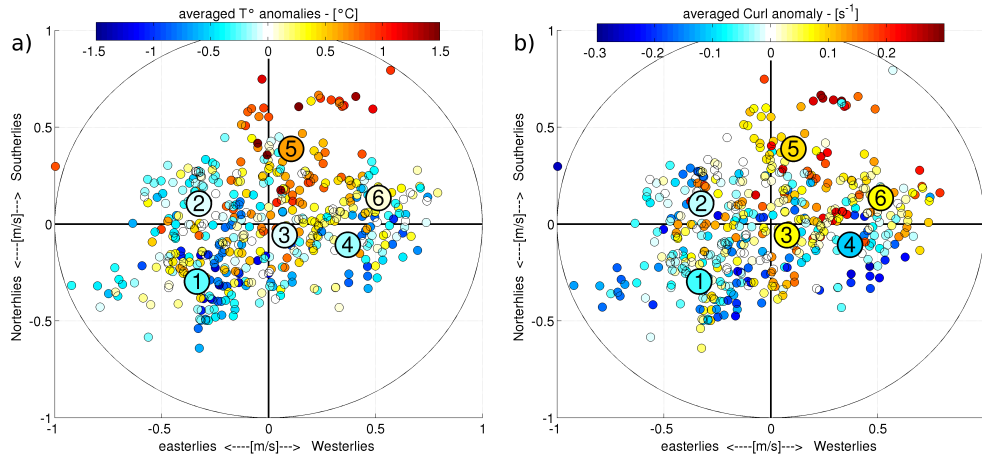


Figure 4.9: Small circles: monthly anomalies of the basin scale averaged of the meridional and zonal winds components (all the months between 1962-2000 are plotted). Large circles: recurrent patterns identified by the SOM analysis and illustrated in Figure 4.7. Left: with the basin average AT anomaly superimposed. Right: with the basin average wind curl anomaly superimposed.

The lowest temperature anomalies are described by either pattern 1 or pattern 4 and are associated either to north-eastern winds (pattern 1) or north-western winds (pattern 4).

The spatial repartition of the AT anomaly illustrated in Figure 4.7 shows that the NWS presents an enhanced positive anomaly compared to the rest of the basin in association with western winds (i.e. patterns 4 and 6) while an enhanced negative anomaly is associated with eastern winds (i.e. patterns 1 and 2). East winds have indeed been found to promote the westward extension of the cold air mass from the Siberian weather system (Shapiro et al., 2010a).

South-western winds generate anticyclonic wind (positive curl) over the Black Sea (patterns 5,6) while northern winds promote a cyclonic circulation (patterns 1 and 4).

5.2 Influence of the large scale teleconnection patterns

The potential impacts of large scale climate variability on the recurrent patterns of atmospheric conditions illustrated in Figure 4.7 is assessed by estimating for each recurrent pattern the value of the climate indexes (i.e. NAO, EAWR, ENSO) obtained for the different months mapped towards this pattern. This allows assessing whether a recurrent pattern is significantly associated to a positive or negative value of a climate index and hence a connection between atmospheric conditions over the Black Sea and large scale climate features. Monthly average values of the climate indexes are provided by the NOAA Climate Prediction Center ⁵.

Figure 4.10 indicates for each atmospheric pattern, the distribution of positive and negative phases of the three teleconnection indexes during the months mapped towards this atmospheric pattern.

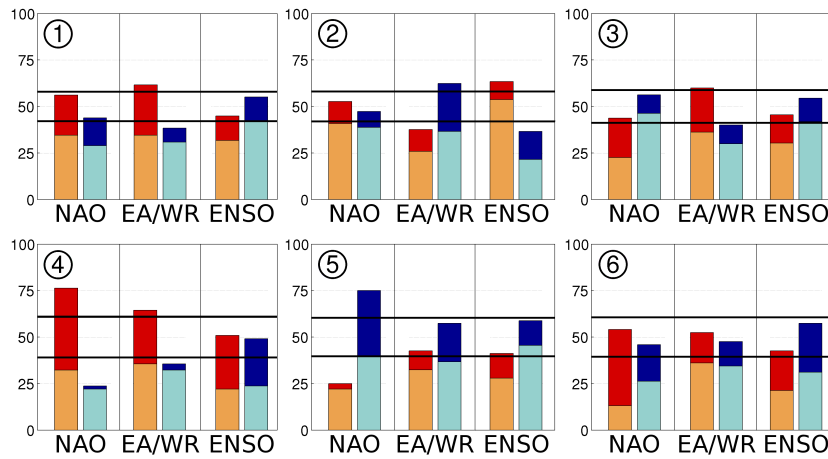


Figure 4.10: Distribution for each atmospheric pattern (identified in Figure 4.7, one panel by pattern) between positive (red) and negative (blue) phases of the teleconnections indexes. We conclude that the phase of an index has a significant ($p < 0.05$) impact on the atmospheric pattern when its distribution amongst positive and negative values fall both outside the bold lines (see Appendix D for details).

This Figure shows that the EA/WR index is significantly negative during months mapped towards patterns 2 and 5 which means that this index promotes the occurrence of south-easterlies (pattern 2) and southerlies (pattern 5). EA/WR is significantly positive during months mapped towards patterns 1,3 and 4 characterized by the occurrence of northerlies. Therefore, EA/WR significantly impacts the occurrence of northerlies and southerlies and hence influences the AT anomaly as already described in section 5.1 and further analyzed in section 5.3.

Strong positive NAO index are more frequent in patterns 4 and 6 characterized by western winds. The negative phase, however is not related to eastern winds but rather, amplifies the negative phase of EA/WR to promote extreme southern anomalies, as can be seen by comparing the cases of patterns 2 and 5. The highest wind curls (patterns 4 and 5) correspond to the most significant distribution of the NAO index among positive and negative values: cyclonic (resp. anticyclonic) wind fields being promoted by positive

⁵ <http://www.cpc.ncep.noaa.gov/data/teledoc/telecontents.shtml>

(resp. negative) phases. However this relationship between the NAO index and the wind curl can not be extended to moderate wind curl anomalies (patterns 1, 2, 3 and 6). Therefore, NAO significantly influences the occurrence of western winds and of extreme wind curls but is not systematically linked to anomalies of AT.

5.3 Comparison with previous studies

[Kazmin and Zatsepin \(2007\)](#) found no relationships between the EA/WR index and the wind regimes, nor with the AT, while these relationship appear clearly in the present work. Conversely, they mentioned a relationship between NAO and AT, also evidenced in the work of [Oguz et al. \(2006\)](#) while this relationship is not found significant in the present work (see section 5.2). These different conclusions are not surprising and stress the influence of the spatial and temporal scales taken into account to perform this type of study. Indeed, conclusions depend notably whether the spatial variability of the atmospheric fields is considered or not (in [Kazmin and Zatsepin \(2007\)](#) basin wide averages are considered, here the spatial variability is considered), the type of temporal averages that have been performed (monthly in this study, seasonal in [Kazmin and Zatsepin \(2007\)](#)), the smoothing window (1 year in this study against 5 years in [Kazmin and Zatsepin \(2007\)](#)) and the removal of a seasonal cycle (in this study we are working with anomaly).

To highlight the importance of these factors, Figure 4.11 illustrates the evolution over 1962-2000 of the basin averaged AT, NAO and EA/WR indexes after smoothing with a 1-year and 5-year average for comparison. It is shown that on a short term (1-5 years), the AT anomaly follows the oscillation of the EA/WR index while, the longer term trends of SST (>5 years), as those depicted by [Ginzburg et al. \(2004\)](#); [Nardelli et al. \(2010\)](#) seems to follow the trends of the NAO index. This partly reconciles the two studies. In fact, the impact of NAO may be indirect through an effect on the localization of EA/WR associated poles of sea level pressure anomaly as reported by [Krichak et al. \(2002\)](#).

No systematic influence of the ENSO index could be deduced from the present analysis. This is in contradiction with [Ginzburg et al. \(2004\)](#) who found that the extreme anomalies of SST occur during the El Niño phases. The absence in this study of a clear relationship between ENSO and the atmospheric patterns identified in Figure 4.7 does not imply that ENSO has no impact on the Black Sea SST but if ENSO impacts the SST it is not through an air temperature anomaly resulting from modification of the winds pathways. Indeed, the recurrent atmospheric patterns identified by the SOM analysis correspond to coincident anomalies of the winds (direction and curl) and AT.

An important remark in [Oguz et al. \(2006\)](#) reminds that the indexes values do not account for the relative positions of the teleconnection's centers of action. This oversimplification can explain some discrepancies in the results with the depicted relationships.

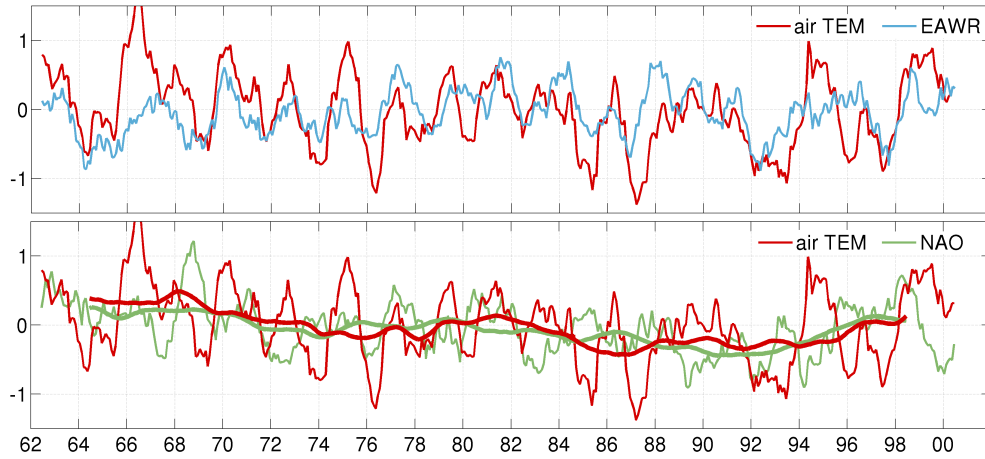


Figure 4.11: Evolution over 1962-2000 of the basin averaged AT (red), EA/WR (blue, upper panel) and NAO (green, lower panel) indexes after smoothing with 1-year (thin lines) and 5-year (bold lines) moving averages. On a short temporal scale (a), the variations of the AT follows those of the EA/WR oscillation while the longer scale (>5 years) trends of AT follow the trends of the NAO index.

6 Discussion

In this section we first discuss and interpret the different modes of variability of SST and SLA identified over the period 1962-2000 in connection with the variability of the hydrodynamics and of meteorological conditions and river discharges. A particular focus is put on the various impacts of the Rim current intensity. Then, this variability is connected with the drastic changes in the ecosystem that mainly occurred at the end of the 80s. Finally, we investigate the possible existence of long term trend (over the 38 years of simulation) in the hydrodynamical variables and we propose some elements of answer to the complex issue of climate change impact on the Black Sea.

6.1 Sea surface temperature

The most important mode of variability of the anomaly of SST occurs at basin scale and governs the short term oscillation of the dominant mode of variability of the MLD by impacting on the thermal stratification. This first mode of variability of the SST anomaly is closely related to the AT ($r = 0.88$, Figure 4.12), and follows both the rapid oscillation governed by the EA-WR index and the long term influence of the NAO (see section 5.3). The close response of SST to AT is modulated by the intensity of the Rim current (Figure 4.12): by deepening the MLD at basin scale, an intense Rim current enhances the thermal inertia of surface waters and reduces the response to AT changes ($0.55\text{ }^{\circ}\text{C}_{sea}\text{ }^{\circ}\text{C}_{air}$ against $0.74\text{ }^{\circ}\text{C}_{sea}\text{ }^{\circ}\text{C}_{air}$ in low Rim current conditions).

The zonal repartition of SST anomaly (SST-2, Figure 4.5) is not significantly correlated with any circulation related variables (i.e. SLA, MKE) and is thus mainly governed by the repartition of the AT anomaly. Its influence on the CIL formation is discussed in section 6.3.

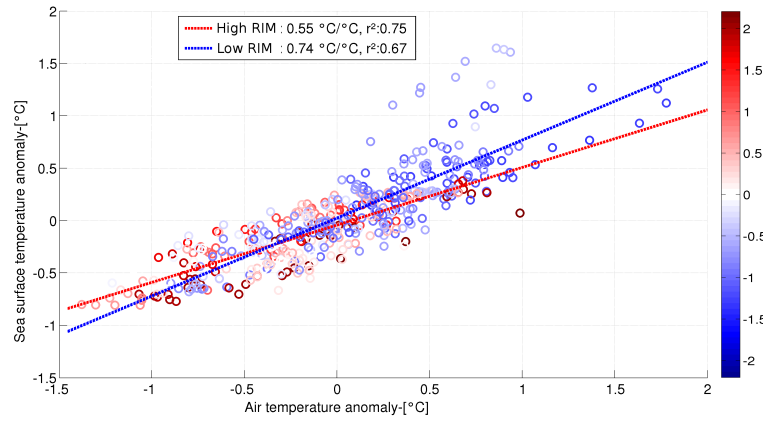


Figure 4.12: Scatter plot of SST-1 (Y-axis) against basin averaged AT (X-axis) anomalies. SST-1 scaling is chosen so that the value on the Y-axis represents the basin wide averaged SST anomaly. The color code represents the Rim current intensity (red: intense, blue: weak as estimated from MKE-1 temporal mode). The dotted lines represent the regressions computed over the months characterized by an intense or weak Rim current and illustrates the different response of SST to AT anomalies.

The meridional gradient of SST anomaly (SST-3) is related to the Rim current (Figure 4.6). This can be explained by considering the Rim current as a conveyor belt bringing warmer waters from the South to the North, and colder water from the North to the South. Interestingly, the whole shelf area is warmer when the Rim current is active. As the NWS is colder in general than the rest of the basin (not shown), this indicates that an intensified Rim current enhances the exchanges between the shelf and the open basin part. An important part of this exchange is mediated by the Sevastopol eddy (Figure 4.1) as already mentioned by Shapiro et al. (2010b).

6.2 Sea level anomaly

SLA-1 is strongly related to the Rim current intensity (i.e. MKE-1 see Figure 4.6) and is also highly correlated with the basin wide averaged Mean Sea Level (MSL) ($r = -0.97$). This suggests a closed link between the MSL and the Rim current as confirmed by the high (negative) correlation found between these two variables ($r = -0.86$) and illustrated in Figure 4.13.

This tight coupling between the interannual variations of the MSL and the Rim current intensity can be understood when considering the impact of the Rim current on the surface curvature. Intense Rim current increases the surface elevation in the periphery and decreases it in the central part. At interannual scales, the sea level at the Bosphorus entrance is mainly imposed by the quasi-direct (Staneva et al., 2001) balancing response of the Bosphorus barotropic transport. Therefore, considering that the sea level at the periphery is maintained, enhanced Rim circulation mainly results in a decrease of the central basin elevation, hence its averaged effect on the MSL. An important consequence of this tight coupling is that the long term variations of the Rim current intensity can be reconstructed based on the MSL signal, which can be retrieved from tide gauge data, as shown by Peneva et al. (2001).

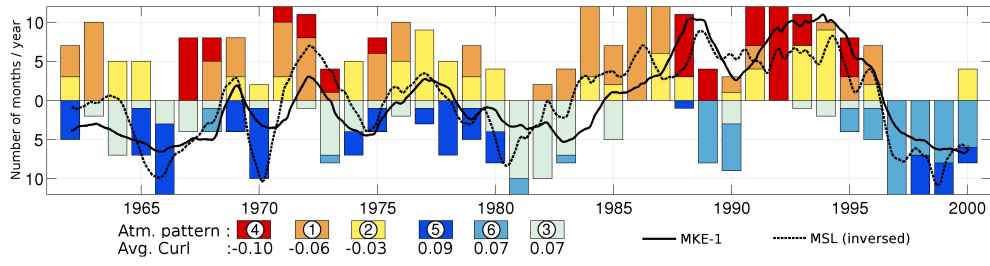


Figure 4.13: Temporal evolution over 1962-2000 of (1) the anomaly of the Rim current intensity (bold line, estimated from MKE-1 temporal evolution), (2) the anomaly of MSL (dotted line, scaled) computed from the modeled free surface elevation and inversed on the plot for facilitating the connection with the anomaly of the Rim current (i.e. a positive anomaly of MSL corresponds to a decrease of MSL). These two curves highlight that the variations of the anomalies of the (negative) MSL and the Rim current intensity are correlated ($r = 0.86$): the MSL decreases (resp. rises) during the active (resp. weak) phases of the Rim current intensity. Additionally, in order to assess the impact of the atmospheric patterns (more specifically of the wind curl) on the anomaly of the Rim current intensity, the bars present for each year the number of months mapped towards patterns 1, 2, 4 (characterized by cyclonic winds), 3, 5 and 6 (characterized by anticyclonic winds).

The second EOF of the SLA (not discussed in section 4) does not correspond to a physically independent mode (see Monahan et al. (2009) for a discussion on the physical interpretation of EOFs) and acts as a complement to SLA-1 to account for the part of MSL which is not directly linked to the Rim current but rather is linked to the water budget. The correspondence of this mode with the river discharges (which are the main terms of the Black Sea water budget (Stanev and Peneva, 2002)) is illustrated in Figure 4.14. The spatial pattern depicted by this mode is a consequence of this complementarity.

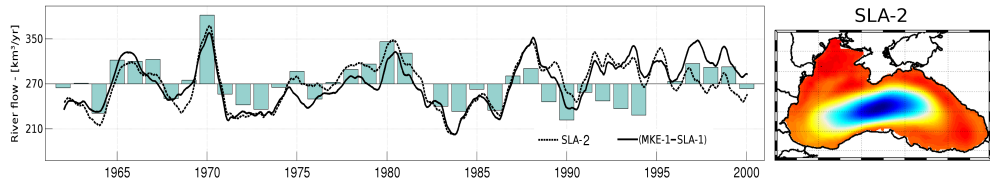


Figure 4.14: Left: Long term evolution of (1) the second EOF of the SLA (dotted line, scaled). (2) the difference between scaled MKE-1 and SLA-1 (bold line) which represents the part of MSL variability that is not accounted for by the variability of the Rim current and corresponds to the variability of the riverine flow (blue bars). Right: the spatial pattern of SLA-2.

Our interpretation of the main modes of variability of the SLA differs from that of Stanev and Peneva (2002); Grayek et al. (2010). For these authors, the first mode of SLA variability is only linked to the water budget (and not to the Rim current as shown here) while the second mode is connected to the Rim current due to its spatial pattern. These different conclusions can partly be explained by the different temporal scales considered in our study and in Stanev and Peneva (2002); Grayek et al. (2010). Indeed, here the seasonal cycle has been removed which is not the case in the other studies. This may change the interpretation of the variability of the SLA since at seasonal scales the time of adjustment through water exchanges to a rising of SLA in the Bosphorus area is not

negligible anymore. However, the comparison of the EOFs associated to the modeled SLA (Figure 4.3) or its anomalies (Figures 4.6 and 4.14) shows that the removal of the seasonal cycle does not impact substantially on the spatial patterns depicted by the obtained EOFs.

6.3 Cold intermediate layer

Figure 4.4 (right panel illustrating the temporal component of the EOF) shows that the dynamic of CCC is rather slow, in agreement with the scale of CIL waters renewal of 5.5 years found by Staneva and Stanev (2002).

Interestingly the positive and negative phases of CCC correspond to similar phases of the intensity of the Rim current (MKE-1, Figure 4.6), suggesting that an intensified circulation favors the formation of CIW. Indeed, an intense Rim current accentuates the doming shape of the main pycnocline by intensifying the upwellings in the central part and the downwellings in the periphery. This enhanced curvature of the pycnocline has a positive impact on the CCC because (1) the formation of CIW waters is facilitated in the open basin by the outcropping of the deep isopycnals as shown by Stanev et al. (2003), and (2) the deepening of CIL along the periphery reduces its erosion by the summer heating.

The second mode, CCC-2 (Figure 4.5), interestingly highlights and opposes the two main areas of CIW formation (cf. Introduction). Figure 4.5 indicates that the CCC in the southern part of the basin is mainly affected by the CIL waters formed on the NWS. Figure 4.15 illustrates that a positive anomaly of CCC-2 (stronger CIL formation in the open basin) is frequently associated to atmospheric conditions characterized by a higher positive anomaly of AT on the NWS compared to the open sea (i.e. patterns 4 and 6) while a negative anomaly of CCC-2 (stronger CIL formation on the NWS) is associated to a higher negative anomaly of the NWS AT compared to the rest of the basin (i.e. patterns 1 and 2).

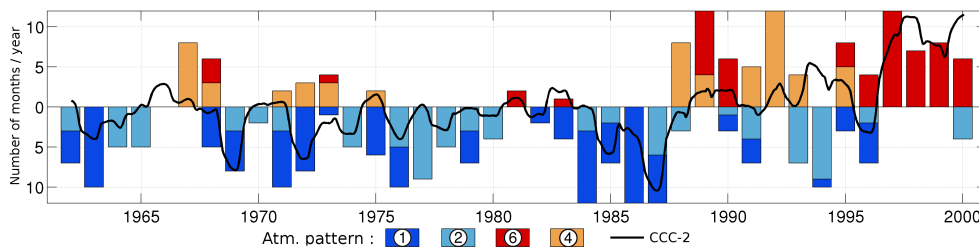


Figure 4.15: Long term evolution of the second temporal EOF mode of the CCC (bold line, CCC-2 shown in Figure 4.5). Positive (resp. negative) phases correspond to a relative enhancement of CIL formation in the open basin (resp. in the NWS). The histograms present for each year the number of months mapped towards patterns 1,2 (both characterized by a negative anomaly of the NWS AT), 4 and 6 (both characterized by a positive anomaly of the NWS AT).

6.4 Impacts on the Black Sea environment

During the second part of the 80s and first part of the 90s, drastic environmental changes affected the Black Sea deep sea ecosystem. Among these changes are the sharp increase of phytoplankton blooms in the open basin (Yunev et al., 2003; Oguz, 2008), the outburst of the invasive ctenophore *Mnemiopsis* responsible for the 10-fold reduction of the biomass of copepods and other zooplankton in the late 1980s (Kovalev and Piontkovski, 1998; Shiganova, 1998), an increase in the inventory of sulfide and nutrients (ammonia, silicate, phosphate) in the anoxic zone and a decrease in the inventory of oxygen in the upper layer (Konovalov and Murray, 2001).

Figures 4.6, (right panels), highlight that most of the physical variables present a singular behavior during the period 1985-1996. This is the case for SLA, MKE, MLD and CCC.

For instance, we note an important enhancement of the Rim current between 1983 (weak circulation) to 1988 (maximum circulation observed during 1962-2000). As explained previously (see section 6.3), enhancement of the Rim current is generally accompanied by an intensification of the CIL formation (see CCC-1 (Figure 4.6)). Additionally, during these particular years the enhancement of the Rim current coincides with an enhancement of the NWS specific CIL formation, as indicated by the strongly negative phase of CCC-2 (Figure 4.15). Since the Rim current and the NWS CIL formation and propagation are responsible for the exchanges of water and materials from the NWS to the deep basin, the intensification of these two processes during the second part of the 80s has promoted the export to the central basin of the products of eutrophication accumulated in the NWS waters and sediments during the long period of weak Rim current and high nutrient riverine discharge (late 70's and early 80's). These materials were then suddenly delivered to the open basin in 1985 and promoted phytoplankton blooms. Conversely, the general decrease of the deep basin phytoplankton biomass during the second part of the 90s corresponds to a general decrease of the Rim current intensity and to reduced CIL formation in the NWS.

The different regimes of the Rim current may have had an important impact on the possibilities of fish larvae retentions and hence, may have played a role in the collapse of small pelagic fishes in favor to the invasive *Mnemiopsis leydi*.

6.5 Climate change

Figures 4.4, 4.5, 4.6 and 4.11 show that none of the investigated variables (SST, MKE, MLD, CCC, AT) presents a consistent trend over the period 1962-2000.

It has been shown (see section 5.3) that the SST trends follow the long term trends of the NAO index. If global warming affected the Black Sea during this period it was by impacting on the air masses circulation, as no AT trends superimposed to its relationship with the NAO can be evidenced. A displacement of the relative position of the teleconnection (see discussion in Hurrell and Deser (2010)) would probably affect the Black Sea response to teleconnection system phases, but as mentioned in section 5.3, the use of the NOAA times series does not allows to take into account these displacements.

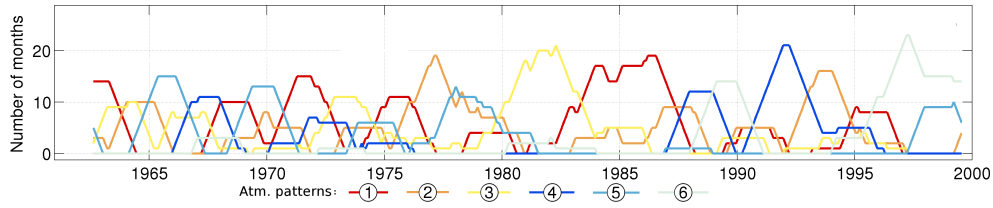


Figure 4.16: Evolution of the duration of the atmospheric anomalies shown in Figure 4.7, estimated as the number of months mapped towards each pattern (a color is attributed to each pattern) in a moving window of 2 years. An increase is observed in the duration of the anomalies regime. For example, the SOM pattern 6 lasted for almost two entire years (23 months over 24) between 1996 and 1998, while no patterns occurred more than 15 months over 24 before 1978.

No increase of the occurrence of a particular atmospheric anomaly pattern can be evidenced during this period neither. However, Figure 4.16 shows that the Black Sea is affected by similar (as identified by the SOM analysis) atmospheric conditions lasting over longer period after 1980. For instance, atmospheric patterns lasting more than a year occurred in 1986, 1992 and 1997 (Figure 4.16). This is of course not straightforward to connect this observed tendency to global warming and this trend has to be confirmed for the 2000-2010 decade.

These types of long lasting anomalies regimes have the potentials to drive the system away from its average state. This occurred during the late 80's during which the Black Sea was affected during 5 years by dominant cold and cyclonic atmospheric anomalies (pattern 1, Figure 4.16) which led to the changes described in section 6.4.

7 Conclusion

The long term (1962-2000) variability of the Black Sea hydrodynamics has been assessed using a 3D high resolution hydrodynamical model. First, the performances of the model in simulating the Black Sea physical properties at interannual scales have been assessed by comparing model outputs with multi-year satellite SST (1985-2000) and SLA (1993-2000). We chose to compare the dominant EOFs of modeled and satellite SST and SLA since this level of validation allows to assess the performances of the model in simulating surface variables but also the dynamics of connected hydrodynamical variables. The correlations between the modeled and satellite spatial and temporal dominant EOFs are most of the time significant and thus the model has the potentials to simulate the Black Sea physical processes at interannual scales. Model simulations have been performed over 40 years and the variability of SST, SLA, MLD, Rim current intensity and CCC were assessed and correlated. The synoptic perspective provided by the model approach allowed to evidence the preponderating role of the variability of the Rim current intensity in various aspects of the Black Sea hydrodynamics.

In particular active (resp. weak) Rim current circulation was shown (1) to lower (resp. raise) the MSL. (2) to promote (resp. reduce) the CIL formation, being in this regard as effective as the Negative (resp. positive) SST anomalies. (3) to enhance (resp. reduce)

the MLD and hence the thermal inertia of surface waters, reducing the SST response to AT anomalies, (4) to convey more (resp. less) effectively heat across the average SST meridional gradient. (5) to enhance (resp. reduce) the exchange between the NWS and the open basin.

In order to connect the variability of the Black Sea hydrodynamics with that of atmospheric conditions over the Black Sea, spatial atmospheric fields (i.e. AT, wind stress and curl) have been analyzed during 1962-2000. Recurrent atmospheric patterns (i.e. various regimes of coincident AT and wind circulation anomalies) have been identified using a SOM analysis. The impact on these patterns of the NAO, EA/WR and ENSO oscillations has also been assessed.

The study shows that the EA/WR and the NAO oscillations both impact on the AT, but with distinct time scales : the rapid oscillations of AT (1-5 years) are driven by the EA/WR oscillation which drives the meridional component of the winds, while on larger time scales (>5 year), the AT variations follow those of the NAO oscillations, as was previously identified by [Oguz et al. \(2006\)](#). Both time scales of the AT variations are followed by the SST. We found no significant relationship between ENSO and the atmospheric patterns which does not imply that ENSO has no impact on the Black Sea SST but rather it means that if ENSO impacts the SST it is not through an AT anomaly resulting from modification of the winds pathways.

It should be noted that the conclusions on the potential influence of large scale climate patterns on the Black Sea local atmospheric conditions are sensitive to the selected temporal and spatial scales (not) considered and this explains why our conclusions are in some points different from other studies. The study address the interannual variability of the Black Sea hydrodynamics.

We have tried to connect the long term variability of the physical environment with that of the ecosystem and in particular, with the drastic environmental changes that occurred at the end of the 80s. We found that, during the period 1985-1995, the intensification of the Rim current and CIL formation process on the NWS have promoted the export to the central basin of the products of eutrophication accumulated in the NWS waters and sediments during the long period of weak Rim current and high nutrient riverine discharge (late 70s and early 80s). These materials were then suddenly delivered to the open basin in 1985 and promoted phytoplankton blooms. Conversely, the general decrease of the deep basin phytoplankton biomass during the second part of the 90s corresponds to a general decrease of the Rim current intensity. The different regimes of the Rim current may have had an important impact on the possibilities of fish larvae retentions and hence, may have played in the collapse of small pelagic fishes in favor to the invasive *Mnemiopsis leydyi*.

We also investigated the existence of a global trend in the hydrodynamical and atmospheric variables during 1962-2000. The only significant trend we found is an increase of the duration of persistent atmospheric anomalies regime over 1962-2000. These types of long lasting anomalies regimes have the potentials to drive the system away from its average state as exemplified by the pronounced enhancement of the Rim current at the end of the 80s as a consequence of a persistent cyclonic wind anomaly affecting the Black Sea over 5 years. This is of course not straightforward to assess whether this trend of an

increase of long lasting atmospheric anomalies regimes is a consequence of climate change but if this tendency is confirmed, we could expect an intensification of the drastic changes affecting marine systems in response to the foreseen increasing global warming (Hansen et al., 2010).

This increase instability of the physical environment may affect the ecosystems by making them more sensitive to human perturbations in the future. This underlines the utmost importance of preserving and promoting the ecosystem resilience (Costanza and Mageau, 1999) by a sound management, as it was already shown to be significantly affected in the Black Sea by human activity (Llope et al., 2011).

8 Appendixes

8.1 Construction of the anomalies compared to a climatological seasonal cycle

Construction of the climatological seasonal cycle : The climatology consists of 366 daily climatological fields and is computed for each day by averaging all the fields present within a 20 day moving window, over the whole period (e.g. 38 years). In the case of model results, for example, each field corresponds to a weekly average. When the corresponding week is only partly covered by the averaging window its contribution to the average is weighed proportionally to the part of the week covered by the averaging window.

Computation of the anomalies : For each original weekly or monthly average field, the anomaly is produced by subtracting from this field the average of the climatological corresponding days.

8.2 Empirical Orthogonal Functions

Each hydrodynamical variable considered in this study is decomposed into its Empirical Orthogonal Functions (EOFs). The EOFs are orthogonal spatial patterns that can be thought of as empirically derived basis functions. The time coefficients obtained by projecting the observed field onto the EOFs are uncorrelated and represent the variability of the field efficiently (Von Storch and Zwiers, 1999)

The EOFs are ordered according to the part of the original signal's variance they represent. Usually, only a few EOFs are required to describe most of the variability of the original variables.

In some circumstances, the spatial modes have a physical meaning and represent the main processes affecting the evolution of the variable but this is, however, not systematically true (Monahan et al., 2009), and the EOFs should in general rather be viewed as axis of main variability allowing a more convenient description of the variable's evolution.

There are several options concerning the normalization of the EOFs. When a mode is homogeneous in sign, this mode is normalized by its basin scale average implying that the

spatial average of this mode is 1 and its temporal mode gives directly the basin average of the variable (e.g. the temporal mode associated to SST-1 shown in Figure 4.4 directly gives the basin wide average of the SST anomaly). Other EOFs are normalized in order to have a standard deviation of the temporal mode equals to 1.

8.3 Definition of the hydrodynamical variables

The mixed layer depth (MLD) is retrieved by linear interpolation of the density profile. It is defined (Kara et al., 2009) as the first depth where a density difference of $\Delta\rho = 0.125 \text{ kg/m}^3$ compared to the density at 3m is found. MLD is expressed in meters counted negatively from the surface.

The CIL Cold Content (CCC) (Staneva and Stanev, 2002) corresponds to $\int (T - 8)dz$, where T is the temperature in $^{\circ}\text{C}$, and the integration is carried out between the upper and lower 8°C isotherms.

The Mean Kinetic Energy (MKE) , $\frac{1}{2}\rho u^2$, where ρ is the density and u the norm of mean velocity, is vertically averaged over the upper 100m.

8.4 Self Organizing Maps (SOM)

We refer to Kohonen (1998) for a mathematical description of the SOM algorithm, and to Richardson et al. (2003) for an illustration of the ways it can be used in oceanography.

The SOM algorithm allows to identify from an initial set of vector elements a subset of vector (the "typical" patterns) optimally representative of the initial set distribution. In the present case, for example, each initial element consist of the fields of AT, wind curl, zonal and meridional component anomalies of one particular month, gathered in a single vector. The representative patterns are those presented in Figure 4.7. The key issue is that it allows to reduce the dimensionality of the initial dataset to a discrete number (chosen prior the analysis) of representative patterns, which facilitates the analysis of the initial dataset. In this case, the SOM analysis allows us to refer to one of the six identified pattern wich are multivariate and contain spatial information, rather than, for example, to the averaged AT.

The procedure allows then to map each element toward one of the representative patterns, based on euclidean distance considerations. As in our case each element corresponds to one month it allows us in particular to relate the teleconnection monthly time series to the identified atmospheric patterns.

If the distribution associated to one pattern, amongst the positive and negative phases of a given teleconnection, is significantly different from a random distribution, it indicates a relationship between the occurrence of this pattern and a given phase of the teleconnection.

As some patterns occurs more often than others, however, the significance of uneven distribution is not the same for each pattern. In order to provide a quantified appreciation of this significance, we assess, for each pattern, the probability of getting the observed distribution for a number of trials equal to this pattern occurrence and under the hypothesis

that each trial as an equal probability of being positive or negative.

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Part II

Biogeochemistry

Chapter 5

Biogeochemical Model : BAMHBI



The Sun Is in Love with the Moon, Mr. Dejo, 2009

This chapter describes the biogeochemical model and its implementation in the Black Sea. It focuses on the pelagic part, as the benthic model and its coupling with the pelagic model are developed in Chapter 6. Model skills in resolving the distribution of nutrients and oxygen reflected by in situ observations are assessed in the last section.

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1 The BAMHBI model

1.1 General approach

The acronym BAMHBI goes for BiogeochemicAl Model for Hypoxic and Benthic Influenced areas. This model resolves the cycling of carbon, nitrogen, phosphorus, silica and oxygen through living, non-living and inorganic forms (26 state variables), across a wide range of environmental contexts.

The 3D BAMHBI model has been developed on the basis of an earlier model described in detail in [Grégoire et al. \(2008\)](#). This earlier version was initially coupled with a vertical (1D) physical model and implemented to study the evolution of the open Black Sea ecosystem during the eutrophication phase. This previous implementation has been validated with in-situ data collected in the open basin area (see [Grégoire et al. \(2008\)](#) for further details).

During this study we extended and adapted this model to meet the requirements of a 3D implementation coupled with the hydrodynamical model (Chap. 3) over the entire Black Sea domain. This required to make sure that the model can adequately resolve the contrasting dynamics across the eutrophic shelf, the oligotrophic basin interior and the deep suboxic and anoxic zones.

The complete description of the BAMHBI model hereafter thus merges previous achievements described in [Grégoire et al. \(2008\)](#) and original developments.

In addition to transposing the model in a 3D context, a major enhancement includes the introduction of the phosphate dynamics, the development of a detailed light penetration scheme and that of the benthic/pelagic coupling module. The benthic module is detailed in the next chapter (Chap. 6).

The state variables of the model are described in Section 1.2 and listed in Table 5.2. In Fig. 6.2 we show a schematic representation of the interactions between the main groups of variables of the ecosystem model. The corresponding equations are given in Tables 5.4 (State equations) and 5.5 (Biogeochemical processes) and are described in Section 1.3. The parameters used in these formulations are listed in Table 5.6 along with corresponding references.

1.2 State Variables

The phytoplankton community is represented by three groups : diatoms, dinoflagellates and small phototrophic flagellates. The diatoms group has been included because several authors report that the planktonic community shifts from siliceous to non-siliceous during the eutrophication phase ([Eker et al., 2000](#); [Moncheva et al., 2001](#); [Eker-Develi and Kideys, 2003](#)). The small phototrophic flagellates group aggregates pico- and nanophototrophic flagellates, amongst them coccolithophorids. To dissociate the carbon and nitrogen internal content for these three functional groups (cf. 1.3), phytoplankton are described in the model by six independent state variables.

The model considers micro- (mainly ciliates and protozoa), meso-zooplankton (mainly copepods) and gelatinous zooplankton.

Four species of gelatinous carnivores are common in the Black Sea: two scyphozoans, *Aurelia aurita* and *Rhyzostoma pulmo*, and two ctenophores, *Pleurobrachia pileus* and *Mnemiopsis*. While *Rhyzostoma pulmo* is most common in coastal areas, the three other species are distributed in all parts of the Black Sea (Mutlu et al., 1994). In the model, the latter three species are joined within the carnivorous gelatinous functional group. The complexity of the gelatinous life cycle combined to the lack of data and knowledge prevents an accurate description of the gelatinous dynamics and these have mainly to be perceived here as a sophisticated closure term to the lower trophic levels. The model also involves an explicit representation of an omnivorous gelatinous group (mainly *Noctiluca scintillans*). These two gelatinous zooplankton functional groups are 'top-predators' and no trophic link exists between them.

Along with the bacteria, the microbial loop is represented through particulate (POM), semi-labile and labile dissolved organic forms (DOM), for both nitrogen and carbon. A distinct particulate forms is considered for siliceous detritus, while the phosphate content in detrital matter is assumed to be stoichiometrically linked to the nitrogen content.

Three limiting nutrients are considered: phosphate, silicate and nitrogen. Due to their different dynamics in anoxic environment, inorganic nitrogen is divided amongst ammonium and "nitrate+nitrite" (further termed as "nitrate"). Oxygen is explicitly represented with an additional compartment, the Oxygen Demanding Unit (ODU), that lumps all the reduced substances present in the suboxic and anoxic environment specific to the Black Sea.

1.3 Biogeochemical Processes

Living groups

Autotrophs Temporal decoupling of carbon and nutrient dynamics may result from metabolic instabilities in algae, as reported after bloom events (Engel et al., 2002; Wetz and Wheeler, 2003) or under environmental stresses (e.g. light or nutrients limitation) (Mague et al., 1980). This is reflected, for instance, in the accumulation of carbon-rich dissolved organic matter (DOM) (Søndergaard et al., 2000), an increase in the particulate C:N ratio, and the formation of transparent, carbon-rich, exopolymeric particles (Alldredge et al., 1995).

The unbalanced growth model (Tett, 1998; Smith and Tett, 2000) permits to dissociate the internal carbon and nitrogen content, and allows for a potential control of growth by several nutrients and light.

Carbon assimilation (photosynthesis) is directly synonymous with growth. Phytoplanktonic growth rates increase with higher N:C ratios and are limited by nutrients and light (5.34, 5.35).

The uncoupling between nitrogen and carbon occurs by allowing uptake of nutrients

in excess of immediate need for growth. Nitrogen uptake increases at low phytoplankton N:C ratios and is unaffected by light (e.g. [Laws and Wong, 1978](#)). Ammonium inhibits the uptake of nitrate. Growth is also limited by the availability of phosphate and, for diatoms, by silicate.

The necessary uptake of phosphate and silicate are computed to maintain the group specific N:P and N:Si ratios (Table 5.6). The vertical sinking speed of diatoms increases with high C:N ratio([5.44](#)).

A fixed fraction of the phytoplankton carbon uptake is excreted through leakage (Eq. [5.39](#)). An 'overflow' of photosynthesis may also occurs under nutrient limitation and produce 'extra' carbon excretion, depending on the difference between the actual and optimal internal N:C ratio (Eq. [5.40](#)) ([Van den Meersche et al., 2004](#)). Passive and active excretion are distributed among the labile and semi-labile pool of DOM ([5.16](#), [5.18](#), [Anderson and Pondaven \(2003\)](#)). In addition, phytoplankton mortality ([5.41](#)) contributes to both POM and DOM pools and dissolved inorganic carbon is released through basal and activity respiration ([5.38](#)).

Heterotrophs P:N:C ratios are considered fixed for bacteria and zooplankton groups. The bioenergetic model ([Anderson, 1992](#); [Anderson and le B Williams, 1998](#); [Anderson and Pondaven, 2003](#)) simulates the effect of food availability and quality (its relative carbon and nitrogen content) on growth rates, nitrogen excretion and carbon respiration.

The food ingested by micro- and mesozooplankton is used for growth and respiration, considering fractions of unassimilation and messy feeding losses ([5.49](#)). N:C ratios are maintained on a constant level through excretion and respiration: surplus nitrogen in the assimilated food is excreted while surplus carbon is oxygenated by respiration ([5.50](#), [5.51](#), [5.52](#), [5.53](#)).

The mortality terms gathers a density-dependent term (a closure term including the predation from fishes) and a term reflecting mortality in oxygen deficient conditions ([5.54](#)).

Bacterial growth is first sustained by labile DOM. Ammonium uptake is permitted to supplement DON when the N:C ratio of DOM is low. Otherwise ammonium is released from the bacterial remineralization of the DON ([5.68](#), [5.69](#), [5.70](#), [5.71](#) and [5.72](#)). Bacterial mortality is distributed among labile and semi-labile DOM ([5.73](#)).

Gelatinous Zooplankton The representation of gelatinous zooplankton is based on the works of [Lancelot et al. \(2002\)](#)). *Noctiluca* is known to feed on a large spectrum of prey (e.g. [Kirchner et al., 1996](#); [Shanks and Walters, 1996](#); [Nakamura, 1998](#)), including mainly phytoplankton cells but also copepods eggs, fish eggs, protozoans in marine snow and possibly bacteria. Laboratory culture experiments ([Nakamura, 1998](#)) have shown that *Noctiluca* has a grazing rate that increases linearly with prey carbon concentrations without any threshold. In the model, the clearance rate has been chosen about one order of magnitude lower than that of mesozooplankton. A relatively important growth threshold makes *Noctiluca* more adapted to eutrophic conditions. The growth efficiency defined as the ratio between the grazing rate and the growth rate is attributed according to culture experiments ([Nakamura, 1998](#)).

Gelatinous carnivores feed at high rates on zooplankton and ichthyoplankton, and thereby may be detrimental to fish populations. In the model, these animals are strictly carnivorous and only eat mesozooplankton.

For both omnivore and carnivore, feeding by the gelatinous does not saturate at natural prey concentrations and the grazing rate increases linearly with respect to food without saturation at high concentration (5.55, 5.56).

Internal composition is maintained constant by adjusting the excretion and respiration terms (5.63, 5.64, 5.65). Kremer (1994) found that three factors act in a hierarchy to determine the abundance of *Mnemiopsis*, with temperature being the most important, food availability second, and mortality (predation) third (in their native environment, their biomass is controlled by predators). In the model *Mnemiopsis* presents a strong response to temperature

Gelatinous organisms represent trophic dead-ends and their mortality is represented by the sum of a first-order kinetics (Lancelot et al., 2002) and an additional term traducing the rapid mortality of these organisms in anoxic conditions (equation 5.66).

Detrital Matter

Dissolved Organic Matter

The 'labile' pool is the only pool directly taken up by bacteria. The assimilation of the 'semi-labile' pool requires first ectoenzyme hydrolysis to the labile pool which is described by Michaelis-Menten kinetics (5.74, 5.75) with bacterial biomass as the limiting variable. Both labile and semi-labile pools have a variable C:N ratio and a fixed P:N ratio. Fluxes to the DOM pool (i.e. phytoplankton excretion and lysis (5.39, 5.41), zooplankton 'messy feeding' (5.49), bacterial lysis (5.73) and detrital breakdown (5.76, 5.77)) are distributed between the labile and semi-labile pools in fixed proportions (Anderson and Pondaven, 2003). Phytoplankton leakage is assumed to produce only labile DOM.

Particulate Organic matter (non-living) We consider a preferential decomposition of PON relative to POC (Anderson and Pondaven, 2003). POM sinking is described using the aggregation model developed by Kriest (2002) (5.79, 5.80, 5.81 and 5.82), which adds a state variable to describe the number of aggregates in each cell. This model assumes that the number of particles $n(d_i)$ of size d_i , the mass of particles $m(d_i)$ and their sinking speeds $w(d_i)$ can be represented by a two-parameter power law of the form: $y(d_i) = Ad_i^{-\alpha}$, where d_i is the diameter of a particle, and A and α are specific constants. It is supposed that only detritus can form aggregates and these are assumed to be produced/removed at the same rate as detritus (5.26). The stickiness parameter, i.e. the probability that two particles stick together, has been calibrated in Grégoire et al. (2008) based on sediment trap data (Karl and Knauer, 1991).

Inorganic Dissolved constituents In the oxygenated part of the water column, ammonium is converted into nitrate through nitrification (5.88). Dissolved silicate is pro-

duced by the chemical dissolution of siliceous detritus (5.78). Phosphate dynamics is stoichiometrically linked to nitrogen in the organic forms and is only released in specific phosphate units in the final step of mineralization by bacteria.

Anoxic and suboxic conditions

Chemical processes in the anoxic layer In anoxic marine basins such as the Black Sea, the remineralization of organic matter by bacteria occurs with different types of oxidants: oxygen in the upper oxygenated layer, nitrate in the suboxic layer (i.e. denitrification) and other oxidants (e.g. manganese oxides, iron oxides, sulphate) in the anoxic layer. Due to the similarity of this vertical structure with that of sediments, an early diagenetic model developed for the sediments (Soetaert et al., 1996) has been used to describe the chemical processes in the water column.

The consumption of oxygen and of nitrate by bacterial respiration are respectively limited by the availability of oxygen and nitrate. Additionally, nitrate consumption is inhibited by the presence of oxygen (5.84, 5.85).

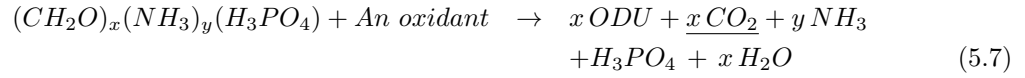
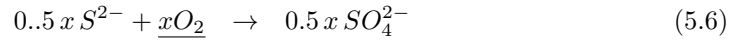
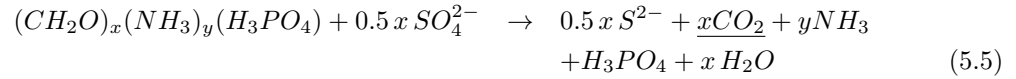
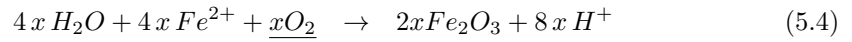
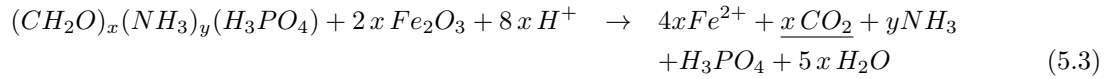
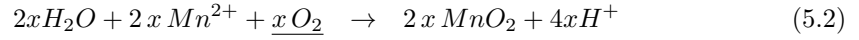
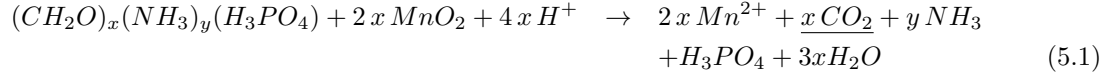
The anaerobic respiration process involves manganese, iron and sulfate as oxidants and produces reduced substances (5.1, 5.3 and 5.5). Complete re-oxidation of these reduced substances, formed through the oxidation of x moles of carbon, requires x moles of oxygen, whatever the anoxic pathway considered (5.2, 5.4 and 5.6). These processes are therefore lumped together into one process termed "anoxic mineralization" (5.1, 5.7, 5.8), in which degradation is only limited by carbon (the quantity of oxidants is assumed non-limiting) and which is inhibited by the presence of oxygen and nitrate (5.86). The state variable lumping the reduced substance is termed ODU (i.e. Apparent Oxygen Demand Unit) with $ODU = 0.5 H_2S + 2 Mn^{2+} + 4 Fe^{2+}$. This approach is convenient for our modeling purposes because we do not aim at resolving the details of manganese and iron cycling.

The oxidation of ODU and ammonium diffusing towards the suboxic layer is represented as a chemical reaction, limited by the availability of oxidants. Oxidation by nitrate is inhibited when oxygen is present in sufficiency (5.88, 5.89, 5.90, 5.91). The denitrification process as well as the oxidation of ammonium and ODU by nitrate constitute a loss of nitrogen for the system (in the form of dissolved dinitrogen, not represented in the model).

It should be noted that the use of limiting and inhibiting functions in our numerical model allows us to use a single model system across the oxygenation gradient.

POM degradation in the anoxic layer Observations in the Black Sea have shown that organic matter decomposition under anaerobic conditions is not as rapid and/or complete as oxic decomposition (R.V. KNORR cruise, Mopper and Kieber (1991)). The question why and how this is so led to much debate (see Hedges et al. (1999), Grégoire et al. (2008), and references therein) but is not addressed here specifically. In the model, the low efficiency of POM degradation in anaerobic conditions is attributed to the absence of oxygen and therefore is represented with an oxygen limiting function (5.76, 5.77).

Table 5.1: Idealized chemical reactions lumped in the model in the expression of Eqs. 5.7 and 5.8. The amount of CO_2 produced and the amount of O_2 needed to oxidize the reduced substance are underlined. y denotes the molar N:P ratio, x the molar C:P ratio in organic matter per mole of phosphorus (for Redfield Stoichiometry, $x=106$, $y=16$). ODU stands for Oxygen Demand Units.



Metal sulfide formation Muramoto et al. (1991) found that the observed sulfide concentrations in the 75-200 m depth interval of the Black Sea are consistently lower than expected if sulfide was considered as a conservative tracer of water mixing. This indicates that this area is a site of net consumption of dissolved sulfide due to oxidation and/or precipitation of pyrite, metal sulfides and other sulfur compounds as well as scavenging with the sinking organic matter. In agreement, the study of the relationship between reduced sulfur and organic carbon content in Black Sea sediments suggests that sulfide precipitation should be occurring in the anoxic water column above sediments (Jørgensen et al., 1991) and could be associated to the formation of metal sulfide as evidenced by the maximum FeS concentration at 50-100 m below the sulfidic interface (e.g. Jørgensen et al., 1991).

In the model, a part of the formed ODU is permanently removed as metal sulfides in the upper part of the anoxic layer where dissolved metals are available. This process is limited by iron availability according to a Michaelis Menten function (a fixed iron profile obtained from observations is imposed to the model)(equation 5.87).

Temperature dependency of all biogeochemical processes All the modeled processes depend on temperature, with a specific increase for each 10°C of temperature

increase (Q_{10} formulation, equation 5.28).

1.4 Light penetration scheme - Extension for the biogeochemical simulations

The enhancement of the water optical properties constitutes an original development. Given the peculiar optical properties of Black Sea waters, this development was applied to resolve more accurately the control that the restriction of light penetration exerts on phytoplankton dynamics.

The traditional use of optical case-types (Jerlov, 1976) to derive the extinction coefficient (Kara et al., 2005, e.g.) is an approximation usually made necessary by the non-resolution of the seawater optical constituents (Morel and Maritorena, 2001; Mobley et al., 2004). Because our model is resolving the concentrations of most of these constituents, and in particular the mechanism of resuspension required to represent the dynamics of inert mineral particles, we took the opportunity to develop an optical model considering the specific inherent optical properties as initiated by (Bissett et al., 1999).

The surface insolation is divided in three bandwidths as in the physical model, but the attenuation coefficients for the long and short wave bands are now computed interactively at each model grid and time step.

The attenuation coefficients, k_s and k_l (respectively for short and long waves), are computed from the total absorption (a_s and a_l) and backscattering (b_s and b_l) coefficients, according to Lee et al. (2005a) (5.30). The inherent optical properties (IOPs), a and b sums up the contributions of sea water optical constituents.

Light is absorbed by the seawater, the chlorophyll content, particulate organic carbon and colored dissolved organic matter (CDOM) (5.32). The absorption is constant for pure seawater (Smith and Baker, 1981). It is derived from specific absorption rates and concentrations for particulate organic carbon and suspended minerals (Neukermans et al., 2012). Chlorophyll's specific absorption is expressed as a power law of the chlorophyll content (Bricaud et al., 1995). CDOM concentration is influenced by past phytoplankton concentrations and photo-bleaching (Mobley et al., 2004). As the dynamics of CDOM is not resolved by the model, a dominant river origin is assumed (Mobley et al., 2004). CDOM absorption is therefore computed using salinity as a proxy (Kowalczyk et al., 2003; Xu et al., 2005), and the corresponding coefficients were calibrated on the basis of in situ light extinction profiles (Churilova, 2001), after having computed the other terms using simulated concentrations.

Backscattering is very small for pure seawater (Smith and Baker, 1981). As specific backscattering differs with the size and shape of phytoplankton cells, average values for the model groups were interpreted from Vaillancourt et al. (2004). Backscattering of suspended minerals is obtained by considering the backscattering fraction (Doerffer and Schiller, 2007) of the total specific scattering coefficients (Mobley et al., 2004). Particulate organic matter specific backscattering coefficients are obtained from Neukermans et al. (2012). Finally, backscattering may be neglected for the CDOM (Bissett et al., 1999).

1.5 Equations and parameters

Table 5.2: List of biogeochemical state variables, description, and units.

STATE VARIABLES	DESCRIPTION	UNITS
<i>NOS</i>	Nitrate + nitrite	mmolN m^{-3}
<i>NHS</i>	Ammonium	mmolN m^{-3}
<i>PHO</i>	Phosphate	mmolP m^{-3}
<i>SIO</i>	Silicate	mmolSi m^{-3}
<i>DOX</i>	Dissolved oxygen	mmolO ₂ m^{-3}
<i>DIC</i>	Dissolved inorganic carbon	mmolC m^{-3}
<i>ODU</i>	Oxygen demand unit	mmolODU m^{-3}
<i>SMI</i>	Suspended minerals (inert)	mg m^{-3}
<i>NPHY</i> ₁ , <i>CPHY</i> ₁	Small phototrophic flagellates	mmolN m^{-3} , mmolN m^{-3}
<i>NPHY</i> ₂ , <i>CPHY</i> ₂	Dinoflagellates	mmolN m^{-3} , mmolN m^{-3}
<i>NPHY</i> ₃ , <i>CPHY</i> ₃	Diatoms	mmolC m^{-3} , mmolN m^{-3}
<i>CZOO</i> ₁	Microzooplankton	mmolC m^{-3}
<i>CZOO</i> ₂	Mesozooplankton	mmolC m^{-3}
<i>CGEL</i> ₁	Omnivorous gelatinous	mmolC m^{-3}
<i>CGEL</i> ₂	Carnivorous gelatinous	mmolC m^{-3}
<i>BAC</i>	Bacteria	mmolC m^{-3}
<i>DOCL</i> , <i>DONL</i>	Labile dissolved organic C and N	mmol C m^{-3} , mmolN m^{-3}
<i>DOCSL</i> , <i>DONSL</i>	Semi-labile dissolved organic C and N	mmol C m^{-3} , mmol N m^{-3}
<i>POC</i> , <i>PON</i>	Particulate organic carbon and nitrogen	mmol C m^{-3} , mmol N m^{-3}
<i>SID</i>	Detrital particulate silicate	mmolSi m^{-3}
<i>AGG</i>	Number of aggregates	m^{-3}

Table 5.3: List of variables used in Tables 5.4 and 5.5

VARIABLES	DESCRIPTION	UNITS
$\tilde{\lambda}$	Turbulent diffusion coefficient	m^2s^{-1}
$f(T)$	Temperature factor	-
<i>PAR</i>	Photosynthetic Active Radiation	Wm ⁻²
<i>Q</i>	Solar Radiation at the sea surface	Wm ⁻²
k_s	Attenuation coef. for short waves ([400-580] nm)	m^{-1}
a_s	total absorption coef. for short waves	m^{-1}
b_s	total backscattering coef. for short waves	m^{-1}
k_l	Attenuation coef. for long waves ([580-700] nm)	m^{-1}
a_l	total absorption coef. for long waves	m^{-1}
b_l	total backscattering coef. for long waves	m^{-1}
<i>Chl</i>	Chlorophyll	mgChl m^{-3}
$(Chl : C)_{PHY_i}$	Phytoplankton <i>i</i> chlorophyll:carbon ratio	gChl molC ⁻¹
$(N : C)_{PHY_i}$	Phytoplankton <i>i</i> nitrogen:carbon ratio	molN molC ⁻¹

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VARIABLES	DESCRIPTION	UNITS
$(N : Si)_{PHY_3}$	Phytoplankton 3 nitrogen:silicate ratio	molN molSi ⁻¹
$(N : P)_{PHY_i}$	Phytoplankton i nitrogen:phosphate ratio	molN molP ⁻¹
$PhotosynthPHY_i$	Phytoplankton i photosynthesis	mmolC m ⁻³ d ⁻¹
$RespirationPHY_i$	Phytoplankton i respiration	mmolC m ⁻³ d ⁻¹
$LeakagePHY_{C,i}$	Phytoplankton i passive leakage in carbon	mmolC m ⁻³ d ⁻¹
$ExtraExcrPHY_i$	Phytoplankton i extra-excretion	mmolC m ⁻³ d ⁻¹
U_i^{*NOS}	Phytoplankton i potential nitrate uptake	mmolN m ⁻³ d ⁻¹
U_i^{NOS}	Phytoplankton i nitrate uptake	mmolN m ⁻³ d ⁻¹
U_i^{*NHS}	Phytoplankton i potential ammonium uptake	mmolN m ⁻³ d ⁻¹
U_i^{NHS}	Phytoplankton i ammonium uptake	mmolN m ⁻³ d ⁻¹
U_i^{*PHO}	Phytoplankton i potential phosphate uptake	mmolN m ⁻³ d ⁻¹
U_i^{PHO}	Phytoplankton i phosphate uptake	mmolN m ⁻³ d ⁻¹
U_i^{*SIO}	Diatoms silicate potential uptake	mmolSi m ⁻³ d ⁻¹
U_i^{SIO}	Diatoms silicate uptake	mmolSi m ⁻³ d ⁻¹
v_{PHY_3}	Diatoms sinking rate	m d ⁻¹
$DissolutionSID$	Dissolution rate of detrital particulate silicate	mmolSi m ⁻³ d ⁻¹
$LeakagePHY_{N,i}$	Phytoplankton i passive leakage in nitrogen	mmolN m ⁻³ d ⁻¹
$MortPHY_{C,i}$	Phytoplankton i mortality flux in carbon	mmolC m ⁻³ d ⁻¹
$MortPHY_{N,i}$	Phytoplankton i mortality flux in nitrogen	mmolN m ⁻³ d ⁻¹
$GrazZOO_{C,j}$	Grazing flux of zooplankton j in carbon	mmolC m ⁻³ d ⁻¹
$GrazZOO_{N,j}$	Grazing flux of zooplankton j in nitrogen	mmolN m ⁻³ d ⁻¹
$GrazPrey_i$	Grazing flux of prey i by all its predators	mmol m ⁻³ d ⁻¹
$I_{C,j}$	Zooplankton j intake of carbon	mmolC m ⁻³ d ⁻¹
$I_{N,j}$	Zooplankton j intake of nitrogen	mmolN m ⁻³ d ⁻¹
$GrowthZOO_{C,j}$	Zooplankton j growth flux in carbon	mmolC m ⁻³ d ⁻¹
$GrowthZOO_{N,j}$	Zooplankton j growth flux in nitrogen	mmolN m ⁻³ d ⁻¹
$ExcrZOO_j$	Zooplankton j excretion flux of ammonium	mmolN m ⁻³ d ⁻¹
$RespZOO_j$	Zooplankton j respiration flux	mmolC m ⁻³ d ⁻¹
$MortZOO_{C,j}$	Zooplankton j mortality flux	mmolC m ⁻³ d ⁻¹
$GrazGEL_{C,j}$	Grazing flux of gelatinous j in carbon	mmolC m ⁻³
$GrazGEL_{N,j}$	Grazing flux of gelatinous j in nitrogen	mmolN m ⁻³
$GrowthGEL_{C,j}$	Gelatinous j growth in carbon	mmolC m ⁻³ d ⁻¹
$EgestGEL_{C,j}$	Gelatinous j Egestion flux in carbon	mmolC m ⁻³ d ⁻¹
$EgestGEL_{N,j}$	Gelatinous j Egestion flux in nitrogen	mmolN m ⁻³ d ⁻¹
$RespGEL_j$	Gelatinous j respiration flux	mmolC m ⁻³ d ⁻¹
$AdjExcrGEL_j$	Potential Excretion flux necessary to maintain constant the N:C ratio of Gelatinous j	mmol N m ⁻³ d ⁻¹
$AdjRespGEL_j$	Potential Additional respiration flux necessary to maintain constant the N:C ratio of Gelatinous j	mmol C m ⁻³ d ⁻¹
$MortGEL_{C,j}$	Gelatinous j mortality flux	mmolC m ⁻³ d ⁻¹
U_{BAC}^{DOC}	Bacteria uptake of DOC	mmolC m ⁻³ d ⁻¹
U_{BAC}^{DON}	Bacteria uptake of DON	mmolN m ⁻³ d ⁻¹

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VARIABLES	DESCRIPTION	UNITS
U_{BAC}^{*NHS}	Bacteria potential uptake of ammonium	$\text{mmolN m}^{-3}\text{d}^{-1}$
U_{BAC}^{NHS}	Bacteria uptake of ammonium	$\text{mmolN m}^{-3}\text{d}^{-1}$
$GrowthBAC$	Bacteria growth flux	$\text{mmolC m}^{-3}\text{d}^{-1}$
$RespBAC$	Bacteria respiration flux	$\text{mmolC m}^{-3}\text{d}^{-1}$
$ExcrBAC$	Bacteria excretion flux of ammonium	$\text{mmolN m}^{-3}\text{d}^{-1}$
$TestBAC$	intermediary variable	$\text{mmolN m}^{-3}\text{d}^{-1}$
$MortBAC_C$	Bacteria mortality flux in carbon	$\text{mmolC m}^{-3}\text{d}^{-1}$
$HydrolDOCSL$	Hydrolysis rate of Semi-labile DOC into Labile DOC	$\text{mmolC m}^{-3}\text{d}^{-1}$
$HydrolDONSL$	Hydrolysis rate of Semi-labile DON into Labile DON	$\text{mmolN m}^{-3}\text{d}^{-1}$
$HydrolPOC$	Hydrolysis rate of POC into Labile and Semi-Labile DOC	$\text{mmolC m}^{-3}\text{d}^{-1}$
$HydrolPON$	Hydrolysis rate of PON into Labile and Semi-Labile DON	$\text{mmolN m}^{-3}\text{d}^{-1}$
v_{POM}	POM sinking rate	m d^{-1}
v_{AGG}	Aggregates sinking rate	m d^{-1}
$Aggregation$	Aggregation rate of particles after collision due to differential settelment and shear	number of particles $\text{m}^{-3}\text{d}^{-1}$
$RespBACOxygen$	Oxic bacterial respiration flux	$\text{mmolC m}^{-3}\text{d}^{-1}$
$RespBACNitrate$	Bacterial respiration flux using nitrate as oxidant	$\text{mmolC m}^{-3}\text{d}^{-1}$
$AnoxicRespBAC$	Anoxic bacterial respiration flux	$\text{mmolC m}^{-3}\text{d}^{-1}$
$SolidODU$	the amount of ODU deposited as solids (metal sulfide formation)	$\text{mmolODU m}^{-3}\text{d}^{-1}$
$ODUoxid_{DOX}$	oxidation rate of ODU by oxygen	d^{-1}
$ODUoxid_{NOS}$	oxidation rate of ODU by nitrate	d^{-1}
$NHSoxid_{DOX}$	oxidation rate of NHS by oxygen (Nitrification)	d^{-1}
$NHSoxid_{NOS}$	oxidation rate of NHS by nitrate	d^{-1}

Table 5.4: Biogeochemical variables state equations

$$\frac{dX}{dt} = \kappa_h \nabla_h^2 X + \frac{\partial}{\partial z} \left(\tilde{\lambda} \frac{\partial X}{\partial z} \right) - \frac{\partial(v_X X)}{\partial z} + Q_X \quad (5.9)$$

$$Q_{CPHY_i} = PhotosynthPHY_i - RespirationPHY_i - LeakagePHY_{C,i} - MortPHY_{C,i} - GrazCPHY_i \quad i = 1, 2, 3 \quad (5.10)$$

$$Q_{NPHY_i} = (U_i^{NOS} + U_i^{NHS}) - LeakagePHY_{N,i} - MortPHY_{N,i} - GrazNPHY_i \quad i = 1, 2, 3 \quad (5.11)$$

$$Q_{CZOO_j} = GrowthZOO_{C,j} - MortZOO_{C,j} - GrazCZOO_j \quad j = 1, 2 \quad (5.12)$$

$$Q_{CGEL_j} = GrowthGEL_{C,j} - MortGEL_{C,j} - AdjRespGEL_j \quad j = 1, 2$$

$$Q_{BAC} = GrowthBAC - MortBAC_C - GrazBAC$$

$$Q_{NOS} = - \sum_{j=1}^3 NO_{3,j}^{up} + NHS_{oxid_{DOX}} NHS - RespBAC_{Nitrate} \gamma_{NOS}^{POC} - NHS_{oxid_{NOS}} NHS \gamma_{NOS}^{NHS} - ODU_{oxid_{NOS}} ODU \gamma_{NOS}^{ODU} \quad (5.13)$$

$$Q_{NHS} = \sum_{j=1}^2 (ExcrZOO_j + AdjExcrGEL_j) + ExcrBAC - \sum_{j=1}^3 NHS_j^{up} - U_{BAC}^{NHS} - NHS_{oxid_{NOS}} NHS - NHS_{oxid_{DOX}} NHS \quad (5.14)$$

$$Q_{SIO} = -U_i^{SIO} + DissolutionSID \quad (5.15)$$

$$Q_{PHO} = - \sum_{j=1}^3 PHO_j^{up} + ExcrBAC / (N : P) - U_{BAC}^{NHS} / (N : P) + \sum_{j=1}^2 (ExcrZOO_j + AdjExcrGEL_j) / (N : P)$$

$$Q_{DOCL} = \sum_{i=1}^3 [LeakagePHY_{C,i} + \gamma_1 ExtraExcrPHY_i + (1 - \gamma_1) \delta_2 ExtraExcrPHY_i] + \delta_1 \left[\epsilon \sum_{i=1}^3 MortPHY_{C,i} + \phi_i \sum_{j=1}^2 GrazZOO_{C,j} + MortBAC_C + HydrolPOC \right] + HydrolDOCSL - U_{BAC}^{DOC} \quad (5.16)$$

$$Q_{DONL} = \sum_{i=1}^3 [LeakagePHY_{N,i}] + \delta_1 \left[\epsilon \sum_{i=1}^3 MortPHY_{N,i} + \phi_i \sum_{j=1}^2 GrazZOO_{N,j} + \frac{MortBAC_C}{(C : N)_{BAC}} + HydrolPON \right] + HydrolDONSL - U_{BAC}^{DON} \quad (5.17)$$

$$Q_{DOCSL} = \sum_{i=1}^3 [(1 - \gamma_1)(1 - \delta_2)ExtraExcrPHY_i] \quad (5.18)$$

$$Q_{DONSL} = (1 - \delta_1) \left[\epsilon \sum_{i=1}^3 MortPHY_{C,i} + \phi_i \sum_{j=1}^2 GrazZOO_{C,j} + HydrolPOC + MortBAC_C \right] - HydrolDOCSL$$

$$= (1 - \delta_1) \left[\epsilon \sum_{i=1}^3 MortPHY_{N,i} + \phi_i \sum_{j=1}^2 GrazZOO_{N,j} + HydrolPON + \frac{MortBAC_C}{(C : N)_{BAC}} \right] - HydrolDONSL \quad (5.19)$$

$$Q_{POC} = \sum_{i=1}^3 (1 - \epsilon) MortPHY_{C,j} + \sum_{j=1}^2 [MortZOO_{C,j} + MortGEL_{C,j}] \quad (5.20)$$

$$+ \sum_{j=1}^2 [(1 - \beta_C) I_{C,j} + (1 - AssEffGEL_j) GrazGEL_{C,j}] - HydrolPOC - GrazPOC$$

$$Q_{PON} = \sum_{i=1}^3 (1 - \epsilon) MortPHY_{N,j} \quad (5.21)$$

$$+ \sum_{j=1}^2 \left[\frac{MortZOO_{C,j}}{(C : N)_{ZOO_j}} + \frac{MortGEL_{C,j}}{(C : N)_{GEL_j}} + (1 - \beta_N) I_{N,j} + (1 - AssEffGEL_j) GrazGEL_{N,j} \right] - HydrolPON - GrazPON$$

$$Q_{SID} = \frac{\partial}{\partial z} \left(\tilde{\lambda} \frac{\partial SID}{\partial z} \right) - \frac{\partial (v_{SID} SID)}{\partial z} - DissolutionSID \quad (5.22)$$

$$+ (MortPHY_{N,3} + GrazNPHY_3)(Si : N)_{PHY_3}$$

$$Q_{ODU} = \gamma_{ODU}^{POC} AnoxicRespBAC - ODUoxid_{NOS} ODU - ODUoxid_{DOX} ODU - SolidODU \quad (5.23)$$

$$Q_{DOX} = \sum_{i=1}^3 (PhotosynthPHY_i + ExtraExcrPHY_i) \gamma_{DOX}^C \quad (5.24)$$

$$- \sum_{j=1}^2 (RespZOO_j + RespGEL_j + AdjRespGEL_j) \gamma_{DOX}^C$$

$$- RespBAC_{Oxygen} \gamma_{DOX}^C - NHSoxid_{DOX} NHS \gamma_{DOX}^{NHS} - ODUoxid_{DOX} ODU \gamma_{DOX}^{ODU}$$

$$Q_{DIC} = RespBAC + \sum_{j=1}^2 (RespZOO_j + RespGEL_j + AdjRespGEL_j) - \quad (5.25)$$

$$\sum_{i=1}^3 (PhotosynthPHY_i + ExtraExcrPHY_i)$$

$$Q_{AGG} = Q_{PON} \frac{AGG}{PON} - Aggregation \quad (5.26)$$

$$Q_{SMI} = 0 \quad (5.27)$$

Table 5.5: Biogeochemical processes equations

$$f^T = Q_{10}^{\frac{T-20}{10}} \quad (5.28)$$

Optical properties

$$PAR = |Q_s| [(p_{IR}) \exp(k_{IR}z) + (1 - p_{IR}) \cdot ((p_l) \exp(k_l z) + (1 - p_l) \exp(k_s z))] \quad (5.29)$$

$$k_\lambda = m_0 a_\lambda + m_1 (1 - m_2 e^{m_3 a_\lambda}) b_\lambda, \text{ for } \lambda = s, l \quad (5.30)$$

$$m_0 = 1 + 0.005\theta \quad (5.31)$$

$$a_\lambda = a_{\lambda,sw} + [(a_{\lambda,Chl}^* \cdot Chl^{\hat{a}_{\lambda,Chl}}) \cdot Chl] + [a_{\lambda,SMI}^* SMI] + [a_{\lambda,POC}^* POC] \\ + [a_{\lambda,CDOM}^* - a_{\lambda,CDOM}^{**} S] \quad , \text{ where } S \text{ is the salinity.} \quad (5.32)$$

$$b_\lambda = b_{\lambda,sw} + b_{\lambda,PHY_1}^* CPHY_1 + b_{\lambda,PHY_2}^* CPHY_2 + b_{\lambda,PHY_3}^* CPHY_3 \\ + b_{\lambda,SMI}^* SMI + b_{\lambda,POC}^* POC \quad (5.33)$$

Phytoplankton, $(i = 1, 2, 3)$

$$PhotosynthPHY_i = \mu_{max,i} f^T \min(lim_{nut,i}, lim_{light,i}) CPHY_i \quad (5.34)$$

$$\text{with } \begin{cases} lim_{light,i} = 1 - \exp\left[-\frac{\alpha_i I(z)}{\mu_{max,i}}\right] \\ lim_{nut,i} = \left(1 - \frac{(N:C)_{PHY_i,min}}{(N:C)_{PHY_i}}\right) \text{ for } (i = 1, 2) \\ lim_{nut,3} = \min\left[\left(1 - \frac{(N:C)_{PHY_3,min}}{(N:C)_{PHY_3}}\right), \left(1 - \frac{(Si:C)_{PHY_3,min}}{(Si:C)_{PHY_3}}\right)\right] \text{ for } (i = 3) \end{cases} \quad (5.35)$$

Chlorophyll

$$Chl = \sum_{i=1}^3 CPHY_i (Chl : C)_{PHY_i} \quad (5.36)$$

Chl:C

$$\begin{cases} \text{for } (N : C)_{PHY_i,min} \leq (N : C)_{PHY_i} \leq (N : C)_{PHY_i,max} : \\ (Chl : C)_{PHY_i} = (N : C)_{PHY_i} \left\{ (Chl : N)_{PHY_i,min} + [(Chl : N)_{PHY_i,max} \dots \right. \\ \left. \dots - (Chl : N)_{PHY_i,min}] \times \frac{(N:C)_{PHY_i} - (N:C)_{PHY_i,min}}{(N:C)_{PHY_i,max} - (N:C)_{PHY_i,min}} \right\} \\ \text{for } (N : C)_{PHY_i} \leq (N : C)_{PHY_i,min} \\ (Chl : C)_{PHY_i} = (N : C)_{PHY_i,min} (Chl : N)_{PHY_i,min} \\ \text{for } (N : C)_{PHY_i} \geq (N : C)_{PHY_i,max} \\ (Chl : C)_{PHY_i} = (N : C)_{PHY_i,max} (Chl : N)_{PHY_i,max} \end{cases} \quad (5.37)$$

$$RespirationPHY_i = ActivityRespPHY_i + BasalRespPHY_i \quad (5.38)$$

$$\text{with } \begin{cases} ActivityRespPHY_i = ProdResp_i PhotosynthPHY_i \\ BasalRespPHY_i = Resp_i f^T CPHY_i \end{cases} \quad (5.39)$$

$$\begin{cases} LeakagePHY_{N,i} = \gamma_1 (NHS_1^{up} + NOS_1^{up}) \\ LeakagePHY_{N,i} = 0 \text{ when } (N : C)_{PHY_i} > (N : C)_{PHY_i,max} \\ LeakagePHY_{C,i} = \gamma_1 PhotosynthPHY_i \end{cases}$$

$$ExtraExrPHY_i = \gamma_2 \left[PhotosynthPHY_i |_{(N:C)_{PHY_i} = (N:C)_{PHY_i,max}} - PhotosynthPHY_i \right] \quad (5.40)$$

$$MortPHY_{X,i} = mort_{PHY_i} f^T XPHY_i, \quad X = C, N \quad (5.41)$$

Nutrient Uptake (5.42)

for $(N : C)_{PHY_i} \leq (N : C)_{PHY_i, max}$

$$\begin{aligned} U_i^{*NOS} &= U_i^{NOS max} f^T \left(1 - \frac{(N:C)_{PHY_i}}{(N:C)_{PHY_i, max}} \right) \frac{NOS}{NOS + k_{NOS_i}} \frac{k_{in}}{k_{in} + NHS} CPHY_i \\ U_i^{*NHS} &= U_i^{NHS max} f^T \left(1 - \frac{(N:C)_{PHY_i}}{(N:C)_{PHY_i, max}} \right) \frac{NHS}{NHS + k_{NHS_i}} CPHY_i \\ U_i^{*PHO} &= U_i^{PHO max} f^T \left(1 - \frac{(P:C)_{PHY_i}}{(P:C)_{PHY_i, max}} \right) \frac{PHO}{PHO + k_{PHO_i}} CPHY_i \\ U_3^{*SIO} &= U_3^{SIO max} f^T \left(1 - \frac{(Si:C)_{PHY_3}}{(Si:C)_{PHY_3, max}} \right) \frac{SIO}{SIO + k_{SIO_3}} CPHY_i \end{aligned}$$

for $i=1,2$

$$\begin{aligned} U_i^{*NOS} &= \min \left(U_i^{*NOS} + U_i^{*NHS}, \frac{U_i^{*PHO}}{(P:N)_{PHY_i}} \right) \frac{U_i^{*NOS}}{U_i^{*NOS} + U_i^{*NHS}} \\ U_i^{*NHS} &= \min \left(U_i^{*NOS} + U_i^{*NHS}, \frac{U_i^{*PHO}}{(P:N)_{PHY_i}} \right) \frac{U_i^{*NHS}}{U_i^{*NOS} + U_i^{*NHS}} \\ U_i^{*PHO} &= \min \left(U_i^{*NOS} + U_i^{*NHS}, \frac{U_i^{*PHO}}{(P:N)_{PHY_i}} \right) (P : N)_{PHY_i} \end{aligned}$$

for $i=3$ (Diatoms)

$$\begin{aligned} U_3^{*NOS} &= \min \left(U_3^{*NOS} + U_3^{*NHS}, \frac{U_3^{*SIO}}{(Si:N)_{PHY_3}}, \frac{U_3^{*PHO}}{(P:N)_{PHY_3}} \right) \frac{U_3^{*NOS}}{U_3^{*NOS} + U_3^{*NHS}} \\ U_3^{*NHS} &= \min \left(U_3^{*NOS} + U_3^{*NHS}, \frac{U_3^{*SIO}}{(Si:N)_{PHY_3}}, \frac{U_3^{*PHO}}{(P:N)_{PHY_3}} \right) \frac{U_3^{*NHS}}{U_3^{*NOS} + U_3^{*NHS}} \\ U_3^{*SIO} &= \left[\min \left(U_3^{*NOS} + U_3^{*NHS}, \frac{U_3^{*SIO}}{(Si:N)_{PHY_3}}, \frac{U_3^{*PHO}}{(P:N)_{PHY_3}} \right) - LeakagePHY_{N,3} \right] (Si : N)_{PHY_3} \\ U_3^{*PHO} &= \min \left(U_3^{*NOS} + U_3^{*NHS}, \frac{U_3^{*SIO}}{(Si:N)_{PHY_3}}, \frac{U_3^{*PHO}}{(P:N)_{PHY_3}} \right) (P : N)_{PHY_3} \end{aligned}$$

for $(N : C)_{PHY_i} > (N : C)_{PHY_i, max}$ (negative uptake corresponds to excretion)

$$\begin{aligned} U_i^{*NOS} &= 0 \\ U_i^{*NHS} &= U_i^{NHS max} f^T \left(1 - \frac{(N:C)_{PHY_3}}{(N:C)_{PHY_3, max}} \right) CPHY_i \\ U_i^{*PHO} &= U_i^{NHS} (P : N)_{PHY_i} \\ U_3^{*SIO} &= [U_3^{*NHS} - LeakagePHY_{N,3}] (Si : N)_{PHY_3} \end{aligned} \tag{5.43}$$

Sedimentation of Diatoms

$$v_{PHY_3} = v_{PHY_3, min} + (v_{PHY_3, max} - v_{PHY_3, min}) \frac{((N : C)_{PHY_3, max} - (N : C)_{PHY_3})}{((N : C)_{PHY_3, max} - (N : C)_{PHY_3, min})} \tag{5.44}$$

Zooplankton, ($j = 1, 2$)

$$GrazZOO_{C,j} = f^T MaxGrazZOO_j \frac{Ba_{C,ZOO_j}}{Ba_{C,ZOO_j} + k_{sat,ZOO_j}} CZOO_j \tag{5.45}$$

$$GrazZOO_{N,j} = GrazZOO_{C,j} (N : C)_{food,j} \tag{5.46}$$

$$Ba_{X,ZOO_j} = \sum_{preys} e_{prey,Zoo_j} XPrey, \quad X = C, N \tag{5.47}$$

$$(N : C)_{food,j} = Ba_{N,ZOO_j} / Ba_{C,ZOO_j} \tag{5.48}$$

$$I_{X,j} = (1 - \phi_i) GrazX_j, \quad X = C, N \tag{5.49}$$

$$(N : C)_j^* = (N : C)_{ZOO_j} \frac{k_{C,j} \beta_{C,j}}{\beta_{N,j}} \rightarrow \begin{cases} (N : C)_{food,j} < (N : C)_j^* \Rightarrow N \text{ limitation} \\ (N : C)_{food,j} > (N : C)_j^* \Rightarrow C \text{ limitation} \end{cases} \tag{5.50}$$

$$\text{If N limits: } \begin{cases} \text{GrowthZOO}_{N,j} = \beta_{N,j} I_{N,j} \\ \text{GrowthZOO}_{C,j} = \text{GrowthZOO}_{N,j} / (N : C)_{ZOO} \\ \text{ExcrZOO}_j = 0 \end{cases} \quad (5.51)$$

$$\text{If C limits: } \begin{cases} \text{GrowthZOO}_{C,j} = k_{C,j} \beta_{C,j} I_{C,j} \\ \text{GrowthZOO}_{N,j} = \text{GrowthZOO}_{C,j} (N : C)_{ZOO_j} \\ \text{ExcrZOO}_j = \beta_{N,j} I_{N,j} - \text{GrowthZOO}_{N,j} \end{cases} \quad (5.52)$$

$$\text{RespZOO}_j = \beta_{C,j} I_{C,j} - \text{GrowthZOO}_{C,j} \quad (5.53)$$

$$\text{MortZOO}_{C,j} = f^T CZOO_i \left(\text{mortZOO}_j \frac{CZOO_i}{CZOO_i + k_{\text{satMortZOO}_i}} + \left(1 - \frac{DOX}{DOX + k_{\text{satAnoxMort}}} \right) \text{AnoxMort} \right) \quad (5.54)$$

Gelatinous, ($j = 1, 2$)

$$\text{GrazGEL}_{C,j} = f^T \text{MaxGrazGEL}_j \text{Ba}_{C,GEL_j} \text{CGEL}_j \quad (5.55)$$

$$\text{GrazGEL}_{N,j} = \text{GrazGEL}_{C,j} (N : C)_{\text{food},j} \quad (5.56)$$

$$\text{Ba}_{x,GEL_j} = \sum_{\text{preys}} e_{\text{prey},GEL_j} X\text{Prey}_j, \quad X = C, N \quad (5.57)$$

$$(N : C)_{\text{food},GEL_j} = \text{Ba}_{n,GEL_j} / \text{Ba}_{C,GEL_j} \quad (5.58)$$

$$\text{GrowthGEL}_{C,j} = \text{GrowthEffGEL}_j \text{AssEffGEL}_j \text{GrazGEL}_{C,j} \quad (5.59)$$

$$\text{EgestGEL}_{C,j} = (1 - \text{AssEffGEL}_j) \text{GrazGEL}_{C,j} \quad (5.60)$$

$$\text{EgestGEL}_{N,j} = (1 - \text{AssEffGEL}_j) \text{GrazGEL}_{N,j} \quad (5.61)$$

$$\text{RespGEL}_j = (1 - \text{GrowthEffGEL}_j) \text{AssEffGEL}_j \text{GrazGEL}_{C,j} \quad (5.62)$$

$$(N : C)^* = \frac{\text{GrazGEL}_{C,j} (N : C)_{\text{food},GEL_j} - \text{EgestGEL}_{N,j}}{\text{GrazGEL}_{C,j} - \text{EgestGEL}_{C,j} - \text{RespGEL}_j} \quad (5.63)$$

if $(N:C)_{GEL} \leq (N:C)^*$

$$\rightarrow \begin{cases} \text{AdjRespGEL}_j = 0 \\ \text{AdjExcrGEL}_j = (\text{GrazGEL}_{C,j} (N : C)_{\text{food},GEL_j} - \text{EgestGEL}_{N,j}) \\ \quad - (N : C)_{GEL_i} (\text{GrazGEL}_{C,j} - \text{EgestGEL}_{C,j} - \text{RespGEL}_{C,j}) \end{cases} \quad (5.64)$$

if $(N:C)_{GEL} > (N:C)^*$

$$\rightarrow \begin{cases} \text{AdjRespGEL}_j = (\text{GrazGEL}_{C,j} - \text{EgestGEL}_{C,i} - \text{RespGEL}_j) \\ \quad - (\text{GrazGEL}_{C,j} (N : C)_{\text{food},GEL_j} - \text{EgestGEL}_{N,j}) / (N : C)_{GEL_i} \\ \text{AdjExcrGEL}_j = 0 \end{cases} \quad (5.65)$$

$$\text{MortGEL}_{C,j} = f^T \text{CGEL}_j \left(\text{mortGEL}_j + \left(1 - \frac{DOX}{DOX + k_{\text{satAnoxMort}}} \right) \text{AnoxMort} \right) \quad (5.66)$$

$$\text{GrazXPrey}_i = \sum_{j=1}^2 \left[\frac{\text{GrazZOO}_{X,j}}{\text{Ba}_{X,ZOO_j}} e_{X\text{Prey}_i,ZOO_j} X\text{Prey}_i + \frac{\text{GrazGEL}_{X,j}}{\text{Ba}_{X,GEL_j}} e_{X\text{Prey}_i,GEL_j} X\text{Prey}_i \right] , \quad X = C, N \quad (5.67)$$

Bacteria

$$U_{BAC}^{DOC} = f^T \mu_{BAC} \frac{DOCL}{k_{BAC,DOC} + DOCL} BAC, \quad U_{BAC}^{DON} = U_{BAC}^{DOC} \left(\frac{DONL}{DOCL} \right) \quad (5.68)$$

$$U_A^* = f^T \mu_{BAC} \frac{NHS}{k_{BAC,NHS} + NHS} BAC (N : C)_{BAC} \quad (5.69)$$

$$\text{TestBAC} = U_{BAC}^{DON} - \omega_B U_{BAC}^{DOC} (N : C)_{BAC} \quad (5.70)$$

if $U_A^* > -TestBAC \rightarrow$ Carbon limitation case:

$$GrowthBAC = \omega_B U_{BAC}^{DOC}$$

$$RespBAC = (1 - \omega_B) U_{BAC}^{DOC}$$

if $TestBAC \leq 0 \rightarrow$ NHS uptake is necessary to consume all the DOCL

$$U_{BAC}^{NHS} = -TestBAC$$

$$ExcrBAC = 0$$

if $TestBAC \leq 0 \rightarrow$ Bacteria act as remineralizers:

$$U_{BAC}^{NHS} = 0$$

$$ExcrBAC = TestBAC$$

if $U_A^* \leq -TestBAC \rightarrow$ Nitrogen Limitation case:

$$U_{BAC}^{NHS} = U_{BAC}^{*NHS}$$

$$GrowthBAC = (U_{BAC}^{DON} + U_{BAC}^{NHS}) / (N : C)_{BAC}$$

$$RespBAC = GrowthBAC (1/\omega_B - 1)$$

$$ExcrBAC = 0$$

(5.71)

(5.72)

$$MortBAC = f^T mort_{BAC} BAC$$

(5.73)

Detritus

Labile and Semi-labile Dissolved Organic Matter

$$HydrolDOCSL = f^T MaxHydDOM \frac{DOCSL}{DOCSL + k_{sat,hydDOM}} BAC \quad (5.74)$$

$$HydrolDONSL = HydrolDOCSL \frac{DONSL}{DOCSL} \quad (5.75)$$

Particulate Detrital Matter

$$HydrolPOC = f^T MaxHydPOC \frac{DOX + 0.1}{DOX + 0.1 + k_{sat,OxicHydrol}} POC \quad (5.76)$$

$$HydrolPON = f^T MaxHydPON \frac{DOX + 0.1}{DOX + 0.1 + k_{sat,OxicHydrol}} PON \quad (5.77)$$

$$DissolutionSidet = f^T diss_{SID} SID \quad (5.78)$$

Sedimentation of Particulate Organic Matter

$$v_{POM} = \frac{(\epsilon - \zeta - 1) v_{sed,cell}}{(\epsilon - \eta - \zeta - 1)} - \frac{G_M \eta v_{sed,max}}{(\epsilon - \zeta - \eta - 1)} \quad (5.79)$$

$$v_{AGG} = \frac{(\epsilon - 1) v_{sed,cell}}{(\epsilon - \eta - 1)} - \frac{F_M \eta v_{sed,max}}{(\epsilon - \eta - 1)} \quad (5.80)$$

$$\text{with } \begin{cases} v_{sed,max} = BL^\eta \\ v_{sed,cell} = Bl^\eta \\ G_M = \left(\frac{L}{l}\right)^{1+\zeta-\epsilon} \\ F_M = \left(\frac{L}{l}\right)^{1+\zeta-\epsilon} \end{cases} \quad (5.81)$$

Number of Aggregates

$$Aggregation = 0.5 stick (AggregSettlement + AggregShear) \quad (5.82)$$

where AggregSettlement and AggregShear are the number of particles colliding due to respectively differential settlement and shear rate. These two quantities are computed according to [Kriest \(2002\)](#).

(5.83)

Chemical submodel

$$RespBAC_{Oxygen} = RespBAC \frac{DOX}{DOX + k_{sat,DOX}^{OxicMin}} \quad (5.84)$$

$$RespBAC_{Nitrate} = RespBAC \frac{NOS}{NOS + k_{sat,NOS}^{Denit}} \left(1 - \frac{DOX}{DOX + k_{in,DOX}^{Denit}} \right) \quad (5.85)$$

$$AnoxicRespBAC = RespBAC \left(1 - \frac{NOS}{NOS + k_{in,NOS}^{AnoxMin}} \right) \left(1 - \frac{DOX}{DOX + k_{in,DOX}^{AnoxMin}} \right) \quad (5.86)$$

$$SolidODU = R_{solid} IronLimitation \gamma_{POC}^{ODU} AnoxicRespBAC \quad (5.87)$$

with $IronLimitation = \frac{Iron}{Iron + k_{sat,iron}^{SolForm}}$

where $Iron$ is an imposed profile from observations

$$NHSoxid_{DOX} = f^T \mu_{NHS}^{DOX} \frac{DOX}{DOX + k_{sat,DOX}^{NHSoxid}} \quad (5.88)$$

$$NHSoxid_{NOS} = f^T \mu_{NHS}^{NOS} \frac{NOS}{NOS + k_{sat,NOS}^{NHSoxid_{NOS}}} \left(1 - \frac{DOX}{DOX + k_{in,DOX}^{NHSoxid_{NOS}}} \right) \quad (5.89)$$

$$ODUoxid_{DOX} = f^T \mu_{ODU}^{DOX} \frac{DOX}{DOX + k_{sat,DOX}^{ODUoxid}} \quad (5.90)$$

$$ODUoxid_{NOS} = f^T \mu_{ODU}^{NOS} \frac{NOS}{NOS + k_{sat,NOS}^{ODUoxid_{NOS}}} \left(1 - \frac{DOX}{DOX + k_{in,DOX}^{ODUoxid_{NOS}}} \right) \quad (5.91)$$

Table 5.6: Parameters values for biological processes.

PAR.	UNITS	VALUE	DESCRIPTION	REF.
Q_{10}	-	2	Temperature coefficient	(2)
$Q_{10,diatoms}$	-	1.8	Temperature coefficient for diatoms	(c)
p_{IR}	-	0.54	Part of PAR with a infra-red wave length (λ 700 nm)	(12)
p_l	-	0.63	Part of visible PAR with a long wave length ([580-700nm])	(c)
θ	deg	var.	Solar zenith angle above surface	(C)
m_1	-	4.18		(13)
m_2	-	0.52		(13)
m_3	-	10.8		(13)
<u>Specific IOPs</u>				
$a_{\lambda,sw}$	m^{-1}	short waves		
$a_{\lambda,chl}^*$		0.0196	long waves	(14)
$\hat{a}_{\lambda,chl}$		0.029		(15)
$a_{\lambda,SMI}^*$		0.6		(15)
$a_{\lambda,POC}^*$	m^2mg^{-1}	0.1		(16)
$a_{\lambda,CDDOM}^*$	m^2mmolC^{-1}	0.6		(16)
$a_{\lambda,CDDOM}^{**}$	m^{-1}	0.2522		(c)
$b_{\lambda,sw}$	$m^{-1}p.s.u^{-1}$	0.0122		(c)
b_{λ,PHY_1}^*	m^{-1}	0.0015		(14)
b_{λ,PHY_2}^*	m^2mmolC^{-1}	12.1e-5		(17)
b_{λ,PHY_3}^*	m^2mmolC^{-1}	9.8e-5		(17)
$b_{\lambda,SMI}^*$	m^2mg^{-1}	7.344e-5		(17)
$b_{\lambda,POC}^*$	m^2mmolC^{-1}	6.96e-5		(17)
		0.0155		(16,18)
		0.0055		(16)
<u>Phytoplankton</u>				
$(N:C)_{PHY,min}$	molN molC $^{-1}$	PHY ₁	PHY ₃	
$(N:C)_{PHY,max}$	molN molC $^{-1}$	0.05	0.05	(2)
$(N:Si)$	molN molSi $^{-1}$	0.2	0.2	(2)
$(N:P)$	molN molP $^{-1}$	-	5/6	(10)
$(Chl:N)_{min}$	gChl molN $^{-1}$	16	16	(10)
		1	1	(2)
			Min. Chl:N ratio	

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PAR.	UNITS			2	2			
$(Chl : N)_{max}$	gChl molN ⁻¹			0.03	0.03	Max. Chl:N ratio		(2)
α	d (W m ⁻²) ⁻¹			0.01	0.01	Initial slope P-I curve		(c)
<i>Resp</i>	d ⁻¹			0.1	0.01	Basal Respiration rate		(3)
<i>ProdResp</i>	-			0.1	0.1	Part of Primary Production used for respiration		(3)
μ_{max}	d ⁻¹			3	1.5	Max. spec. growth rate		(c)
$U_{iNOSmax}$	molN molC ⁻¹ d ⁻¹			1.5	0.5	Max. NOS uptake rate		(c)
$U_{iNHSmax}$	molN molC ⁻¹ d ⁻¹			1.5	0.5	Max. NHS uptake rate		(c)
$U_{iSIOmax}$	molSi molC ⁻¹ d ⁻¹			0	0	Max. SIO uptake rate		(c)
$U_{iPHOMax}$	molP molC ⁻¹ d ⁻¹			1.5/16	0.5/16	Max. PHO uptake rate		(c)
k_{NOS}	mmolN m ⁻³			0.05	3	Half-Sat. Cst for NOS uptake		(c)
k_{NHS}	mmolN m ⁻³			0.05	3	Half-Sat. Cst for NHS uptake		(c)
k_{in}	mmolN m ⁻³			0.5	0.5	Inhibition coefficient for NOS uptake by the presence of NHS		(2)
k_{SIO}	mmolSi m ⁻³			-	-	Half-Sat. Cst for SIO uptake		(7)
k_{PHO}	mmolP m ⁻³			0.2	0.1	Half-Sat. Cst for PHO uptake		()
γ_1	-			0.02	0.02	Phyto. leakage fraction		(3)
γ_2	-			0.05	0.05	Ratio of extra DOC produced by N lim.		(3)
$mort_{PHY}$	d ⁻¹			0.03	0.03	Mortality rate		(2)
ϵ	-			0.34	0.34	DOM fraction of phytoplankton mortality		(1)
$v_{PHY3,max}$	m d ⁻¹			0	0	Max. diatoms sinking rate		(c)
$v_{PHY3,min}$	m d ⁻¹			0	0	Min. diatoms sinking rate		(c)
<i>Zooplankton</i>								
$(C:N)_{ZOO}$	molC molN ⁻¹			ZOO_1	ZOO_2	internal ratio		(1)
$MaxGrazZOO$	d ⁻¹			5.5	4.67	Max. grazing rate		(c)
$k_{sat,ZOO}$	mmolC m ⁻³			3.6	1	Half-sat cst		(c)
β_N	-			5	5	Assimilation N effc.		(1)
β_C	-			0.77	0.77	Assimilation C effc.		(1)
k_c	-			0.64	0.64	Net growth effc.		(1)
ϕ	-			0.8	0.8	Messy feeding frac.		(1)
$mortZOO$	d ⁻¹			0.23	0.23	Max mortality rate		(3)
$ksat_{MortZOO}$	mmolC m ⁻³			0.3	0.3	Half-sat for mortality		(3)
$AnoxMort$	d ⁻¹			1	1	Mortality rate in anoxia		(c)
$ksat_{AnoxMort}$	mmolO2 m ⁻³			0.25	0.25	Half-sat for mortality in anoxia		(c)
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PAR.		UNITS			VALUE		DESCRIPTION		REF.
X:	Phy1	Phy2	Phy3	Zoo1	Zoo2	Bac	POM		
eX_{Zoo1}	1	0	0	0	0	0.7	0	Capture efficiencies	(c)
eX_{Zoo2}	0.4	0.5	1	1	0	0	0.8		
<i>Gelatinous</i>									
$(C:N)_{GEL}$					molC molN ⁻¹		$\frac{GEL_1}{GEL_2}$	internal ratio	(6,9)
$Q_{10gelatinous}$							4.76	Q_{10} factor	(8)
$MaxGrazGEL$					d ⁻¹		3.5	Max. grazing rate	(c)
$AssEffGEL$					-		0.07	Assimilation efficiency	(6)
$GrowthEffGEL$					-		0.75	Growth efficiency	(6)
$mortGEL$					d ⁻¹		0.2	Max mortality rate	(c)
$AnoxMort$					d ⁻¹		0.06	Mortality rate in anoxia	(c)
$ksat_{AnoxMort}$					mmolO2 m ⁻³		0.25	Half-sat for mortality in anoxia	(c)
							8		
X:	Phy1	Phy2	Phy3	Zoo1	Zoo2	Bac	POM		
eX_{GEL1}	1	0.2	1.0	1	0.4	0	1	Capture efficiencies	(c)
eX_{GEL2}	0	0	0	0	1	0	0		
<i>Bacteria and dissolved organic matter</i>									
$(C:N)_{BAC}$					molN molC ⁻¹		5.1	Bacteria internal ratio	(1)
μ_{BAC}					d ⁻¹		13.3	Max. labile DOC or NHS uptake	(1)
$k_{BAC,DOC}$					mmolC m ⁻³		25	Half-sat. for labile DOC uptake	(1)
$k_{BAC,NHS}$					mmolN m ⁻³		0.5	Half-sat. for NH ₄ uptake	(1)
ω_B					-		0.17	Bacterial gross growth efficiency	(1)
$mort_{BAC}$					d ⁻¹		0.04	Mortality rate	(1)
$MaxHydDOM$					d ⁻¹		4	Max. semi-labile DOC hydrolysis	(1)
$ksat_{hydDOM}$					mmolC m ⁻³		417	Half Sat. for semi-labile DOC uptake	(1)
δ_1							0.65	Lab. frac. phyto and non-phyto produced DOM	(3)
<i>Detritus</i>									
$MaxHydPOC$					d ⁻¹		0.04	Hydrolysis rate of POC	(1)
$MaxHydPON$					d ⁻¹		0.055	Hydrolysis rate of PON	(1)
$ksat_{OxicHydrOl}$					mmolDOX m ⁻³		0.009	Half Sat. for oxic hydrolysis	(c)
$diss_{SID}$					d ⁻¹		0.1	Dissolution rate of SID	(10)
vs_{SID}					m d ⁻¹		2	Sinking rate of SID	(c)
$\frac{Aggregation}{\eta}$					-		0.62	Sinking exponent	(5)
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PAR.	UNITS	VALUE	DESCRIPTION		
B	$m^{-\eta} d^{-1}$	2294	Sinking factor	(5)	
stick	-	0.5	Stickiness	(c)	
ℓ	m	$2 \cdot d^{-5}$	Minimal cell size	(5)	
L	m	0.01	Maximal cell size	(5)	
ζ	-	1.62	N content exponent	(5)	
C	$mmolN m^{-\zeta}$	0.4744	N content coefficient	(5)	
ϵ		3.5	Epsilon initial value	(5)	
<i>Chemical Model</i>					
μ_{DOX}^{DOX}	d^{-1}	0.03	Max. NHS oxidation rate by DOX	(1)	
μ_{NHS}^{NHS}	d^{-1}	0.1	Max. NHS oxidation rate by NOS	(Assumed)	
μ_{DOX}^{DOX}	d^{-1}	0.1	Max. ODU oxidation rate by DOX	(Assumed)	
μ_{ODU}^{ODU}	d^{-1}	0.1	Max. ODU oxidation rate by NOS	(Assumed)	
$k_{sat,DOX}^{NHS}$	$mmolDOX m^{-3}$	1	Half Sat. const. for DOX limit. in NHS oxid. by DOX	(4)	
$k_{in,DOX}^{NHS}$	$mmolDOX m^{-3}$	2.5	Half Sat. const. for DOX inhib. in NHS oxid. by NOS	(c)	
$k_{sat,NOS}^{NHS}$	$mmolN m^{-3}$	2	Half Sat. const. for NOS limit. in NHS oxid. by NOS	(c)	
k_{ODU}^{ODU}	$mmolDOX m^{-3}$	1	Half Sat. const. for DOX limit. in ODU oxid. by DOX	(4)	
$k_{in,DOX}^{ODU}$	$mmolDOX m^{-3}$	2.5	Half Sat. const. for DOX inhib. in ODU oxid. by NOS	(c)	
$k_{sat,NOS}^{ODU}$	$mmolN m^{-3}$	30	Half Sat. const. for NOS limit. in ODU oxid. by NOS	(c)	
$k_{ODU}^{OxicMin}$	$mmolDOX m^{-3}$	3	Half Sat. const. for DOX limit. in oxic respiration	(4)	
$k_{in,DOX}^{Denit}$	$mmolDOX m^{-3}$	10	Half Sat. const. for DOX inhib. in denitrification	(4)	
$k_{sat,NOS}^{Denit}$	$mmolN m^{-3}$	30	Half Sat. const. for NOS limit. in denitrification	(4)	
$k_{in,DOX}^{AnoxMin}$	$mmolDOX m^{-3}$	0.005	Half Sat. const. for DOX inhib. in anoxic respiration	(c)	
$k_{in,NOS}^{AnoxMin}$	$mmolN m^{-3}$	0.005	Half Sat. const. for NOS inhib. in anoxic respiration	(c)	
R_{solid}		0.2	Pourc. of ODU production that is deposited as a solid	(c)	
$k_{sat,iron}^{SolForm}$	$\mu molFe m^{-3}$	100	Half Sat. const. for Iron limit. in solid ODU Formation	(c)	
γ_{DOX}^{DOX}	$molDOX (molC)^{-1}$	1	Mol DOX used per mol C in oxic respiration	(see equ. in Table 1)	
γ_{DOX}^{NHS}	$molDOX (molNHS)^{-1}$	2	Mol DOX needed to oxidize one mol of NHS in nitrification	(see equ. in Table 1)	
γ_{DOX}^{ODU}	$molDOX (molODU)^{-1}$	1	Mol DOX needed to oxidize one mol of ODU	(see equ. in Table 1)	
γ_{DOX}^{POC}	$molODU (molC)^{-1}$	1	Mol ODU formed per mol C in anoxic respiration	(see equ. in Table 1)	
γ_{POC}^{POC}	$molNOS (molC)^{-1}$	0.8	Mol NOS used per mol C in denitrification	(see equ. in Table 1)	
γ_{NOS}^{NHS}	$molNOS (molNHS)^{-1}$	0.6	Mol NOS needed to oxidize one mol of NHS	(see equ. in Table 1)	
γ_{ODU}^{NOS}	$molNOS (molODU)^{-1}$	0.8	Mol NOS needed to oxidize one mol of ODU	(see equ. in Table 1)	
$burial_C$		0.28	Percentage of POC buried in the Sediments	(11)	

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PAR.	UNITS	VALUE	DESCRIPTION REF.
<i>burial_N</i>		0.28	Pourcentage of PON buried in the Sediments (11)
(c) after calibration. (C) Computed. References: (1) Anderson and Pondaven (2003) (2) Soetaert et al. (2001) (3) Van den Meersche et al. (2004) (4) Soetaert et al. (1996) (5) Kriest (2002) (6) Lancelot et al. (2002) (7) Paasche (1980) (8) Kremer (1977) (9) Nakamura (1998) (10) Tusseau (1996) (11) Muramoto et al. (1991) (12) Mobley et al. (2004) (13) Lee et al. (2005b) (14) Smith and Baker (1981) (15) Bricaud et al. (1995) (16) Neukermans et al. (2012) (17) Vaillancourt et al. (2004) (18) Doerffer and Schiller (2007) (16))			

Rivers	DON/DIN		PON/DIN		DOC/DON		POC/PON		[SIO]	
	1970	2000	1970	2000	1970	2000	1970	2000	1970	2000
Danube	0.29	0.34	0.14	0.17	12.29	12.44	11.01	10.93	66.60	67.62
Dnepr	1.15	1.26	0.05	0.06	11.71	12.80	10.60	10.52	7.59	7.53
Dnestr	0.32	0.61	0.07	0.20	12.64	12.14	10.89	10.68	34.21	44.56
Rioni	0.41	0.18	0.73	0.27	16.19	13.48	11.51	11.49	203.17	207.82
Kizilmark	0.64	0.52	1.11	0.50	17.07	9.21	13.56	14.31	284.62	366.67
Sakarya	0.65	0.50	0.48	0.23	9.97	5.82	13.09	12.91	211.42	217.08

Table 5.7: Riverine discharge ratios ([Seitzinger et al., 2010](#)).

2 Black Sea Implementation

2.1 Initial conditions

Initial conditions were reconstructed from the data described in [3.1](#) using layered DIVA analysis ([Troupin et al., 2012](#)).

2.2 Boundary Conditions

Surface Fluxes

Though atmospheric nutrient deposit has generally been overlooked in Black Sea biogeochemical models, these inputs are estimated to be comparable to the riverine loads, so their omission leads to severe gaps when trying to close the nutrient budget at basin scale. Deposit estimates ([Kanakidou et al., 2012](#)) were imposed as uniform values over the domain, an acceptable approximation as spatial variability remains relatively low.

Rivers

Nutrient loads data are issued from the SESAME and PERSEUS project. These are reconstructed through hydrological modelling merged with observations wherever available ([Ludwig et al., 2009](#)). As for freshwater flows, nutrients loads are gathered into the 6 main river entrances represented in the model domain. Again, they consist in annual loads, modulated by repeated seasonal distribution. As organic forms were not available from these sources we relied to ([Seitzinger et al., 2010](#)) to estimate the ratio NHS/DIN , DON/DIN , PON/DIN for the different rivers. These ratios are indicated in [5.7](#) for the 1970 and 2000 estimated periods. To reconstruct to monthly riverine discharges required by the models we used a linear interpolation from these values between 1970 and 2000, and used the 2000 values for the period after 2000.

The nutrients are imposed to the model as concentrations (obtained by dividing the loads by the freshwater discharges) imposed for the surface levels (σ layer 20 to 31) of the riverine boundaries. Null gradient conditions are imposed for the lower levels of river entrances, and for all levels in the case of the Bosphorus.

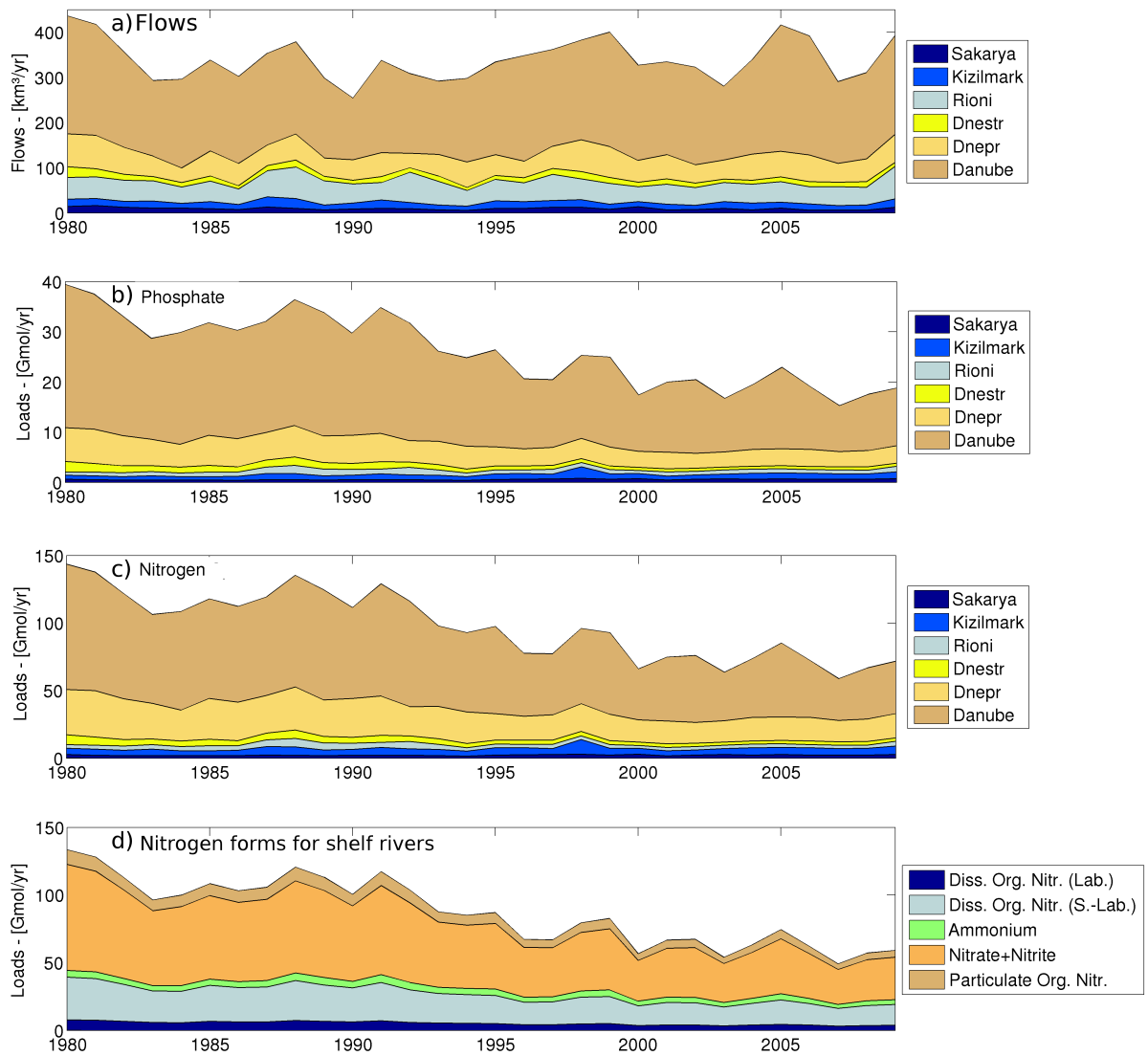


Figure 5.1: (a) Annual riverine flows, (b) annual loads of dissolved inorganic phosphate, (c) annual load of nitrogen (in various forms), (d) speciation of the nitrogen riverine load for the three Shelf river (Danube, Dnepr and Dnestr)

3 Skill Assessment

3.1 In situ observations

In-situ data were assembled by Joassin (2011) for the period 1960-1999 from the NATO-TU (<http://sfp1.ims.metu.edu.tr/TU-BlackSea/>), MEDAR (<http://medar.ieo.es/>), and PANGEA (<http://www.wdc-mare.org/>) databases, and complemented with local databases (Romanian and Bulgarian data from Sesame project partnership) (<http://www.sesame-ip.eu/>).

Hereafter we assess the model skills in reproducing the vertical distribution of oxygen and nutrients and their seasonal and interannual variability. Horizontal variability is only considered by distinguishing between the NWS and central regions.

Given the poor data availability for biogeochemical variables, uneven data distribution may result in spurious apparent variability. Especially when addressing the temporal variability, as monthly and annual medians will be impacted by an uneven data distribution, both horizontally and vertically. While it does not enhance the interpretability of the apparent signal, considering model results *at observations location*, rather than domain averages, minimizes the impact of representativity error on the model skills assessment.

3.2 Vertical profiles

Open Sea

Vertical profiles of Oxygen in the open sea (Fig. 5.2) indicate a deeper penetration of oxygen in the model and good representation of the surface dynamics. The depths of subsurface oxygen maximum concentrations are generally consistent.

Nitrate profiles depict an underestimation of the maximum concentrations in the nitracline, mostly visible during the summer months. Also, observations profiles presents larger seasonal fluctuations of this maximum value than that resolved by the model.

Regarding ammonium, summer months indicate overestimated concentrations below the observed oxycline, ammonium and oxygen profiles overlap more in the model than they do in the observations.

Phosphate profiles are pretty well resolved by the model. The peculiar behavior of phosphate around the halocline is not resolved by the model.

Silicate appears to be systematically underestimated by the model between 50 and 120 m depth.

Northwestern shelf

Vertical profiles of Oxygen in the NWS (Fig. 5.3) match the observations, their seasonal fluctuations as well as the surface/subsurface differences.

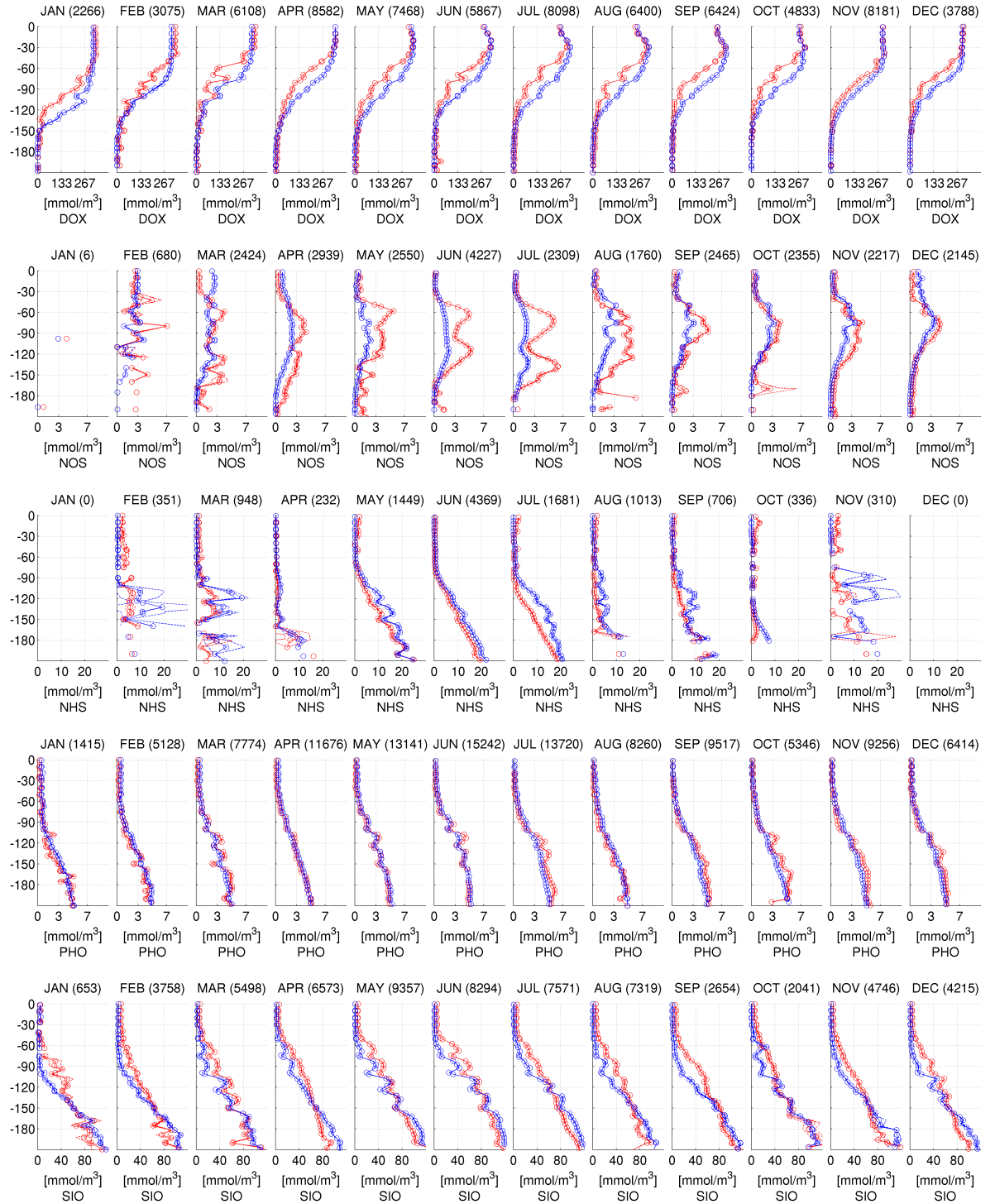


Figure 5.2: Monthly vertical profiles in the open sea : Oxygen, Nitrate, Ammonium, Phosphate, Silicate.

Nitrate profiles are difficult to interpret: high concentrations were observed in Spring, but only near the surface. In fact high concentrations have only been measured very close to the river mouths. Observed nitrate levels rapidly decrease in May, while this decrease is slower in the model and lasts until August. Finally, winter profiles are well reproduced.

Ammonium concentrations seems slightly underestimated from November to April.

Phosphate on the northwestern shelf is systematically overestimated by the model by about 0.4 mmol/m^3 .

Silicate profiles show a high variability which complicates interpretations. It seems however that an underestimation below the 50 m depth is a general rule.

3.3 Temporal variability

Temporal variability is addressed as in Section 3, restricting to data from the upper 40 m.

In the open sea (Fig. 5.4), both seasonal and interannual variations of oxygen are reproduced without any practical bias and with matching variations despite a systematic slight underestimation in spring. Unfortunately, the lower number of data does not allow to state whether the apparent decrease of oxygen after 1995, both observed and resolved by the model, is representative or artificial.

Nitrate is generally overestimated after winter mixing.

Phosphate appears generally overestimated and indicates a marked drift which points towards biased initial conditions.

Skills are most satisfactorily for oxygen in the NWS (Fig. 5.5). This case is addressed more specifically in Chapter 7.

Both nitrate and phosphate concentrations indicate overestimation in spring. Again the important spatial variability hampers the interannual signal visibility (Fig. 5.6).

Ammonium and silicate depicts matching levels, but their apparent variability is difficult to interpret.

3.4 Summary and discussion

The vertical structure of biogeochemical variables are usually very well reproduced by the model. Temporal dynamics is accurate in the case of oxygen, and indicates the consequence of the light winter overmixing in the case of nutrients. Data limited availability generally prohibits clear interpretations of the apparent variabilities.

It is difficult to establish to which extent the mismatches of biogeochemical variables are to be attributed to imperfections of the physical model, or when imperfections of the biogeochemical models formulations and parameters starts to play a role.

For instance the over-mixing identified in Chapter 3 is likely to play a role in the over-estimation of oxygen and the underestimation of nitrate and silicate in the intermediate

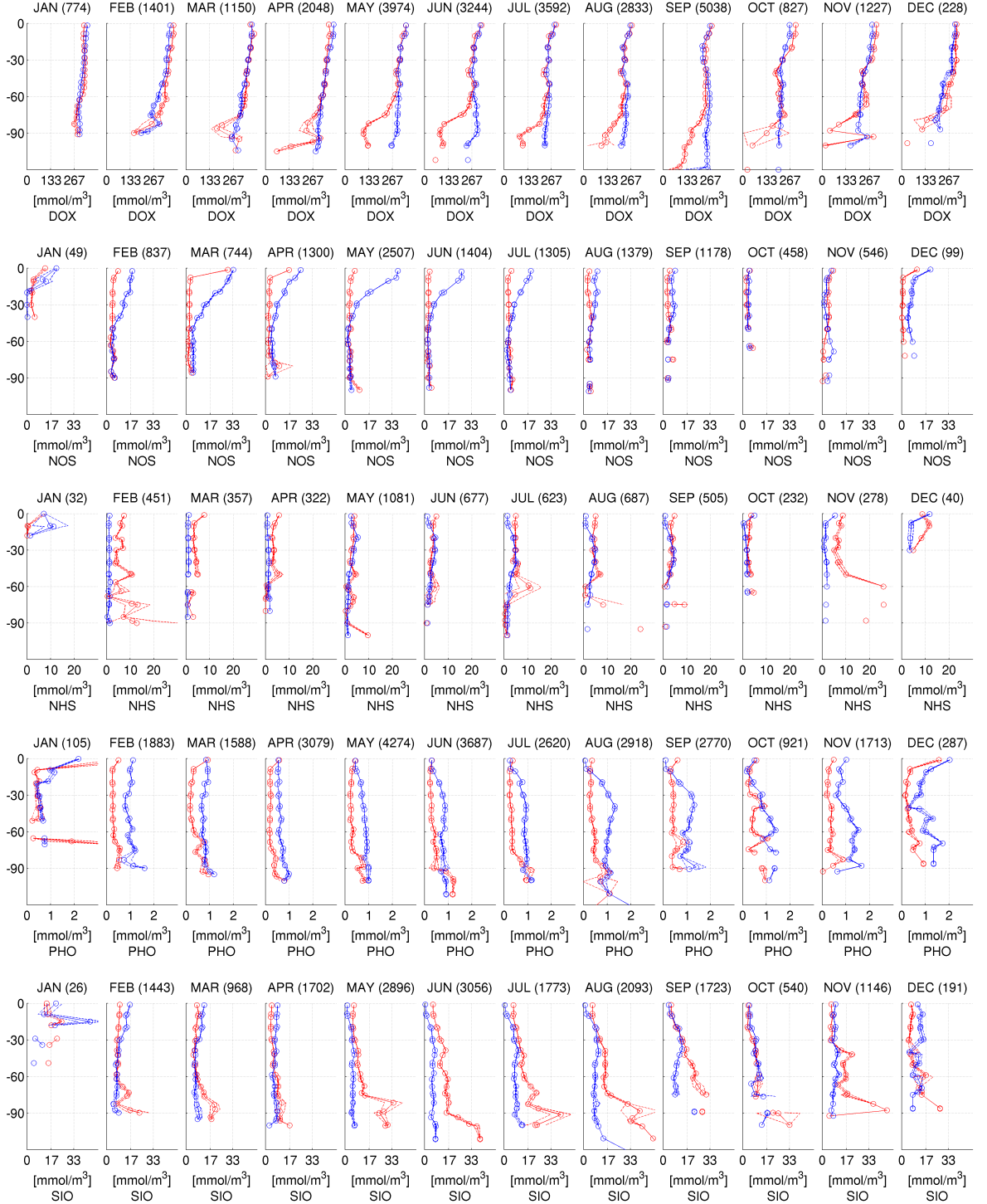


Figure 5.3: Monthly vertical profiles in the NWS : Oxygen, Nitrate, Ammonium, Phosphate, Silicate .

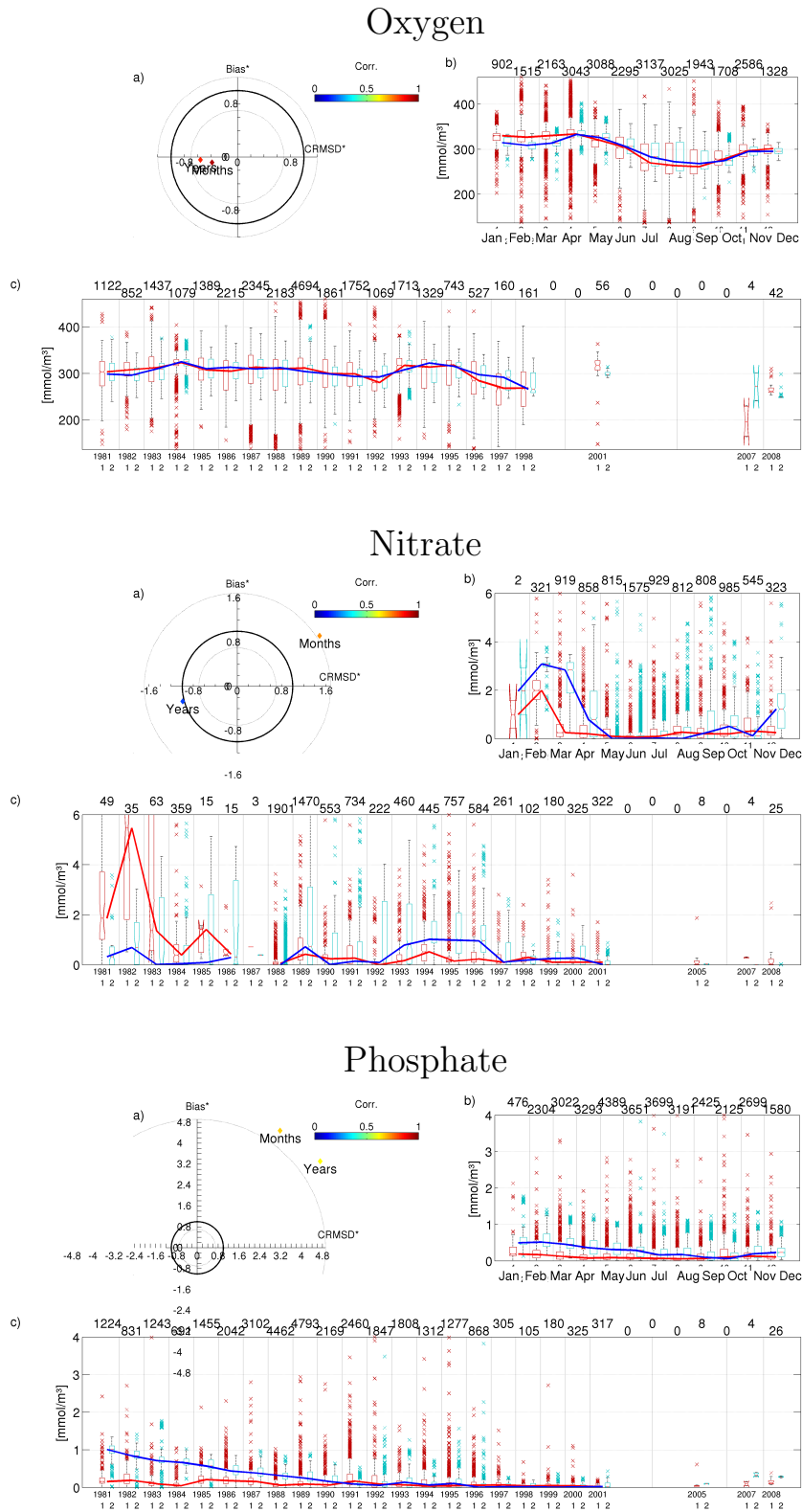


Figure 5.4: Temporal skill assessment in the open sea : Oxygen, Nitrate, Phosphate.

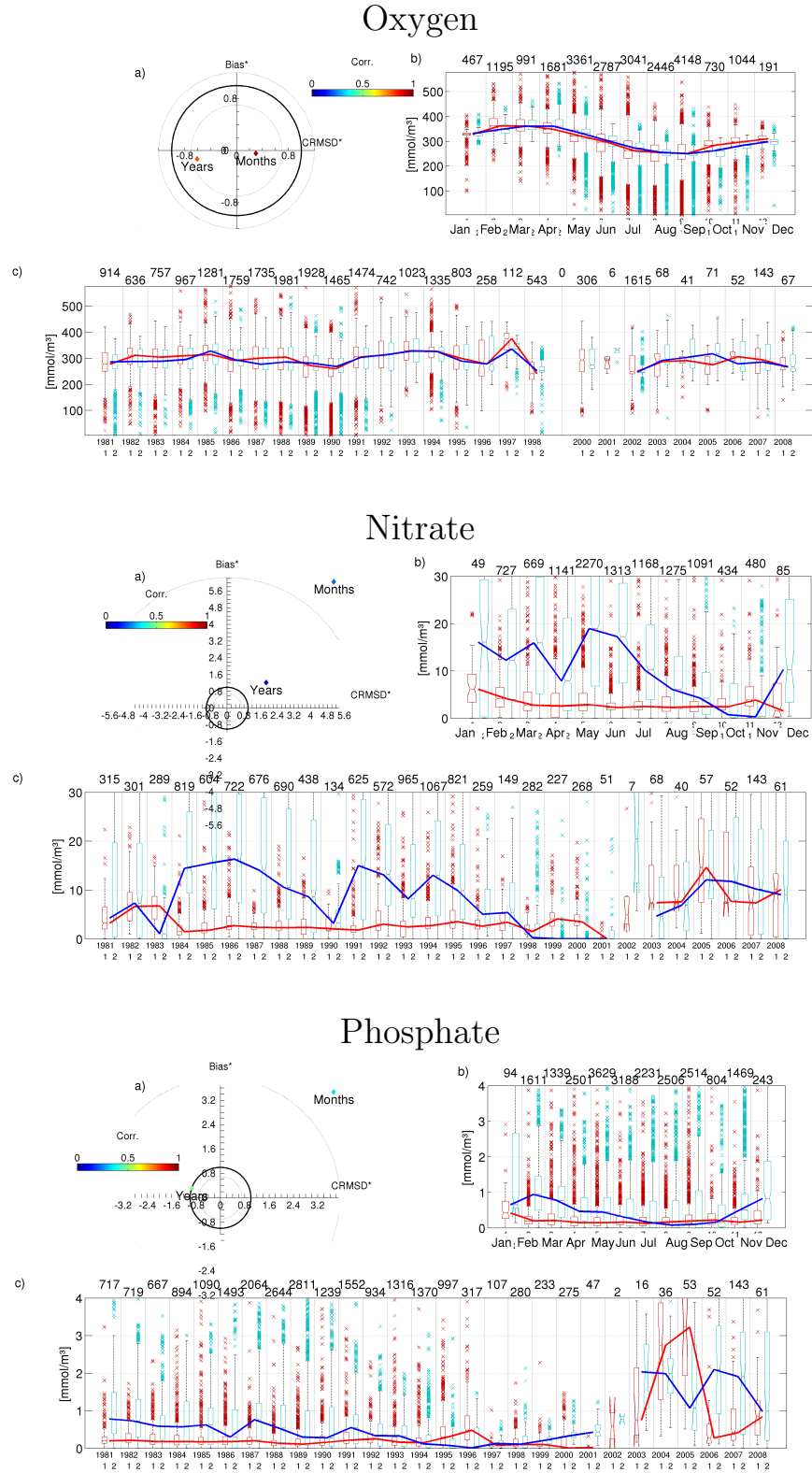


Figure 5.5: Temporal skill assessment in the NWS : Oxygen, Nitrate, Phosphate.

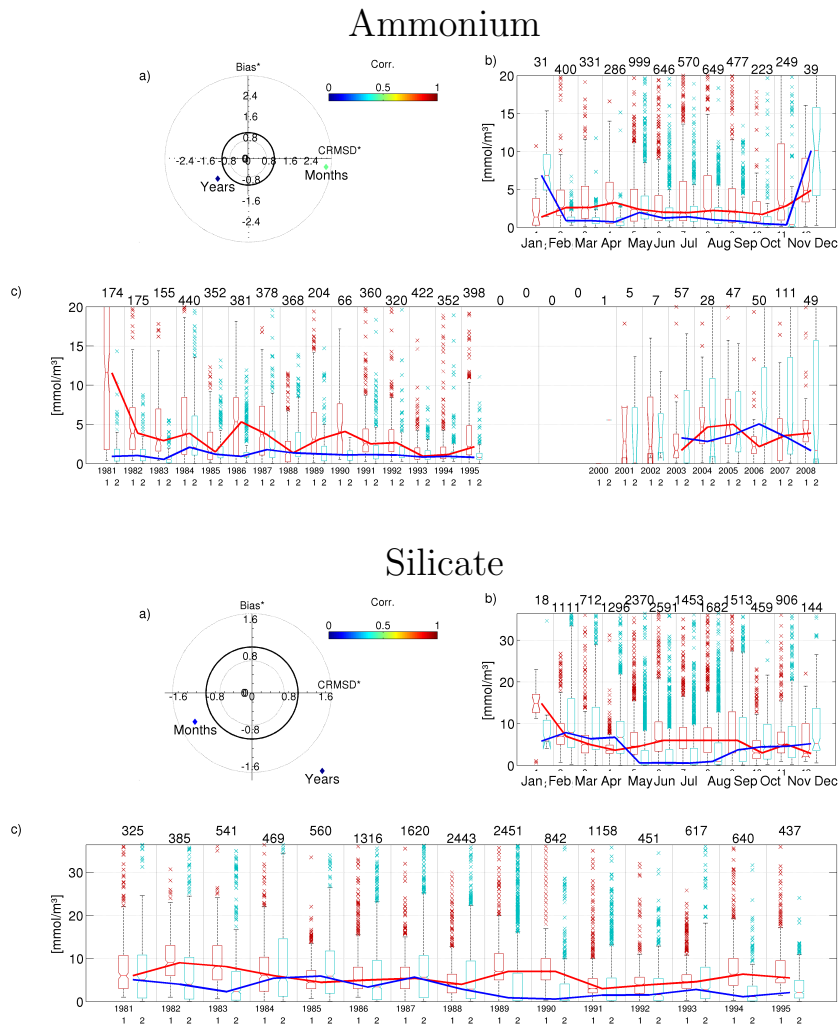


Figure 5.6: Temporal skill assessment in the NWS : Ammonium, Silicate

depths (60-120 m). But it could also be argued that an overestimated sinking velocity for the detritus (and eventually for diatoms) would limit the remineralization of organic matter in this region, hence reduce the oxygen consumption and the release of remineralized nitrogen and silicate. The latter would also explain the overestimation of ammonium just below the oxycline. This specific issue could be partly addressed using sediment trap data but those are only scarcely available.

The matching depth, both in the NWS and open sea areas, of subsurface oxygen maximum and that of increasing nitrate concentrations gives confidence regarding the light penetration scheme.

One main issue affects the model skills in the NWS region. Skill assessment procedures indicate an overestimation of nutrients contents, mainly in spring when the river discharges are high. While it does not appear clearly on the figures, very high nitrate concentrations ($> 200 \text{ mmol/m}^3$) are effectively measured but these are confined to the close vicinity of the Danube delta. It indicates that the model misses some specific dynamics that permit the very strong gradients of nutrients concentration in the vicinity of the river mouths, and the fast absorption of the high spring land inputs of nutrients. We can only be speculative here: While this “fast nutrient absorption” may be associated to specific planktonic populations, we strongly suspect the implication of the benthic ecosystem, in particular benthic phototrophs are known to play an important role in the Black Sea NWS, and are not represented in the model. The overestimation of phosphate may be partially linked to the absence of phosphate retention in the sediments (see discussion in [4.3](#)).

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Chapter 6

Benthic-pelagic coupling in 3D ocean models : An efficient approach tested on the Black Sea northwestern shelf



Sea grasses and blue sea, Avery , 1958

This chapter is to be submitted as :

A. Capet, I. Akoumianaki, F. Meysman, K. Soetaert, and M. Grégoire, Benthic-pelagic coupling in 3D ocean models : An efficient approach tested on the Black Sea northwestern shelf, *Estuarine, Coastal and Shelf Science*.

This publication presents the application in the Black Sea of a method for representing the benthic/pelagic coupling at reduced computational costs. While this method is not original this study constitutes its first implementation in 3D model. The methodology has been completed in that occasion by taking into account the effects of the bottom stress on the sedimentation of organic matter. Such a sound representation of benthic-pelagic coupling is effectively requisite to represent with some realism the biogeochemical dynamics in the wide and shallow Black Sea northwestern shelf.

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Abstract

Three-D ocean models resolving explicitly the benthic compartment are highly demanding in computing resources.

We describe a new approach for modeling the benthic compartment in 3D ocean models that combines an explicit representation of sediment organic matter, a parameterization of mineralization pathways and bottom stress control on organic matter deposition and resuspension.

The efficient representation of the benthic compartment allows running the 3D ocean model for long time periods (i.e. several decades) which is necessary to assess the inertial contribution of the sediment to marine biogeochemical cycles.

The model is applied to analyze benthic-pelagic coupling in the Black Sea northwestern shelf (BS-NWS) over the period 1980-2010. Comparison of modeled benthic-pelagic fluxes with in situ estimates shows that the model results agree well with the magnitude and inter-regional and seasonal variability of measured fluxes.

Based on the analysis of the simulated seasonal cycle of bottom environmental conditions, benthic-pelagic fluxes and diagenetic processes, three distinct areas extending along a gradient from the land-ocean interface to the open sea boundary are identified, each region characterized by a particular diagenetic pathway, in a way similar as they succeed vertically in a sediment profile.

(1) In the hypoxic zone, high remineralization rates lead to a seasonal peak in anoxic diagenesis and under certain conditions to hydrogen sulphide effluxes from the sediment, (2) in the denitrification zone, benthic denitrification rates are maximal and (3) in the oxic zone where organic matter accumulation are low, oxic diagenesis prevails and seasonality is less marked.

The findings of this study underline the importance of dynamically representing resuspension and deposition processes in coupled benthic-pelagic models. This is essential to realistically describe the horizontal distribution of benthic-pelagic fluxes and the export from the shelf region to the deep sea.

1 Introduction

1.1 Benthic-Pelagic Coupling

Marine sediments play an essential role in the functioning of shelf ecosystems ([Middelburg and Soetaert, 2004](#)), and in the oceanic global biogeochemical cycles in general (e.g. [Hedges, 1992](#); [Arndt et al., 2011](#)). The coupling between pelagic and benthic ecosystems is particularly tight in the shallow coastal and shelf areas ([Heip et al., 1995](#)) where a significant part of the primary production (15-50 % according to [Canfield \(1993\)](#) and [Wollast \(1998\)](#)) escapes degradation in the water column and reaches the sediment in a relatively fresh state.

The net contribution of sediments to marine biogeochemistry results from the balance of processes controlling the transfer of organic matter to the sediments and early diagenetic processes affecting the organic matter accumulated in the sediments.

The sediment diagenetic processes are impacted by local environmental conditions, among them the amount of pelagic primary production that reaches the bottom (e.g. [Soetaert et al., 1996b](#); [Dollar et al., 1991](#)), temperature (e.g. [Van Cappellen et al., 2002](#)), bottom oxygen and nutrient concentration, (e.g. [Wijsman et al., 1999](#); [Soetaert et al., 2000](#); [Fulweiler et al., 2008](#); [Dale et al., 2011](#)).

Consequently, diagenetic processes and, by extension, benthic-pelagic exchanges exhibit an important spatial and temporal (e.g. seasonal and interannual) variability (e.g. [Friedrich et al., 2002](#); [Fulweiler et al., 2010](#)).

The magnitude and variability of sediment-water exchanges have significant implications in critical and challenging issues such as carbon sequestration (e.g. [Hedges and Keil, 1995](#)), eutrophication (e.g. [Cерco and Cole, 1993](#); [Gypens et al., 2008](#); [Fulweiler et al., 2010](#); [Bohlen et al., 2012](#)) and deoxygenation (e.g. [Turner et al., 2008](#); [Peña et al., 2010](#); [Capet et al., 2013](#)) and cannot be ignored in a sound management strategy of the Good Environmental Status (GES) of marine waters ([Cardoso et al., 2010](#)).

In the open ocean, the influence of the deep sediments is only relevant to the surface layer at the large time scale of bottom water renewal ([Soetaert et al., 2000](#)). However, an important fraction of the oceanic primary production depends on the transfer of nutrients and organic matter from the shelf zone to the deep sea and this transfer depends on the capacity of the shelf to filter the inputs from the land. As sediments account for a significant part of this filtering, a good representation of the shallow benthic system is necessary, not just for the shelf, but also for the basin scale ecosystem.

In the coming decades and centuries, the ocean will become increasingly stressed by at least three factors: rising temperatures, acidification and deoxygenation. These three stressors will cause substantial changes in the physical, chemical and biological environment, which will then affect the ocean biogeochemical cycles and ecosystems in ways that we are only beginning to comprehend ([Gruber, 2011](#)).

A complicating factor in coastal and shelf waters which are more prone to environmental perturbations, is that marine sediments may act as a buffer to biogeochemical changes. Alternatively, as the benthic biogeochemical balance is in turn responding to environmental conditions, benthic-pelagic coupling could introduce further non-linearities in the ecosystem response to changes in the external driving forces (e.g. [Nixon et al., 2009](#)). The mechanisms of this coupling therefore have to be thoroughly considered within the definition of GES management strategies.

The fluxes of solutes (e.g. oxygen, nitrate, ammonium, phosphate, silicate) across the sediment-water interface can be determined by in situ measurements using benthic chambers, sediments core incubation or by interpreting the vertical profiles of solutes with Ficks law. However, due to logistic constraints, these estimates are limited in space and time and offer only a glimpse of the variation in benthic-pelagic exchanges. These limitations prevent to resolve the important spatial and seasonal variability of benthic-pelagic fluxes ([Cardoso et al., 2010](#)) and hence their upscaling at the scale of the entire

shelf.

Given the number of processes involved, the complexity of interactions and their variability in time and space, three-dimensional (3D) biogeochemical models are indispensable tools to explore the mid- and long-term evolution of marine biogeochemical cycles under environmental stressors. These models offer means to upscale the punctual measurements of highly variable processes and constitute ideal tools to obtain an integrated and holistic picture of the system.

In coupled benthic-pelagic models, the pelagic model provides the deposition rate of particulate substances and environmental conditions in the bottom water (e.g. temperature, salinity, shear stress, oxygen, nutrients, light), while the return flux of dissolved constituents is a result of the benthic (diagenetic) model. Because they are often used to provide answers to global environmental problems (e.g. climate change, eutrophication, pollution, assessment of the Good Environmental Status of marine waters), pelagic models have considerably evolved during these last two decades with increasingly complex 3D hydrodynamic models coupled to increasingly complex biogeochemical descriptions.

Diagenetic models developed somewhat independently and also present a high degree of sophistication, resolving several elemental cycles (e.g. carbon, nitrogen, oxygen, silica and phosphorus cycling) and reproducing the vertical distribution of solids and solute fractions (e.g. [Soetaert et al., 1996a](#); [Dale et al., 2008](#); [Arndt et al., 2013](#), and references therein).

Although pelagic and benthic models have both substantially progressed, their coupling (especially in 3D models) is by far less advanced. To date, the choice of a lower boundary condition in water column models is more a matter of convenience rather than based on careful representation of the essentials of sedimentwater exchange ([Soetaert et al., 2000](#)). Due to computational constraints, when the benthic part of a 3D ocean model explicitly resolves the vertical extent, it either considers one element (e.g. phosphorus in [Palastanga et al. \(2011\)](#)) or is integrated for reduced periods (e.g. $\sim$ one year in [Brigolin et al., 2011](#); [Luff and Moll, 2004](#)), which enhances the sensitivity to initial conditions.

This unsatisfactory incorporation of benthic processes in 3D biogeochemical models severely restricts our ability to upscale site-specific studies and to evaluate past, present and futures changes of the marine biogeochemistry ([Arndt et al., 2013](#)).

The main objective of this paper is to find an efficient and accurate methodology for coupling the benthic and pelagic compartment in 3D models, such that it is usable for long term simulations and offers a reliable representation of benthic-pelagic interactions.

1.2 The Black Sea northwestern shelf

The Black Sea northwestern shelf (BS-NWS) receives the discharge of the largest European river, the Danube, and has been severely disturbed by eutrophication.

Bottom hypoxic events affected the ecosystem hosted in this shallow area since the 1970's ([Zaitsev, 1997](#)) and are still seasonally occurring nowadays in the northern part of the BS-NWS ([UkrSCES, 2002](#); [Capet et al., 2013](#)). On the long term, the organic

sediment accumulation introduces a strong non-linear term in the response of hypoxia to nutrient loads (Capet et al., 2013). This is because on one hand, the mineralization of the organic matter accumulated in the sediments contributes to the depletion of oxygen in bottom waters locked by the thermocline. On the other hand, bottom hypoxia changes the sediment diagenetic processes hence impacts on the nutrient benthic release and eutrophication dynamics. In case of anoxia the sediment layer also releases toxic hydrogen sulphide (UkrSCES, 2002), which may consume oxygen after water-column mixing.

Benthic denitrification has been found to consume an important part of the river-borne nitrogen in the BS-NWS (Grégoire and Friedrich, 2004). As this process removes fixed nitrogen, it has the potential to significantly alter the nitrogen to phosphate (N:P) ratio in the water column compared to the N:P ratio of riverine discharge (Friedrich et al., 2002). Usually, the N:P ratio of the BS-NWS is taken to be similar to the composition of riverine discharge, causing the role of P limitation to be overestimated compared to N with consequences on waste water management policies. A better understanding of the role of benthic fluxes in this area is crucial to allow a proper survey and management of eutrophication issues.

The contribution of benthic fluxes to biogeochemical cycles is conditioned by the spatial distribution of organic matter deposition. In shallow areas, deposition is affected by the action of the bottom currents which may reduce the deposition and induce the resuspension of settled materials (Stanev and Kandilarov, 2012). The impact of bottom stress on sedimentation-resuspension needs therefore to be considered for a sound representation of the benthic-pelagic coupling.

1.3 Outline

The main objective of this paper is to propose a novel formulation of benthic-pelagic coupling in 3D models that offers a good balance between computational demand and attained accuracy. The representation of the benthic compartment combines a semi-empirical modeling of diagenesis with an explicit consideration of the bottom stress impacts on particulate matter deposition and resuspension. To the best of our knowledge this is the first study that combines these two aspects in a single modeling framework although these two aspects are crucial for representing benthic-pelagic coupling in shallow shelves.

The manuscript is organized as follows. Section 2 describes the mathematical model and the observations of benthic fluxes used to validate our modeling approach. Section 3 presents the results of the model focusing on the spatial and seasonal variability of benthic-pelagic fluxes, and comparing model estimates with available data. The discussion then elaborates on (Sect. 4.1) the biogeochemical implications of benthic-pelagic coupling in the BS-NWS, (Sect. 4.2) the importance of bottom stress effects on the biogeochemical role of the shelf area and (Sect. 4.3) the limitations of the current modeling approach and perspectives for further development. Sect. 5 provides a general conclusion.

2 Materials and Methods

2.1 In-situ benthic fluxes measurements

Benthic chamber fluxes of O_2 , NH_4^+ , NO_2^- , NO_3^- , HPO_4^{2-} and $Si(OH)_4$ were measured during the EU EROS21 project in August 1995 (Friedl et al., 1998), and, except for nitrate fluxes, in May 1997 (Friedrich et al., 2002) (Fig. 6.1).

In the frame of the EU SESAME project (2007-2011), flux estimates were obtained in October 2007 by on-board core incubations (Akoumianaki et al., 2013).

Additional benthic chamber measurements of sedimentary oxygen consumption in the offshore region of the NWS were taken in the frame of the EU HYPOX project (2007-2010) (Lichtschlag, 2012).

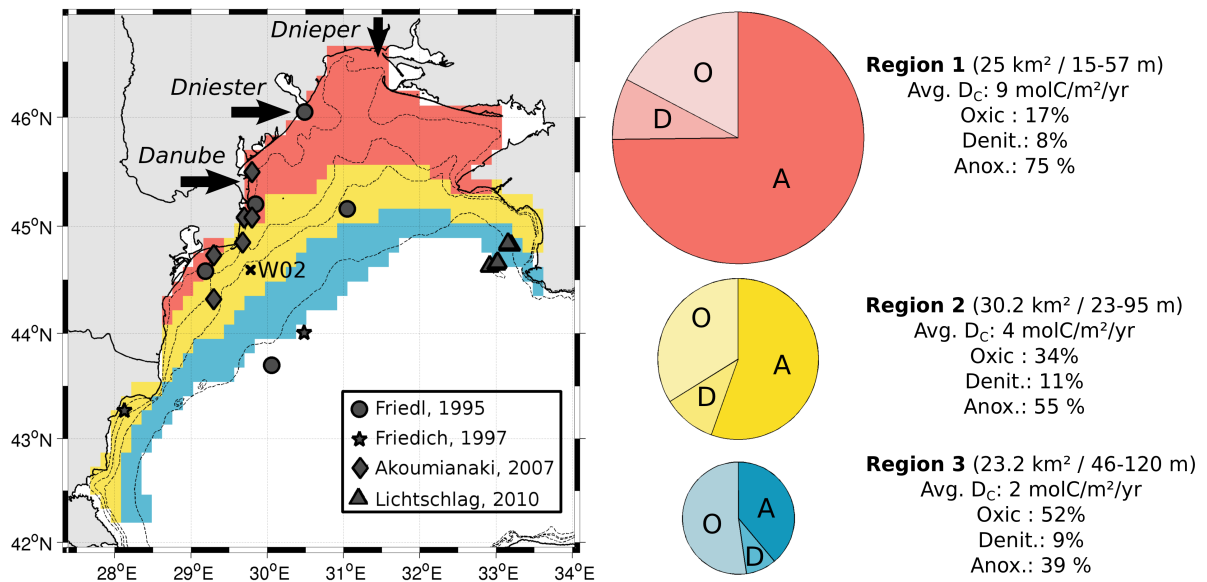


Figure 6.1: Regions of distinct benthic/pelagic coupling regimes, as obtained through the SOM procedure (Sect. 2.3). The map on the left panel indicates the limitation of the different regions (colored areas), the sampling years and locations of benthic fluxes in situ estimates (symbols repeated in the legend for the different sources, Sect. 2.1), and the location of the sediments profiles used to calibrate the WO2 model (marked as WO2, Sect. 2.2). The right panel illustrates the importance of diagenetic processes in each of the three regions (as annual spatial averages) and provides the surface and depth range of each region.

2.2 The Model

The Pelagic component

The physical model is the GHER 3D hydrodynamical model, a finite volume model resolving the currents, temperature, salinity, turbulent kinetic energy and surface elevation on Arakawa-C horizontal grids and double- σ vertical coordinates. The model is described

in Beckers (1991); Delhez (1996) and has been applied to the Black Sea in several studies (Grégoire et al., 1998; Grégoire and Friedrich, 2004; Stanev and Beckers, 1999; Beckers et al., 2002). The implementation used in the frame of our simulations is described in Capet et al. (2012).

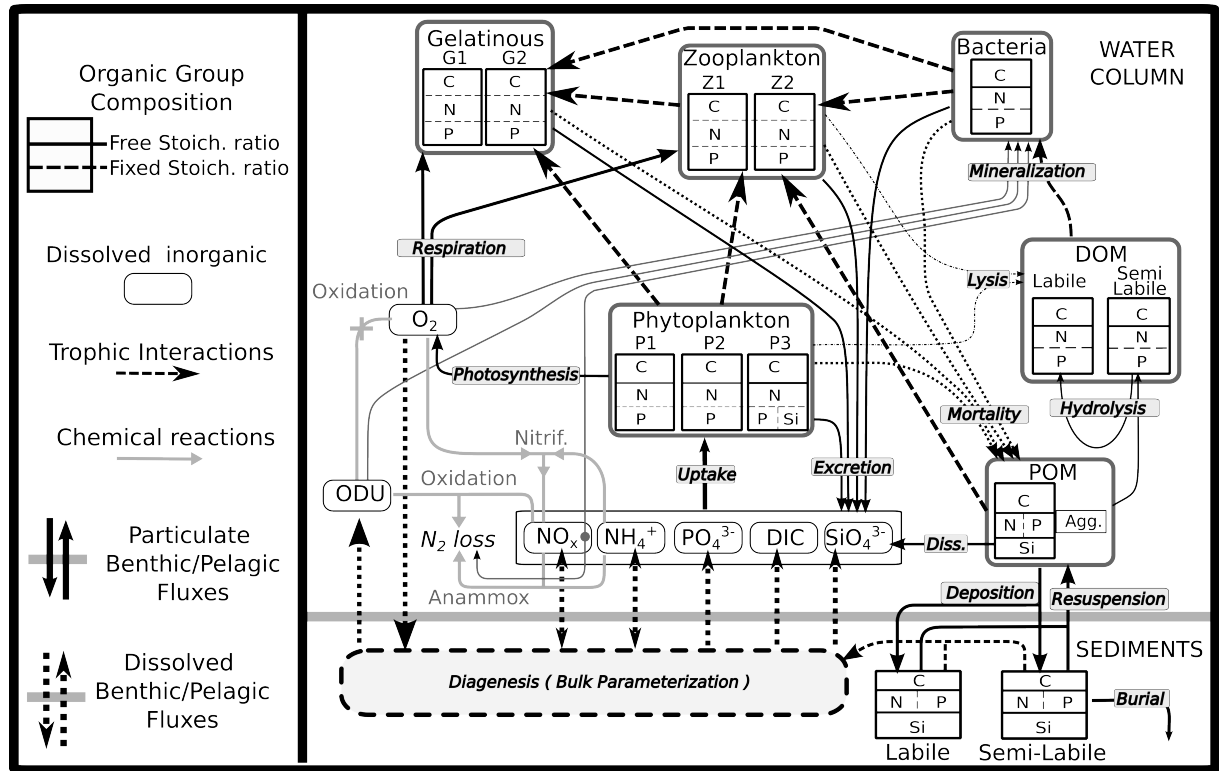


Figure 6.2: Schematic representation of the biogeochemical model.

The biogeochemical model is schematically represented in Fig.6.2 and described in detail in Grégoire et al. (2008). It describes the food web from bacteria to gelatinous carnivores through 30 state variables including three groups of phytoplankton: diatoms, small phototrophic flagellates and dinoflagellates, two zooplankton groups: micro- and mesozooplankton, two groups of gelatinous zooplankton: the omnivorous and carnivorous forms. The bacterial loop is explicitly represented by bacteria, labile and semi-labile dissolved organic matter, and particulate organic matter. The model simulates oxygen, nitrogen, phosphorus, silicate and carbon cycling and, in order to represent the biogeochemistry under hypoxic or anoxic conditions, it involves a lumped representation of reduced substances (Oxygen Demand Unit, ODU). These variables and associated chemical processes allows a dynamic representation of the interfaces between oxygenated, suboxic and anoxic layers.

The hydrodynamical model is coupled (online) with the pelagic biogeochemical model. The physics influences the biogeochemistry through transport processes (i.e. advection, diffusion), and temperature control on metabolic rates and oxygen saturation. The pelagic biogeochemistry influences the radiative heating via the penetration of light in the water that is governed by absorption and backscattering of seawater, phytoplankton and particulate organic matter.

The pelagic model provides the input of organic matter to the benthic compartment,

where sinking velocities of particulate organic materials are represented by a dynamic aggregation model (Kriest, 2002). The benthic model, in turn, provides the boundary conditions at the bottom interface for a subset of the pelagic state variables (listed in Table 6.1), by calculating the sediment-water exchange rates. Pelagic state variables not listed in Table 6.1 experience no-flux bottom boundary condition.

The interannual variability of the Black Sea hydrodynamics and physics resolved by the model has been presented in Capet et al. (2012) and validated in detail with satellite sea surface temperature and sea level elevation data. The biogeochemical model has been validated for the deep sea using all the variables available during the eutrophication period (Grégoire et al., 2008). Additionally, in Capet et al. (2013), all oxygen data have been used to assess the ability of the model to represent the oxygen dynamics (seasonal, interannual and spatial) during the last decades over the whole shelf.

The Benthic Component

In the benthic component, the accumulation in the sediments of sinking organic matter (detritus and sinking diatoms), and its mineralization in the sediment layer is described. The accumulation is controlled by the bottom shear stress, τ , whose intensity controls the deposition or induces resuspension of settled material. The diagenetic alteration of the accumulated organic matter results in fluxes of solutes that provide the boundary conditions for the dissolved pelagic variables (Table 6.1). The modeling of the benthic compartment only implicitly accounts for the dissolved phases in the pore waters and the vertical distribution of solids. Rather, it involves an explicit description of the vertically integrated solids concentrations with two levels of lability for both carbon and silicate, labile or “fast” (S_C^f and S_{Si}^f) and semi-labile or “slow” (S_C^s and S_{Si}^s), all expressed in mmol/m². The benthic organic nitrogen stock is derived from a variable nitrogen to carbon ration that constitute the fifth state variable of the benthic model, $S_{N:C}$. This amounts to imposing a common N:C ratio for both labile and semi-labile stocks and allows one to spare a 2D state-variable. At this stage, it is effectively considered that carbon and nitrogen content of the sediment organic matter is mineralized at equivalent rates.

The sediment phosphate stock is linked to the nitrogen stock by a fixed stoichiometric ratio (see discussion in Sect. 4.3).

The evolution of the four principal stocks (S_C^f , S_{Si}^f , S_C^s and S_{Si}^s) is governed by the balance between deposition/resuspension (P), remineralization/dissolution (D) and burial (B) processes (all expressed in mmol/m²/s, with the convention that upward fluxes are positive). P , D and B are computed at each time step of integration of the 3D pelagic model and the sediments stocks are updated according to equation 6.4.

The evolution of the nitrogen to carbon ratio, $S_{N:C}$, is derived from the algebraic development of $\frac{dS_{N:C}}{dt} = \frac{d}{dt} \left(\frac{S_N}{S_C} \right)$ (Eq. 6.5).

Resuspension/Deposition The exchange of particulate material between the sediment and the overlaying water, noted P , results from a balance between deposition and resuspension, controlled by the relative value of the bottom shear stress τ against critical

thresholds, τ_{dep} and τ_{ero} [Stanev and Kandilarov \(2012\)](#). Low values of τ (i.e. $\tau < \tau_{dep}$) only restrains the deposition of sinking materials (Eq. 6.5), while high values of τ (i.e. $\tau > \tau_{ero}$) cause resuspension of the sediments stock (Eq. 6.8 and 6.9).

In case of deposition, $P < 0$, the downward particulate flux is partitioned between the “fast” and “slow degradable fraction with a fixed ratio (Eq. 6.6).

As the slow decaying fraction penetrates deeper in the sediment (e.g. [Soetaert et al., 1996a](#)) in case of resuspension, $P > 0$, the “fast” fraction is resuspended in priority. The slow fraction only starts to be eroded when the slow fraction is entirely resuspended, with a higher critical threshold (Tab. 6.3).

τ is assumed non-directional and sums the contribution of waves and bottom currents. Bottom currents are computed by the hydrodynamical model while the wave bottom stress is computed separately using the wave model WAM ([WAMDI Group, 1988](#); [Stanev and Kandilarov, 2012](#)) with the bathymetry and atmospheric forcings used to force the hydrodynamical model.

The critical resuspension and deposition thresholds (respectively τ_{ero} and τ_{dep}) depend on various factors such as the nature and the grain size of the sedimenting material, the presence of algae or a biofilm on the bottom. The experimental quantification of these thresholds is a very difficult task ([Berlamont et al., 1993](#)) and usually, these parameters are obtained by calibration or using published values. In the literature, τ_{dep} varies between 0.02 and 1 Pa ([Wang and Pinardi, 2002](#); [Mercier and Delhez, 2007](#), , and references therein). In this study, we use $\tau_{dep} = \tau_{ero} = 0.02$ Pa obtained by [Stanev and Kandilarov \(2012\)](#) for sediment resuspension/deposition modeling on the BS-NWS. The erosion threshold of the slow decaying sediment fraction (which is considered to be below the fast decaying fraction in the sediment) is considered to be 0.02 Pa higher in order to differentiate the behavior of freshly deposited organic matter from that of the accumulated semi-labile materials. In order to test the sensitivity of the biogeochemical model to the value of these two parameters, simulations are performed using different values of these parameters selected within the range found in the literature (i.e. $\tau_{ero} = \tau_{dep} = 0.03, 0.05, 0.07$ Pa and $\tau_{ero,s} = \tau_{ero,f} + 0.02$ Pa) and a very high value (10 Pa) which corresponds to ignore the bottom stress effects.

Burial Burial only affects the slow fraction and its rate is computed as a fixed proportion of the sediment stock (Eq. 6.11)

Mineralization/Dissolution The degradation rate (D), the amount of organic matter degraded in the sediments per unit of time is a function of the stock size and is enhanced by high bottom temperature (Eq. 6.12).

Benthic-pelagic fluxes

The benthic-pelagic exchanges of solutes is parameterized as a function of the degradation rates, as described in [Soetaert et al. \(2000\)](#) (Level 3 formulation). These formulations involve three bulk parameters: p_{nit} , the amount of ammonium oxidized to nitrate relative

to the amount of ammonium produced, p_{denit} , the part of benthic carbon mineralized through denitrification and p_{anox} , the part of benthic carbon mineralized through anoxic processes. The estimation of these parameters is described in Sect. 2.2.

The ammonium flux is estimated from the degradation rate, D_N , minus the part p_{nit} of the produced ammonium that is consumed by nitrification (Eq. 6.20). The nitrate flux results from the balance of nitrification (production) and denitrification (consumption), considering that 0.8 mole of nitrate is required to oxidize 1 mole of organic carbon (Eq. 6.21).

The sediment oxygen consumption equals the amount of oxygen consumed for the degradation of organic carbon, $(1 - p_{denit} - p_{anox}) \cdot D_C$, for nitrification, $(D_N \cdot p_{nit} \cdot ON_{nitrif})$, and for the oxidation of the ODU produced by anoxic remineralization, considering that a part p_{solid} of the ODU produced in the sediments is precipitated by solid formation and escapes oxidation (Eq. 6.23). The latter thus amounts to $(1 - p_{solid}) \cdot p_{anox} \cdot D_C$.

Oxygen availability in the bottom waters may be insufficient to oxidize the ODU produced by anoxic remineralization. This occurs when the oxygen consumption prescribed by the bulk parameterization (Eq. 6.23) is such that $|F_{DOX}| > [DOX] \cdot \Delta z / \Delta t$, where Δz is the height of the bottom cell and Δt the time step. As p_{nit} tends toward zero and p_{anox} towards one for low oxygen concentration, it can be considered that oxygen consumption in these conditions is exclusively due to the oxidation of ODU in the sediments. In that case, the oxygen consumption is therefore limited to the oxygen available in the bottom cell and a release of ODU to the water column is allowed, computed as the difference between the oxygen consumption prescribed by the benthic model and the oxygen availability in the bottom cell (Eq. 6.24).

Despite the fact that bottom concentrations are included in the bulk formulations, their expected asymptotic behavior is not systematically ensured by the fitting procedure. As a results, the bulk computation of the diagenetic processes may results in NOS or NHS consumption rates that surpass their availability in the model bottom cells. Those cases are rare but have to be considered to ensure the numerical stability and the mass conservation of the model. In case NHS consumption becomes critical, p_{nit} is bounded to 1 to ensure no ammonium is consumed. If necessary p_{denit} is adjusted to ensure that F_{NOS} matches the NOS available in the bottom cell.

The benthic fluxes for DIC and SIO are calculated directly from D_C and D_{Si} , respectively (Eq. 6.18, 6.17). F_{PHO} is derived from the degradation of D_N assuming a constant redfield ratio and neglecting the adsorption process (Eq. 6.19).

Remineralization pathways

The parameters p_{nit} , p_{denit} and p_{anox} and their response to environmental conditions are estimated using meta-modeling as described in (Soetaert et al., 2000). The procedure consists in parameterizing processes unresolved by the simplified model by means of a regression model against the results produced from a vertically resolved full diagenetic model. For this exercise we run the full diagenetic model developed for the BS-NWS by Wijsman et al. (2002) (WO2), where we imposed a seasonal cycle of sinking detritus. This model was calibrated by Wijsman et al. (2002) with data collected at station

WO2 (Fig. 6.1). Following a Monte Carlo approach, numerous runs of the WO2 are made while randomly modifying the environmental variables to which this full diagenetic model is the most sensitive, i.e. the particulate flux to the sediments and the bottom concentrations of oxygen and nutrients. The random modifications are allowed within the BS-NWS environmental range derived from early simulations with the 3D pelagic model. The relationships between the integrated rates derived from the Monte Carlo simulations and the corresponding environmental conditions are then used to derive the empirical formulations of the bulk parameters (Eqs. (6.25,6.26,6.27), Fig. 6.3).

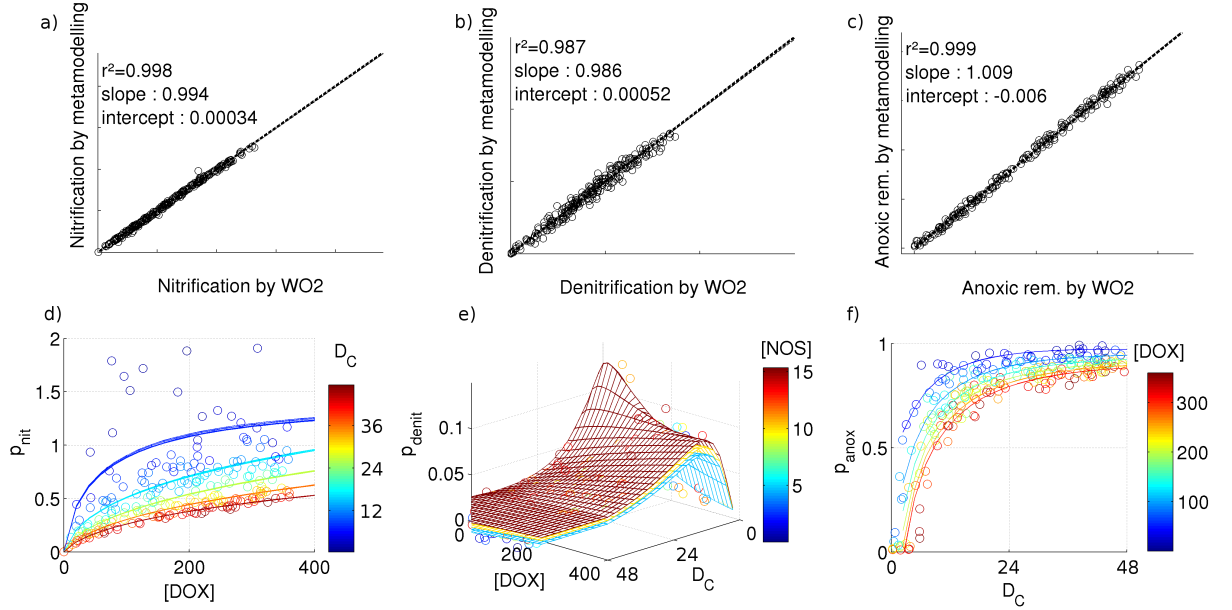


Figure 6.3: Values of (a) nitrification (b) denitrification and (c) anoxic remineralization obtained from the bulk formulations (Eqs 6.25,6.26,6.27), compared to that obtained with the full diagenetic model (WO2). Behavior of the (d) p_{nit} , (e) p_{denit} , and (f) p_{anox} bulk formulations, for various range of the most relevant environmental variables. D_C is expressed in $\text{mmolC/m}^2/\text{d}$, $[DOX]$ and $[NOS]$ in mmol/m^3 .

Following the approach of Soetaert et al. (2000), a stepwise regression procedure is apply to select the variables allowing to render the amount of nitrogen nitrified (resp. denitrified) in the sediments, i.e. the product $p_{nit} \cdot D_N$ (resp. $p_{denit} \cdot D_C$). In the case of p_{anox} best results are obtained by fitting directly p_{anox} rather than the product $p_{anox} \cdot D_C$.

Model implementation

For the present implementation, the model is run on a regular Arakawa-C grid of resolution $\Delta x = \Delta y = 0.135^\circ$ ($\sim 15 \times 11.5$ km), using the terrain following double-sigma vertical coordinates system (Beckers, 1991). The open boundaries are restricted to the Bosphorus and the 6 main rivers: Danube, Dnieper, Dniester, Rioni, Kizilmark and Sakarya. Annual values of rivers flows and nutrients discharges are provided by Ludwig et al. (2009), as well as climatological seasonal repartitions used to construct the monthly river forcings. Concentrations of riverine organic matter are estimated from Cauwet et al. (2002); Reschke et al. (2002); Walling and Fang (2003).

The Bosphorus entrance is parameterized to ensure the representation of the two-layer exchange needed to sustain the halocline, while ensuring long term conservation of the total salt and water contents. Atmospheric data used to force the model are issued from the ECMWF-ERAInterim reanalysis (1.125° resolution), using 10 m winds velocities, 2 m air temperature and dew point temperature, and sea level pressure and precipitations. All atmospheric fields are filtered in order to suppress the erroneous influence of land points on the coastal sea conditions (Kara et al., 2007). Wind stresses, heat fluxes and the pseudo fluxes of salt associated to evaporation and precipitation are computed interactively considering the state of the model surface layer using bulk formulaes (Rosati and Miyakoda, 1988). Air-sea oxygen exchanges coefficients are computed as a function of the wind intensity (Ho et al., 2006). An average atmospheric deposition rate of 0.15 mmolN/m²/d and 6.10⁻⁵ mmolP/m²/d is imposed uniformly across the domain (Kanakidou et al., 2012). The model is run without any relaxation term or data assimilation over the whole Black Sea. The analysis is focused on the northwestern shelf, limited by the 120 m isobathymetric lines. This area of 78300 km² encloses a water volume of 4327 km³ for an average depth of 55 m (Fig. 6.1).

The pelagic biogeochemical model is initialized from climatological fields reconstructed from the MEDAR-MEDATLAS and NATO databases. To minimize the impact of initial conditions, the model is run for 10 years under a perpetual climatological forcing. After this spin-up, the model is integrated for 30 years using realistic forcings starting in 1980. The initialization of the benthic compartment is critical, especially for the two slow degrading stocks, since these compartments are slow to reach steady state and they may not be estimated from in situ observations. The benthic compartments are therefore initialized with equilibrium values, estimated using equation 6.4.

$$S_{i,init}^s = \frac{\overline{P}_i \cdot (1 - f_i)}{k_i^s \cdot f(\overline{T}) + b_i} \quad (6.1)$$

$$S_{i,init}^f = \frac{\overline{P}_i \cdot f_i}{k_i^f \cdot f(\overline{T})} \quad (6.2)$$

$$S_{N:C,init}^f = \frac{\overline{P}_N}{\overline{P}_C}, \quad (6.3)$$

where $\overline{T}$ and $\overline{P}_i$ respectively represent the averaged bottom temperature and net particulate flux to the sediment estimated in preliminary runs (i stand for either C or S).

While benthic dynamics has significant implications for the ecosystem functioning at large interannual scales, as evidenced in Capet et al. (2013), here we focus on the spatial and seasonal variability of the benthic-pelagic coupling.

For this reason, the results presented in the following correspond to climatological values reconstructed from the model simulations over the period 1995-2000. This restricted period is chosen as a compromise to filter out rapid interannual fluctuations related to meteorological variability, while avoiding the inconsistency of climatologies computed over large period marked by interannual trends. Also, the period encompasses the years during which in situ measurements are available.

2.3 Automatic regionalization procedure

The analysis of model results is facilitated by summarizing the spatial variability through regionalization, i.e. by considering averaged quantities over subregions that are characterized by a similar functioning of the benthic system.

The regionalization procedure is based on two successive applications of the Self Organizing Map algorithm (SOM, Kohonen (1998)). The method (Allen et al., 2007) allows the user to choose the number of regions to be distinguished and the set of variables used to constrain the regionalization. Both the average range and the seasonal variability of these variables are considered to constrain the regionalization. Here, the simulated daily distribution of D_C , p_{nit} , p_{denit} , p_{anox} , F_{NHS} , F_{NOS} , F_{DOX} , F_{PHO} and F_{SIO} are considered to identify three distinct regions.

3 Results

3.1 Environmental factors controlling the spatial organization of diagenesis and benthic-pelagic coupling

The 3 regions identified by the SOM procedure are organized along a bathymetric and river influence gradient (Fig. 6.1). These two factors effectively govern most of the dynamics of the environmental variables controlling diagenetic processes.

The range of environmental conditions relevant to diagenesis (temperature, oxygen and nutrients concentrations, organic sediment stocks and bottom shear stress) are illustrated for each region in Fig. 6.4.

In the high flux region 1, where the organic content in the sediments is highest, sediments are affected by seasonal hypoxic/anoxic events and experience the highest concentrations of ammonium and nitrate in the bottom water. Region 2 is characterized by intermediate organic matter content, and is less affected by hypoxic conditions. Region 3 is the deepest and has the lowest organic sediments content, hence exhibits the lowest seasonal variability due to the limited seasonal range of bottom temperature, oxygen and nutrients concentrations.

The high flux area extends over a significant part of the BS-NWS, from the Bay of Constanta (Romania) to the northeast, along the Ukrainian coast. This extension of the high flux area is explained by the seasonal variability of the NWS circulation. From May (when the Danube discharge reaches its peak) to October, the Danube waters are transported northward by an anticyclonic circulation and merge with the plume of the other two main shelf rivers (i.e. the Dnieper and Dniester) for constituting a patch of highly productive waters. From October until end of April the shelf circulation is cyclonic and the river plumes flow along the Romanian and Bulgarian coasts. Around the cape south of the Danube mouth, the strong bottom currents cause high bottom stresses that prevent the accumulation of organic matter in that region and hence reduce the offshore extension of the high flux region in front of Constanta.

The spatial distribution of sedimentary organic carbon stock, S_C^s and S_C^f , and its seasonal cycle (Fig. 6.4) reflect the influences of river discharges, pelagic primary production, bottom stress and bathymetry. The sinking flux of particulate organic carbon is high near the river mouths where allochthonous inputs add to the pelagic primary production sustained by riverine nutrients and permanent stratification. Shallow seafloors are exposed to large amount of sinking detritus, but also to intense bottom stresses.

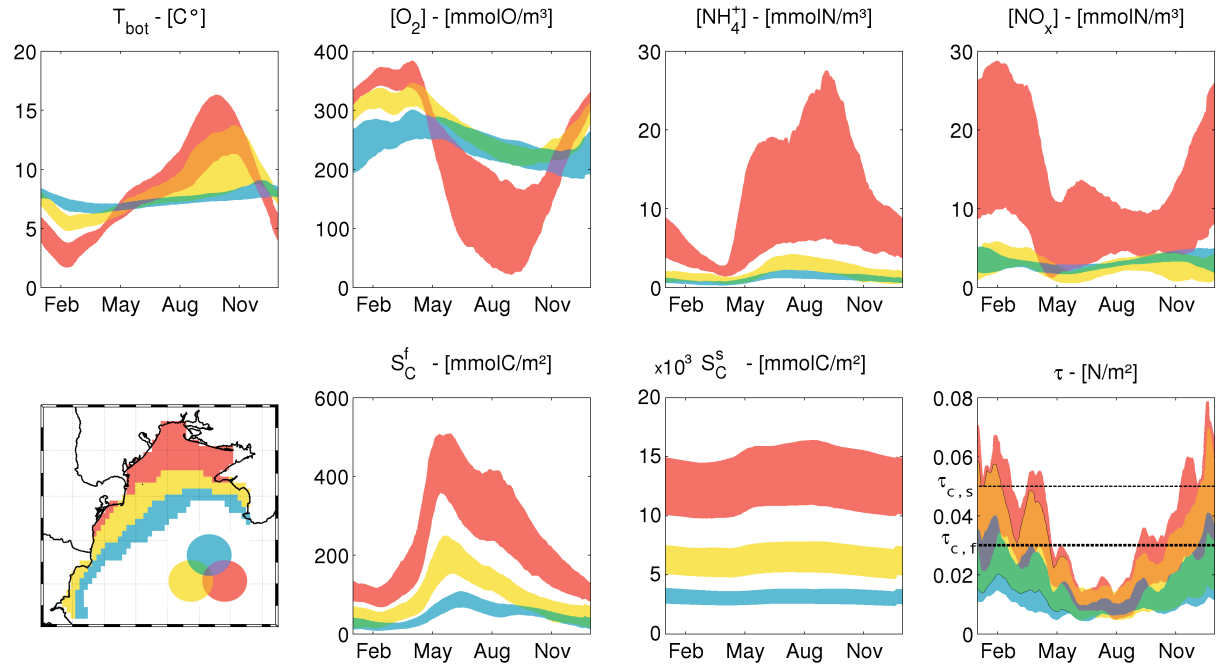


Figure 6.4: Seasonal cycle of bottom environmental conditions typical of each region. The colored areas indicate the interval between the 25th and 75th percentile of the spatial variability for each region.

The dynamics of the two stocks of organic matter (i.e. fast and slow) differ: the fast stock exhibits a pronounced seasonal dynamics while the slow stock is more inertial and may eventually accumulate during the years of important production. In the three regions, the fast stock starts to accumulate in spring (end of March) when planktonic productivity increases and decreasing mixing and bottom stress permit the deposition of the fresh organic matter on the seafloor (Fig. 6.4). This stock peaks in early summer and then starts to decrease due to the intensification of benthic degradation promoted by the increasing temperature.

The seasonal range of temperature, which is closely related to the bathymetry (depth ranges are indicated in Fig. 6.1), thereby conditions the range of seasonal variability of the diagenetic processes.

At the end of fall and during winter, the intensification of wave-induced resuspension events leads to the rapid decrease of the fast stock in regions 1 and 2 (Fig. 6.4).

The deepest region 3 is submitted to lower bottom stress and presents lower seasonal variability in general.

The three regions are also differentiated by their bottom oxygen concentration dynamics

(Fig. 6.4). The higher production and spatial confinement of region 1 make it more sensitive to the occurrence of hypoxia and/or anoxia events.

In the three regions, bottom water oxygen concentrations are generally lower in summer, due to temperature effect on oxygen solubility, the thermal stratification that restricts ventilation of bottom waters and the higher oxygen consumption for remineralization processes (Capet et al., 2013).

Finally, each of the three regions corresponds to a particular diagenetic pathways: region 1 corresponds to a large fraction of anoxic degradation, region 2 depicts the higher denitrification rates, while region 3, near to the open sea border is characterized by mostly oxic remineralization (Fig 6.1).

3.2 Seasonal variability of benthic-pelagic coupling

The contrasting environmental variables, amongst the different regions, results in contrasting seasonal responses.

For instance, in region 1 and 2, increasing D_C induces a reduction of denitrification (in the favor of anoxic processes), while in region 3, increasing D_C provokes an increase of denitrification (at the expense of oxic mineralization).

This is due to the non-linearity of the bulk parameterizations (Eq. 6.25, 6.26, 6.27) depicted in Fig. 6.3.

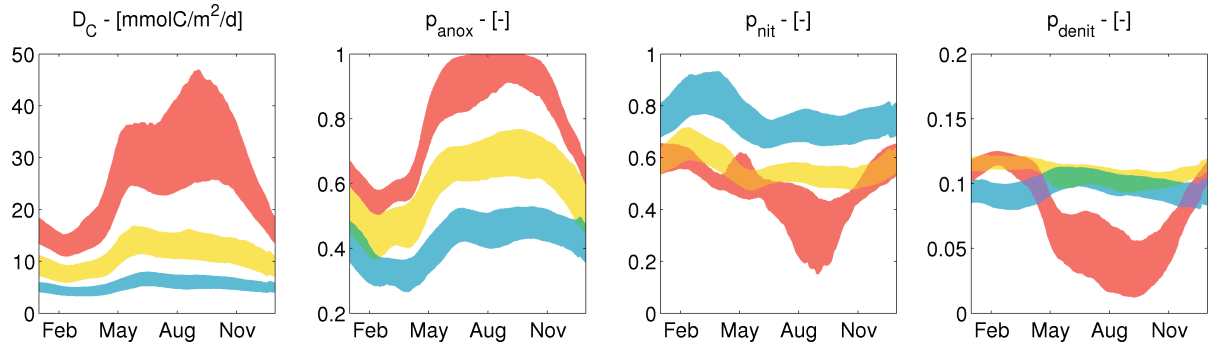


Figure 6.5: Seasonal cycle of the benthic degradation rate (D_C) and remineralization pathways for each region. The colored areas indicate the interval between the 25th and 75th percentile of the spatial variability for each region.

The seasonal cycle of sediment functioning can be summarized as follows. In winter, remineralization rates remain low due to the low organic sediment content and low bottom temperatures. D_C is minimum in March in the three regions (Fig. 6.5). The fast-decaying sediment stocks are mostly absent due to the high bottom stresses and the low pelagic production during this period.

The slowly decaying stock, accumulated during the previous years, maintains a low level of decay, with resulting oxygen consumption and nutrients fluxes that decrease from region 1 to 3 (Fig. 6.6).

The low rates of benthic degradation and the intense ventilation of the water column in winter imply that the oxic degradation pathways and nitrification rates are maximum in the three regions and the ammonium out fluxes are low (Fig. 6.5, 6.6).

Denitrification rates are then maximal in region 1 and 2, permitted by the lower organic sediment contents in winter. In region 3, the low organic content in winter results in minimal denitrification rates.

From mid-February to April, the progressive accumulation in the fast-decaying sediment stock and the increase of bottom temperature provoke an increase of the mineralization rates, especially marked in region 1. This causes an increase of ammonium release and oxygen consumption in all the regions (Fig. 6.6). In regions 2 and 3, D_C and oxygen consumption rapidly reach their maximum in May-June. In regions 1 and 2, the part of degradation due to denitrification decreases due to enhanced anaerobic degradation while in region 3 denitrification increases at the expense of oxic degradation.

In summer, the dynamics in region 1 differs from the two other regions. While D_C slowly decreases in regions 2 and 3 until October, the higher and ongoing primary production and the larger range of bottom temperature cause D_C to keep increasing until October in region 1. Also, bottom waters in region 1 rapidly become depleted in oxygen. Anoxic degradation therefore largely dominates from summer to fall in region 1, and to a lesser extent, in region 2, reaching its maximum just before the October ventilation (Fig. 6.5). Anoxic conditions during this period, causes a release of the reduced compounds (i.e. $H_2S, Fe(II), Mn(II)$) produced by anoxic benthic degradation in the water column. Noteworthy are the irregular shape of the F_{DOX} curve in region 1 (Fig. 6.6), and the difference between this curve and that of D_C in Fig. 6.5, indicating that the intense mineralization is not matched by the corresponding benthic oxygen consumption, as the latter is limited by the oxygen availability in the bottom waters. In late summer, the lack of oxygen in region 1 severely limits the nitrification, which in turn results indirectly in limited denitrification rates. F_{NHS} is then about 4 times bigger than in the other regions and F_{NOS} depicts an important release towards the water column. High nitrification rates in region 3 results generally in positive F_{NOS} (release), while limited nitrification in region 2 leads to generally negative F_{NOS} (uptake by the sediments).

In Fall, around October, the breakdown of the thermocline induces a rapid cooling and oxygenation of bottom waters while increasing bottom stresses start eroding the remaining fast stock. These factors entrain a general decrease of mineralization rates.

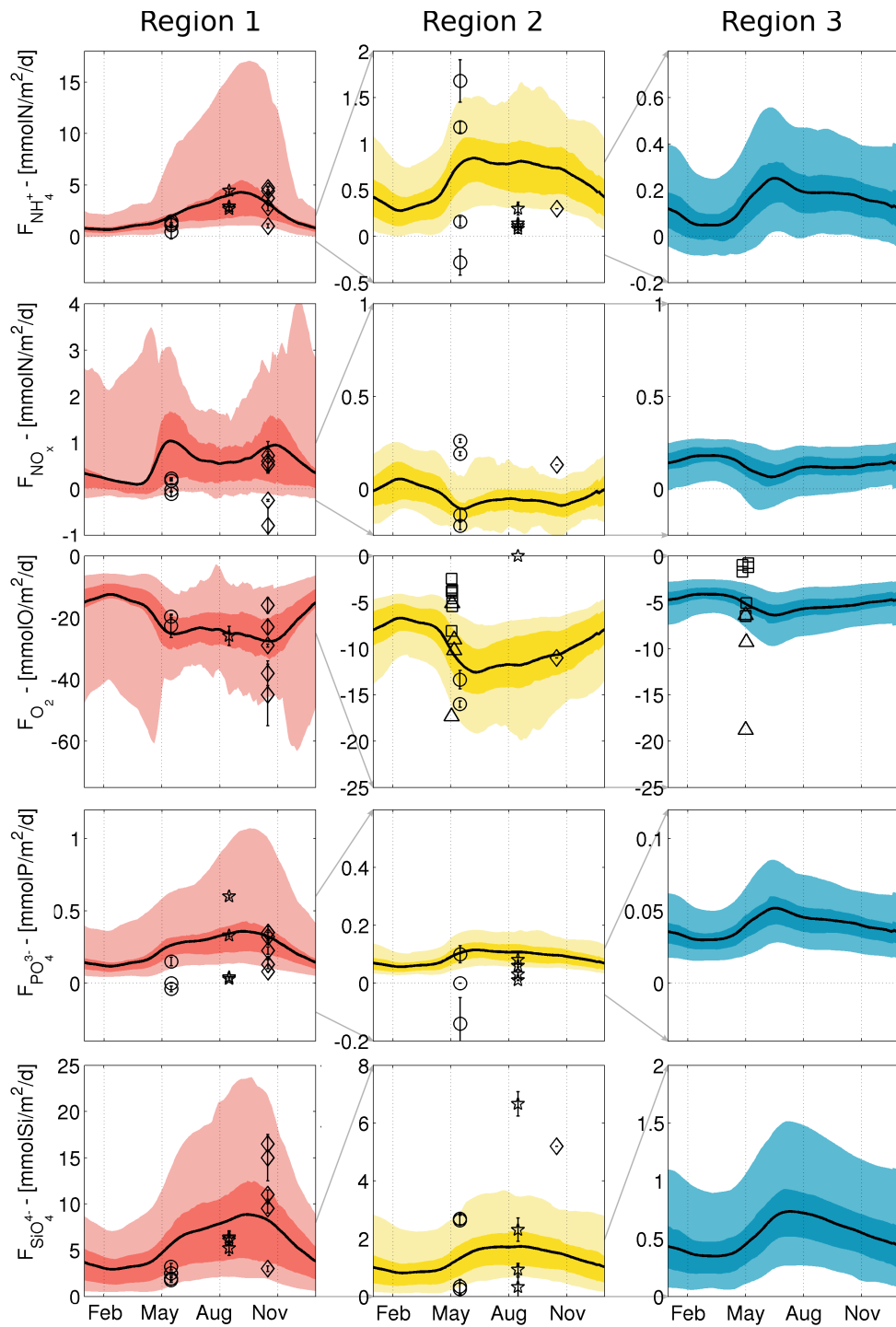


Figure 6.6: Benthic-pelagic fluxes of dissolved substances simulated and observed in the three regions (delimited in Fig. 6.1). The dark (resp. light) colored areas indicate the interval between the 25th and 75th (resp. 2.5th and 97.5th) percentile of the spatial variability for each region. In-situ estimates and corresponding error bars are described in Sect 2.1 (circles: Friedl et al. (1998); stars: Friedrich et al. (2002); diamonds: Akoumianaki et al. (2013); triangles: Lichtschlag et al. (2012), incubation chambers; squares: Lichtschlag et al. (2012), micro-profiling) Fig. 6.1).

3.3 Comparison with in situ estimates of benthic fluxes

In this section, model results are compared to in situ estimates of benthic-pelagic fluxes (Sect. 2.1).

The scarcity (in time and space) of in situ data make the comparison between observations and model results delicate (instantaneous localized observation versus climatological weekly averages computed over a $\sim 15 \times 15$ km square grid over the period 1995-2000). Moreover, in situ observations are gathered over a large period (Sect. 2.1).

These considerations hinder the computation of representative error statistics, so that we restrict ourselves to test whether in situ estimates lie within the variability of model simulations and to detect any inconsistencies between the variability resolved by the model and that apparent from in situ estimates.

The benthic-pelagic fluxes of ammonium, silicate, oxygen, nitrate and phosphate have been estimated in regions 1 and 2 during May, August (not for nitrate) and October while only oxygen fluxes are available for region 3.

In general, both model simulations and observations reveal a decreasing intensity of benthic fluxes from region 1 to 3, (Fig. 6.6), a larger seasonal range in region 1 and an intensification of benthic fluxes from spring to fall.

Nitrogen Measured fluxes of ammonium are in the main range of model spatial variability in region 1 and agree with the seasonal trend.

In summer/fall in region 2, data are systematically below the model climatological values.

Both data and model evidence the occurrence of denitrification. However, the higher range of modeled F_{NHS} in the “high flux” region 1 and the absence of model correspondence to the strong negative F_{NOS} measured in October suggest an underestimation of denitrification in this region.

In general, the measured variability in region 2 is not represented in the model. Also, the model seems to overestimate F_{NHS} in summer and fall while underestimating F_{NOS} which could result from the underestimation of nitrification. Downward ammonium fluxes were recorded during the May 1997 campaign revealing a net consumption of ammonium by the sediment in region 2. Interestingly, this behavior is also resolved by the model in region 3.

Oxygen In the three regions, the variability of in situ observations are in agreement with the range of model variability. In particular, the model is able to simulate the inter-region variability. In region 2, the only measurement available in August gives a zero oxygen consumption by the sediments which coincides with anoxic conditions. This case is punctually resolved by the model but this is filtered by the averaging process.

Phosphate In the model, the dynamics of phosphate is linked to that of nitrogen through a constant Redfield P:N ratio. This is a rough approximation that may compro-

mise the model performances regarding the benthic fluxes F_{PHO} . Simulated and measured phosphate fluxes however show an acceptable agreement regarding the average range and inter-region variability, though in situ estimates generally lie in the lower range of simulated values. Three spring estimates depict sediment consumption of phosphate, which is precluded in the model by Eq. (6.19). This issue is discussed in Sect. 4.3.

Silicate The variability (both the inter-regional and seasonal) of the silicate outflux, F_{SIO} , predicted by the model and derived from in situ observations are in a very good agreement. We can note that two measurements point towards a higher seasonal variability in region 2 than that resolved by the model.

4 Discussion

4.1 Biogeochemical implications of benthic-pelagic coupling

Benthic degradation and associated diagenetic processes are a main aspect of biochemical cycles in shelf areas. Because the open sea biogeochemistry is highly influenced by lateral export from the shelf, benthic diagenesis on the shelf is relevant to the Black Sea biogeochemistry at basin scale.

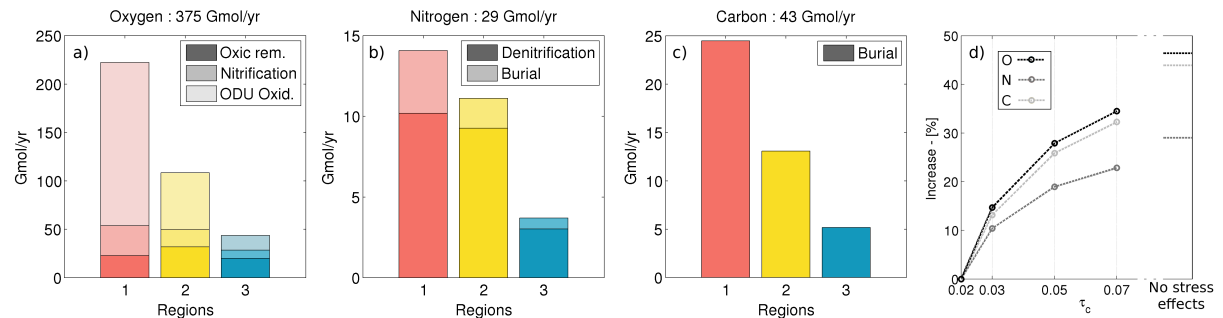


Figure 6.7: Benthic sink terms (annual mean value computed over 1995-2000 and integrated for each region) of the (a) oxygen, (b) nitrogen and (c) carbon budget. The different levels of color in each bar indicate the contribution of various processes to the total consumption. (d) Relative increases in the benthic sink terms (integrated for the total shelf) of the oxygen, nitrogen and carbon budgets for different value of τ_{dep} , i.e. various intensity of bottom stress effects. The sink terms shown in a) b) and c) have been computed with the reference value of $\tau_{\text{dep}} = 0.02$.

Figure 6.7 illustrates the annual sinks of oxygen, nitrogen and carbon in the sediments. Benthic oxygen consumption results from aerobic respiration, nitrification and oxidation of the reduced substance released by anoxic mineralization. In total, it amounts to 375 Gmol/yr and accounts for 48% of the oxygen budget below the mixed layer depth during the stratified period (Capet et al., 2013), and up to 64% if one considers the pelagic oxidation of reduced compounds (ammonium and ODU) released from the sediments. As such, benthic oxygen consumption is a critical factor to resolve the dynamics of seasonal hypoxia (Capet et al., 2013; Fennel et al., 2013). We have found that the spatial

distribution of benthic oxygen consumption is closely related to the spatial extension of hypoxia (Capet et al., 2013).

The annual benthic loss of nitrogen amounts to 29 Gmol/yr with 22.5 Gmol/yr consumed in benthic denitrification, the remaining lost by burial. This represents 62% (resp. 48% for denitrification alone) of the total N inputs to the shelf area, considering the riverine inputs in nitrate and nitrite (27 Gmol/yr), ammonium (5 Gmol/yr) and organic forms (10 Gmol/yr) and atmospheric nitrogen deposit (4.5 Gmol/yr) (see Sect. 2.2 for references). This significant loss of nitrogen associated to benthic denitrification supports the hypothesis that shelf primary production is limited by nitrogen, as suggested by in situ measurements of N:P ratios in shelf waters, while the N:P ratio of riverine waters points to a P limitation (Oguz, 2008). Because of the spatial variability of metabolic pathways (Sect. 3.2), 41% of the benthic denitrification occurs in region 2 while this region only accounts for 29% of total benthic remineralization in terms of carbon. The estimated N burial (6.4 Gmol/yr) lies within the range of previous estimates (3.9-23.1 Gmol/yr, Grégoire and Friedrich (2004)), while carbon burial is equivalent to 4% of the shelf net primary production.

A further consideration of the benthic-pelagic coupling implications at interannual scale indicates that the accumulation of the slow decaying organic matter in the sediments during periods of increased riverine discharge (e.g. eutrophication) introduces a time lag in the environmental response to nutrient reduction policies. For instance, the ongoing oxygen demand alters the global response of hypoxia to a given level of riverine nitrogen load (Capet et al., 2013). Similarly non-linear dynamics may arise from intense resuspension events caused by exceptional storms (e.g. Turner et al., 2008).

At seasonal scale, the benthic fluxes (both particulate and dissolved) modulate the seasonal cycle imposed by river discharges and hence may impact the seasonality of primary production. For instance, the sediment layer acts as a strong sink of nitrogen during the months of April-May, when the highest riverine discharge occurs, and as a net source of nitrogen during the end of the year (Fig. 6.8).

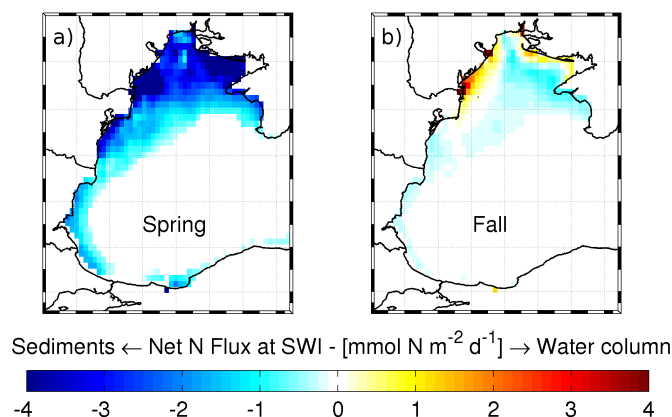


Figure 6.8: Net nitrogen flux at the sediment water interface (SWI) in (a) Spring (April, May, June) and (b) Fall (October, November, December).

4.2 Sediment resuspension: a key process modulating the role of continental shelves in biogeochemical cycles

Sediment resuspension and restriction of the deposition by waves and bottom currents are critical processes that determines the horizontal distribution of sedimentary stocks and thus that of mineralization rates and benthic-pelagic fluxes.

The importance of these physical stresses on sedimentation in the Black Sea was shown by [Stanev and Kandilarov \(2012\)](#), who proposed a numerical model for its representation. Here we look at the consequences of this on the sediment biogeochemical functioning, and on the biogeochemical budgets of the shelf and of the entire basin. Bottom stress effects are particularly important in shallow regions more exposed to wave stress, such as region 1. As it rapidly decreases with depth (Fig. 6.4), bottom stress finally acts as a diffusive factor and transports organic matter away from the locations of highest productivity.

The necessity of modeling the process of sediment resuspension in addition to diagenesis in the BS-NWS was revealed when analyzing a first set of simulations that were performed without this sediment transport. It appeared that neglecting the horizontal transport of sediment stocks led to an overestimation (compared to in situ estimates) of benthic-pelagic fluxes of NH_4^+ , SiOs, PO_4 and O_2 along the coast in the region of river discharges (i.e. Region 1). This overestimation was attributed to the direct sedimentation of riverine and marine organic materials in this region of high production.

The impact of considering bottom stress effects on total shelf budget is illustrated by the sensitivity of the model results to the critical resuspension thresholds τ_{ero} and τ_{dep} (Fig. 6.7d). Figure 6.7d shows that ignoring bottom stress effects enhances the benthic oxygen demand and carbon sequestration by 45 % while nitrogen removal is increased with 30 %.

Sediment resuspension also increases transport of material from the shelf towards the deep sea, causing an increase of deep sea primary production by 30 %.

Bottom stress effects do not affect the BS-NWS homogeneously. Given the strong seasonality of bottom shear stresses (Fig. 6.4, a specific value of τ_{dep} sets the period of the year during which, on the average, sedimentation is permitted.

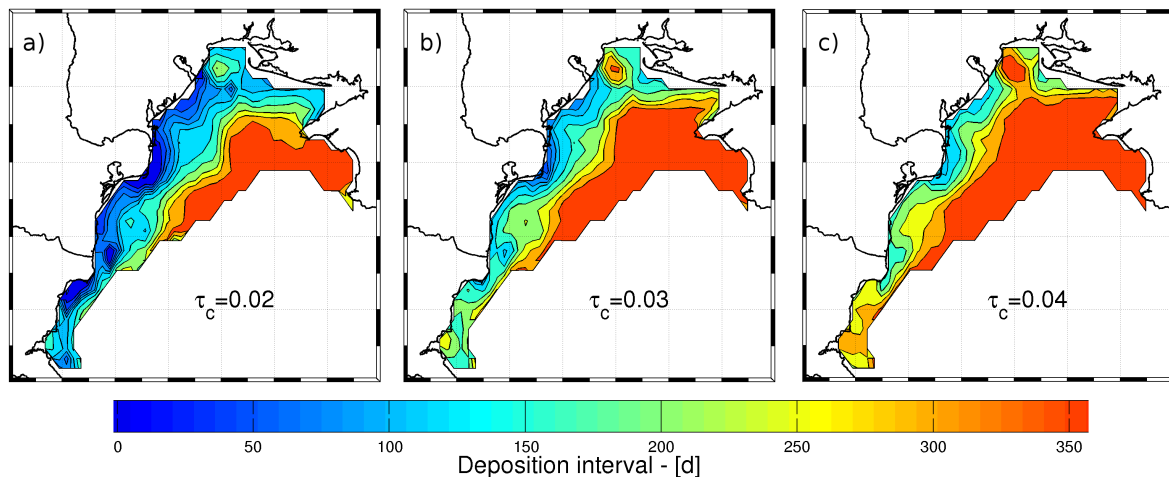


Figure 6.9: Climatological deposition interval for three realistic values of the critical threshold τ_{dep} . The deposition interval is defined as the number of days per year during which deposition is permitted by the bottom stress.

In certain areas, such as the Bay of Constanta or the northern part of the BS-NWS, the duration of this deposition period doubles even for a slight modification of τ_{dep} (Fig. 6.9). In these areas bottom processes are particularly sensitive to the variability of bottom stress intensity. This is especially relevant as on an interannual scale, as it implies that benthic fluxes in these areas may present a strong response to extreme wind events that may cause the resuspension of organic matter accumulated over several years.

4.3 Current limitations and perspectives

Empirical formulation of bulk parameters

In this paper we propose a methodology to couple the pelagic and benthic compartment in a 3D ocean model that combines reliability and tractability for multi-decadal simulations.

To reduce the computation costs, solutes in the benthic compartment are not explicitly represented, but rather the benthic-pelagic fluxes of solutes are derived from the dynamics of vertically integrated sediment stocks using bulk parameterization.

These bulk functions, represent the parametric responses of diagenetic processes to the changing environment are calibrated from Monte Carlo simulations performed with a vertically resolved diagenetic model (see Sect. 2.2 for details). Here we chose a diagenetic model that was specifically devised, calibrated and validated for one specific location of the BS-NWS (Fig. 6.1) (Wijsman et al., 2002). It is thereby implicitly assumed that the diagenetic model used for the calibration has the capacity to reproduce satisfactorily the diagenetic response to the range of environmental conditions encountered in the domain of investigation.

Given the large range of bottom environmental conditions (e.g. from well oxygenated to hypoxia, from eutrophicated to oligotrophic) that may be found on the BS-NWS, it would

obviously be preferable to check the behavior of this model in contrasted conditions, but such extensive data sets are not currently available at other locations.

A second drawback of our approach is the fact that it ignores certain processes, e.g. related to the dynamics of phosphate in the sediments (e.g. precipitation and complex formation, [Slomp and Van Cappellen \(2007\)](#); [Mort et al. \(2010\)](#)). Consequently, the model tends to overestimate phosphate effluxes, and is not able generate phosphate uptake by the sediments, although such influxes have been measured. Clearly, a derivation of integrated bulk parameterization for the phosphate dynamics, similar to nitrogen, may thus be required for a sound application of the present model in P-limited areas.

Benthos and sediment characteristics

Another deficiency of current diagenetic models (including that presented here) is that they do not account for the variable characteristics of the substrate and of the benthos in the formulation of diagenesis and benthic-pelagic coupling ([Arndt et al., 2013](#)).

A more detailed characterization of the sedimentological aspects of the substrate may better constrain the diffusion and advection parameters of diagenetic models, the burial fraction and the distribution of settling organic matter among the various level of biodegradability.

As the type of substrate can be roughly considered as fixed for the timescales targeted by this type of models (decades), this information could be introduced in the model using existing maps of sediment characteristics.

Also, benthic and epibenthic living communities can profoundly affect sediment diagenesis, e.g. they

1. affect the transport of solutes and solids within the sediment layer through respectively bioirrigation and bioturbation ([Kristensen, 2000](#); [Meysman et al., 2006](#));
2. alter the sensitivity of the sediments to bottom stresses ([Murray et al., 2002](#)) by affecting the permeability and by biofilm deposition, and modifies the effective bottom stress by changing the texture roughness of the bottom layer;
3. directly contributes to the biogeochemical budgets through photosynthesis.
4. filter feeders influence water transparency and hence the level of primary production and exported materials to the sediment.

A promising approach for a better dynamic representation of the benthos in biogeochemical models, would be to exploit the notion of habitats ([Diaz et al., 2004](#)).

Unfortunately, unlike sedimentological aspects, the composition of the benthos is subject to changes at short time scales, and the concept of a static habitat is therefore not simply included in a model at the current spatial and temporal extent. As benthic communities change in response to environmental stressors, this in turn will alter functional properties of the ecosystem, in particular regarding diagenetic processes.

Representing this feedback between environmental pressures and ecosystem services is a formidable challenge that is currently missing in our representation of marine ecosystems. This missing link considerably affects our ability to prescribe a sound and integrative management strategy for the coastal eutrophic areas.

5 Conclusions

We propose an original approach to integrate benthic-pelagic coupling in 3D ocean models that offers both reliability and tractability for multidecadal simulations.

The modeling of the benthic compartment involves an explicit description of the vertically integrated solid concentrations in carbon and silicate with two levels of lability, and of the nitrogen to carbon ratio in the sediments. Vertical gradients with sediment depth are not explicitly resolved, which restrains the computational costs. Bottom stress induced by bottom currents and waves determines the deposition of sedimenting organic matter and induces the resuspension of settled organic matter.

The variability of diagenetic processes that conditions the exchanges of solutes at the sediment-water interface is represented by a meta-modeling approach (Soetaert et al., 2000) that statistically fits the response of a complex vertically resolved full diagenetic model to the sediments organic content and the external bottom water environmental conditions.

Implementing this approach for the Black Sea northwestern shelf allowed us to recognize three regions distinguished by different bottom environmental conditions, benthic-pelagic fluxes, sediment stocks and diagenetic processes and by contrasting seasonal variation of the benthic/pelagic coupling mechanisms.

These three regions are organized along a bathymetric–river influence gradient, slightly modified by the main circulation pattern. Region 1, , the high flux region closest to the land-ocean interface, has the higher organic content in the sediments and is affected by seasonal hypoxic/anoxic events. Region 2 still shows significant downward fluxes of organic matter, but is less affected by hypoxic conditions. Region 3, located most offshore, has the lowest organic sediments content and exhibits the lowest seasonal variability due to the limited seasonal variation in bottom temperature, oxygen and nutrient concentrations.

Each of these three regions corresponds to a particular diagenetic pathway, in a way similar as they succeed vertically in a sediment profile. Region 1 exhibits a dominance of anoxic degradation processes, denitrification is maximal in region 2 while oxic remineralization prevails near to the open sea border, in region 3.

The coupled model reasserts the essential role of the benthic compartment in the shelf biogeochemical budgets, removing 62% of the total nitrogen inputs to the BS-NWS. The benthic oxygen demand accounts for 48% of the oxygen consumption below the mixed layer depth during the stratified season, hence significantly sustaining the occurrence of hypoxia.

We show that including the impact of bottom stress on sediment dynamics modifies the distribution of benthic-pelagic fluxes and sediment stocks, hence the benthic role in bio-

geochemical budget at shelf scale, but also has a pronounced qualitative and quantitative effect on the transport of material from the shelf towards the deep sea , which leads to an increase of the deep sea primary production by 30 %.

One of the weaknesses of this study is the limited data for model calibration and validation, and the simplified representation of abiotic and biotic conditions, i.e. by ignoring spatial and temporal variability of the living (biomass, functional traits of animals) and non-living (e.g. grain size) characteristics of the benthic landscape. Both issues require additional field work involving synchronous multivariate measurements. An appropriate methodology has then to be derived to incorporate this information in the actual modeling framework without prohibitively increasing the computing demand.

Acknowledgements

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6 Appendixes : Model state variables, equations and parameters

Table 6.1: State variables of the pelagic model affected by the benthic-pelagic coupling. The bottom concentration for the pelagic variables XXX is noted $[XXX]$ and expressed in mmol/m^3 . The corresponding bottom boundary condition (imposed flux) is noted $F_{XXX}(:, :)$ and expressed in $\text{mmol}/\text{m}^2/\text{s}$. The last column gives the direction allowed for the bottom boundary condition.

Notation	Description	B.C. dir.
$\text{DIC}(:, :, :)$	Dissolved Inorganic Carbon	$\uparrow$
$\text{POC}(:, :, :)$	Labile Particulate Organic Carbon	$\updownarrow$
$\text{CDI}(:, :, :)$	Carbon content of Diatoms	$\downarrow$
$\text{NOS}(:, :, :)$	Nitrate + Nitrite	$\updownarrow$
$\text{NHS}(:, :, :)$	Ammonium	$\updownarrow$
$\text{PON}(:, :, :)$	Labile Particulate Organic Nitrogen	$\updownarrow$
$\text{NDI}(:, :, :)$	Nitrogen content of Diatoms	$\downarrow$
$\text{PHO}(:, :, :)$	Phosphate	$\uparrow$
$\text{ODU}(:, :, :)$	Oxygen Demanding Unit	$\uparrow$
$\text{DOX}(:, :, :)$	Oxygen	$\downarrow$
$\text{SIO}(:, :, :)$	Silicate	$\uparrow$
$\text{SID}(:, :, :)$	Silicious detritus	$\updownarrow$
$\text{SDI}(:, :, :)$	Silicious content of Diatoms	$\downarrow$

Table 6.2: State variables of the benthic model.

Notation	Description	Units
$S_C^s(:, :)$	Vertically integrated organic carbon concentration (slow decay)	$[\text{mmolC}/\text{m}^2]$
$S_C^f(:, :)$	Vertically integrated organic carbon concentration (fast decay)	$[\text{mmolC}/\text{m}^2]$
$S_S^s(:, :)$	Vertically integrated detrital silicate concentration (slow decay)	$[\text{mmolSi}/\text{m}^2]$
$S_S^f(:, :)$	Vertically integrated detrital silicate concentration (fast decay)	$[\text{mmolSi}/\text{m}^2]$
$S_{N:C}(:, :)$	Nitrogen/Carbon ratio of sediment organic matter	$[-]$

Table 6.3: Parameters of the benthic model.

Parameters	Value	Unit	Description	Source
f_C	0.29	-	Part of the particulate C deposition flux that goes to S_C^f	Wijsman et al. (2002)
f_{Si}	0.5	-	Part of the particulate Si deposition flux that goes to S_{Si}^f	Calibrated
k_C^f	0.0753	d^{-1}	Degradation rate for fast decaying C stock	Soetaert et al. (1996a)
k_C^s	0.003	d^{-1}	Degradation rate for slow decaying C stock	Wijsman et al. (2002)
k_{Si}^f	0.0072	d^{-1}	Dissolution rate for fast decaying Si stock	Wijsman et al. (2002)
k_{Si}^s	0.00072	d^{-1}	Dissolution rate for slow decaying Si stock	Wijsman et al. (2002)
Q	2	-	Factor for Temperature effect on mineralization	Wijsman et al. (2002)
b_C, b_S	2.5e-9	/s	Burial rate for the "slow" stocks	Calibrated
p_{solid}	0.11	-	Part of precipitating ODU	Wijsman et al. (2002)
OC_{deg}	1	molO/molC	Oxygen consumed for oxie degradation	Grégoire and Friedrich (2004)
ON_{nit}	2	molO/molN	Oxygen consumed for nitrification	Grégoire and Friedrich (2004)
Me_C^f	10^{-5}	mmolC/m ² /s	Erosion constant for the slow Carbon stock	Stanev and Kandilarov (2012)
Me_C^s	10^{-5}	mmolC/m ² /s	Erosion constant for the fast Carbon stock	Stanev and Kandilarov (2012)
Me_{Si}^f	10^{-5}	mmolC/m ² /s	Erosion constant for the slow Silicious stock	Stanev and Kandilarov (2012)
Me_{Si}^s	10^{-5}	mmolC/m ² /s	Erosion constant for the slow Silicious stock	Stanev and Kandilarov (2012)
τ_{dep}	0.03	N/m ²	Bottom stress threshold for deposition	Calibrated
τ_{ero}^f	0.03	N/m ²	Bottom stress threshold for erosion of the fast stocks	Calibrated
τ_{ero}^s	0.05	N/m ²	Bottom stress threshold for erosion of the slow stocks	Calibrated
w_{POM}	Variable	m/s	Particulate organic matter sinking velocity	Kriest (2002)
w_{DIA}	Variable	m/s	Diatoms sinking velocity	Grégoire and Friedrich (2004)

Benthic Stock Dynamics

$$\begin{aligned}\frac{dS_i^j}{dt} &= P_i^j - D_i^j - B_i^j \\ \frac{dS_{N:C}}{dt} &= \frac{d}{dt}\left(\frac{S_N}{S_C}\right) = \frac{1}{S_C^2} \cdot (S_C \frac{dS_N}{dt} - S_N \frac{dS_C}{dt}) \\ &= \frac{1}{S_C} [(P_N + D_N + B_C \cdot S_{N:C}) - S_{N:C}(P_C + D_C + B_C)] \\ &= \frac{1}{S_C} [(P_N - S_{N:C}P_C)]\end{aligned}\tag{6.4}$$

Particulate Fluxes

if $\tau < \tau_{\text{dep}}$

Deposition

$$P_i = (1 - \frac{\tau}{\tau_{\text{dep}}}) \cdot \sum_{x \in X} w_x[x]\tag{6.5}$$

$X = \{\text{POC}, \text{CDI}\}, \{\text{PON}, \text{NDI}\}, \{\text{SID}, \text{SDI}\}$ for $i = \text{C}, \text{N}, \text{Si}$, resp.

$$P_i^f = P_i \cdot f_i \quad \text{and} \quad P_i^s = P_i \cdot (1 - f_i)\tag{6.6}$$

if $\tau_{\text{dep}} < \tau < \tau_{\text{ero}}^j$

No particulate fluxes

$$P_i^j = 0\tag{6.7}$$

if $\tau > \tau_{\text{ero}}^f$

Resuspension of the fast stock

$$P_i^f = Me_i^{f*} \left(\frac{\tau}{\tau_{\text{ero}}^f} - 1 \right)\tag{6.8}$$

$$Me_i^{f*} = \min(Me_i^f, \frac{S_i^f}{\Delta t} \left(\frac{\tau}{\tau_{\text{ero}}^f} - 1 \right))$$

if $\tau > \tau_{\text{ero}}^s$

Resuspension of the slow stock

$$P_i^s = Me_i^s \left(\frac{\tau}{\tau_{\text{ero}}^s} - 1 \right) \left(1 - \frac{Me_i^{f*}}{Me_i^f} \right)\tag{6.9}$$

When $\tau_{\text{dep}} < \tau$

Resuspension cases

$$P_N = P_C \cdot S_{N:C}\tag{6.10}$$

Burial

$$B_i^s = b_i \cdot S_i^s\tag{6.11}$$

$$B_i^f = 0$$

Remineralization

$$D_i = \sum_{j=f,s} k_j \cdot f_i^j(T) \cdot S_i^j \quad , \quad \text{with} \quad f_i^j(T) = Q_i^j \frac{T-20}{10}\tag{6.12}$$

$$D_N = D_C \cdot S_{N:C}\tag{6.13}$$

For $i = \text{C}, \text{Si}$ and $j = f, s$. The omission of the exponent in Eqs. (6.5,6.10) implicitly represents the sum over the fast and slow components, e.g. $S_C = S_C^s + S_C^f$

Benthic-pelagic boundary conditions.

$$F_{\text{POC}} = P_{\text{C}} \quad (6.14)$$

$$F_{\text{PON}} = P_{\text{N}} \quad (6.15)$$

$$F_{\text{SID}} = P_{\text{Si}} \quad (6.16)$$

$$F_{\text{SIO}} = D_{\text{Si}} \quad (6.17)$$

$$F_{\text{DIC}} = D_{\text{C}} \quad (6.18)$$

$$F_{\text{PHO}} = D_{\text{N}} \cdot r_{P:N} \quad (6.19)$$

$$F_{\text{NHS}} = D_{\text{N}} \cdot (1 - p_{\text{nit}}) \quad (6.20)$$

$$F_{\text{NOS}} = D_{\text{N}} \cdot p_{\text{nit}} - D_{\text{C}} \cdot p_{\text{denit}} \cdot 0.8 \quad (6.21)$$

$$F_{\text{DOX}}^* = -D_{\text{C}} \cdot (1 - p_{\text{denit}} - p_{\text{anox}} \cdot p_{\text{solid}}) \cdot OC_{\text{deg}} - D_{\text{N}} \cdot p_{\text{nit}} \cdot ON_{\text{nit}} \quad (6.22)$$

$$F_{\text{DOX}} = \max(F_{\text{DOX}}^*, -[\text{DOX}] \cdot \frac{\Delta z}{\Delta t}) \quad (6.23)$$

$$F_{\text{ODU}} = \max(0, F_{\text{DOX}} - F_{\text{DOX}}^*) \quad (6.24)$$

Bulk Parameterization

$$\ln(p_{\text{nit}} \cdot D_{\text{N}}) = -6.280 - 0.286 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) + 0.127 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \quad (6.25)$$

$$\begin{aligned} &+ 0.006 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) + 0.098 \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &+ 0.202 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &- 0.021 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &- 0.031 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \cdot \log([\text{DOX}]) - 0.066 \cdot \log(D_{\text{C}}) \cdot \log([\text{NHS}]) \\ &+ 0.009 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{NOS}]) + 0.823 \cdot \log([\text{DOX}]) \\ &- 0.028 \cdot \log([\text{DOX}]) \cdot \log([\text{DOX}]) - 0.012 \cdot \log([\text{DOX}]) \cdot \log([\text{NHS}]) \\ &+ 0.119 \cdot \log([\text{NHS}]) + 0.015 \cdot \log([\text{NHS}]) \cdot \log([\text{NHS}]) \end{aligned}$$

$$\ln(p_{\text{denit}} \cdot D_{\text{C}}) = -5.475 - 0.786 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) + 0.662 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \quad (6.26)$$

$$\begin{aligned} &+ 0.042 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) + 0.064 \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &+ 0.794 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &- 0.082 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &- 0.122 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \cdot \log([\text{DOX}]) \\ &+ 0.077 \cdot \log([\text{DOX}]) \cdot \log([\text{DOX}]) - 0.155 \cdot \log([\text{DOX}]) \cdot \log([\text{NOS}]) \\ &+ 0.875 \cdot \log([\text{NOS}]) + 0.046 \cdot \log([\text{NOS}]) \cdot \log([\text{NOS}]) \end{aligned}$$

$$p_{\text{anox}} = 1.056 - 0.132 \cdot \log(D_{\text{C}}) + 0.005 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \quad (6.27)$$

$$\begin{aligned} &+ 0.057 \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) - 0.017 \cdot \log(D_{\text{C}}) \cdot \log(D_{\text{C}}) \cdot \log([\text{DOX}]) \\ &- 0.008 \cdot \log([\text{DOX}]) \cdot \log([\text{DOX}]) \end{aligned}$$

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Chapter 7

Drivers, mechanisms and long-term variability of seasonal hypoxia on the Black Sea northwestern shelf – is there any recovery after eutrophication?



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It constitutes the most finalized application of this thesis as it relies on the model capacities - representation of the interannual variability of physical-biogeochemical interactions and that of the benthic pelagic coupling - to adress an issue of high socio-economical relevance.

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Abstract

The Black Sea northwestern shelf (NWS) is a shallow eutrophic area in which the seasonal stratification of the water column isolates the bottom waters from the atmosphere. This prevents ventilation from counterbalancing the large consumption of oxygen due to respiration in the bottom waters and in the sediments, and sets the stage for the development of seasonal hypoxia.

A three-dimensional (3-D) coupled physical–biogeochemical model is used to investigate the dynamics of bottom hypoxia in the Black Sea NWS, first at seasonal and then at interannual scales (1981–2009), and to differentiate its driving factors (climatic versus eutrophication).

Model skills are evaluated by a quantitative comparison of the model results to 14 123 in situ oxygen measurements available in the NOAA World Ocean and the Black Sea Commission databases, using different error metrics. This validation exercise shows that the model is able to represent the seasonal and interannual variability of the oxygen concentration and of the occurrence of hypoxia, as well as the spatial distribution of oxygen-depleted waters.

During the period 1981–2009, each year exhibits seasonal bottom hypoxia at the end of summer. This phenomenon essentially covers the northern part of the NWS – which receives large inputs of nutrients from the Danube, Dniester and Dnieper rivers – and extends, during the years of severe hypoxia, towards the Romanian bay of Constanta.

An index H which merges the aspects of the spatial and temporal extension of the hypoxic event is proposed to quantify, for each year, the intensity of hypoxia as an environmental stressor.

In order to explain the interannual variability of H and to disentangle its drivers, we analyze the long time series of model results by means of a stepwise multiple linear regression. This statistical model gives a general relationship that links the intensity of hypoxia to eutrophication and climate-related variables.

A total of 82 % of the interannual variability of H is explained by the combination of four predictors: the annual riverine nitrate load (N), the sea surface temperature in the month preceding stratification (T_s), the amount of semi-labile organic matter accumulated in the sediments (C) and the sea surface temperature during late summer (T_f). Partial regression indicates that the climatic impact on hypoxia is almost as important as that of eutrophication.

Accumulation of organic matter in the sediments introduces an important inertia in the recovery process after eutrophication, with a typical timescale of 9.3 yr.

Seasonal fluctuations and the heterogeneous spatial distribution complicate the monitoring of bottom hypoxia, leading to contradictory conclusions when the interpretation is done from different sets of data. In particular, it appears that the recovery reported in the literature after 1995 was overestimated due to the use of observations concentrated in areas and months not typically affected by hypoxia. This stresses the urgent need for a dedicated monitoring effort in the Black Sea NWS focused on the areas and months concerned by recurrent hypoxic events.

1 Introduction

Hypoxia is a major global environmental problem affecting marine waters and is among the most widespread deleterious anthropogenic influences. The phenomenon of hypoxia is drawing increased attention as dead zones in the coastal ocean have spread exponentially since the 1960s and have been reported from more than 400 sites (Diaz and Rosenberg, 2008) (e.g., Baltic Sea, Black Sea, Kattegat Sea, Gulf of Mexico, East China Sea), 39 % of which are located in Europe (Zhang et al., 2010).

Hypoxia is considered to occur when the concentration of dissolved oxygen decreases below a threshold of 62 mmol m^{-3} ($= 2 \text{ mg L}^{-1}$). However, it has been shown that low oxygen concentrations already affect living organisms above that threshold (Vaquer-Sunyer and Duarte, 2008).

Hypoxic conditions may be encountered in various parts of the ocean (e.g., the coastal area, the shelf and the deep ocean), where water ventilation is not able to renew the oxygen consumed for the degradation of organic matter. The coastal area which receives the input of organic matter from rivers and adjacent land is particularly exposed to this phenomenon. In this shallow area, where the bottom is occupied by a benthic ecosystem, the occurrence of hypoxic conditions may be lethal to these organisms and catastrophic for the benthic biodiversity (Levin et al., 2009).

Hypoxia has important impacts on biogeochemical cycling and may significantly disturb ecosystem functionality as, for instance, it

- directly affects living organisms (e.g., benthic organisms, fishes) (e.g., Vaquer-Sunyer and Duarte, 2008),
- may, in extreme cases, lead to anoxia with the production of greenhouse gases (e.g., CH_4 , N_2O), or toxic substances (e.g., sulfide) (e.g., Naqvi et al., 2010),
- alters the cycling of chemical elements such as nitrogen or phosphate (e.g., Conley et al., 2009),
- modifies the sedimentary geochemical cycling through the removal of bioturbating infauna (e.g., Levin et al., 2009),
- and alters the food web structure by changing the balance of chemical elements (e.g., N, C, P) and by killing some components and hence reducing the transfer of energy towards the higher trophic levels (e.g., Ekau et al., 2010).

The phenomenology of hypoxia events may be classified according to the temporal scales of hypoxia (e.g., permanent, seasonal, episodic, diel) and geomorphological characteristics of the water body (Kemp et al., 2009). The Black Sea northwestern shelf (NWS) is stratified, non-tidal, and affected by recurrent seasonal hypoxia. According to the classification of Kemp et al. (2009) the situation of the Black Sea NWS system is comparable with, for instance, Chesapeake Bay (e.g., Boesch et al., 2001), Pensacola Bay (Hagy III and Murrell, 2007), the Changjiang plume (Chen et al., 2007), and the northern Gulf of Mexico (Turner et al., 2008, 2012).

While it is generally understood that hypoxia in those systems is permitted by stratification and fueled by human-induced eutrophication, non-linearities, indirect and feedback effects involving a number of external and internal factors complicate the situation and prevent direct links between a driver and the intensity of the resulting hypoxia (Kemp et al., 2009; Steckbauer et al., 2011). For instance, we may expect that a temperature rise will intensify hypoxia by strengthening stratification, reducing oxygen solubility and enhancing respiration rates. However a temperature change may also have indirect effects on hypoxia: an increased stratification may for instance reduce the availability of nutrients in the surface layer (and hence limit primary production) and/or intensify the respiration in the upper layer, which would actually reduce the oxygen consumption in bottom waters (Conley et al., 2009).

The organic matter accumulated in the sediments during eutrophication periods introduces an inertia in the response of hypoxia to reduced nutrient load, whose timescale is difficult to estimate although essential to the study of the system recovery. Moreover, hypoxic conditions affect the sediment biogeochemistry by reducing denitrification (Kemp et al., 2009) and causing the release of dissolved inorganic phosphorus from ferric complexes (Slomp and Van Cappellen, 2007). These two processes change the nutrient content of the upper water and hence the level of primary production that can be sustained.

Finally, the modified food web structure of ecosystems affected by hypoxia may also alter the response of the ecosystem to nutrient load (e.g., filter feeders, bioturbators, fish/jellyfish trophic pathways).

For all the reasons mentioned above, which are not exhaustive, hypoxia is a complex process whose dynamics (spatial and temporal scales), understanding (e.g., drivers, impact) and mitigation (e.g., recovery) are challenging to assess (Cardoso et al., 2010). Sound management allowing the preservation and restoration of hypoxia-damaged ecosystems to a healthy state therefore necessitates a good understanding of these interconnected processes (Boesch et al., 2001).

In situ data collection is a key component for this assessment but shows some limitations (Cardoso et al., 2010) that can be alleviated when combined with numerical modeling. Indeed, coupled physical–biogeochemical models are valuable tools for investigating some mechanisms such as the effects of the physics (governed by atmospheric conditions) and biogeochemistry (including the sediments) on the occurrence of hypoxia (Kemp et al., 2009; Peña et al., 2010).

In this paper, a three-dimensional (3-D) physical–biogeochemical model is used to investigate the space-time dynamics of hypoxia and its drivers (atmospheric versus eutrophication) on the Black Sea NWS.

The Black Sea is an almost enclosed sea with restricted exchanges with the Mediterranean Sea through the Bosphorus Strait. It contains a wide shelf (depth < 100 m) on its northwestern part, connected to the deep sea (depth 2000 m) (Fig. 7.1). The deep sea is permanently stratified by a halocline, and hence water ventilation in this area does not extend deeper than ~100–150 m, leading to anoxia of waters below that depth. Moreover, hypoxia on the NWS was first observed in the early 1970s at 30 m depth in a region located between the Danube and Dniester discharge area (Zaitsev, 1997).

The losses of bottom macro-fauna attributed to hypoxia for the 1972–1990 period have been estimated at around 60 million tons, including 5 million tons of fish. The severe decrease in that period of the population of the mussel *Mytilus Galloprovincialis* is also attributed to hypoxia (Zaitsev, 1997). In particular hypoxia affected a unique congregation of Phyllophora named “Zernov’s Phyllophora field” after its first establishment in 1908 by S. A. Zernov (Zernov, 1909). It is not clear whether hypoxia affected directly the Phyllophora field or rather indirectly through the decline of filter feeders that may have decreased water transparency. In return, the decrease of Zernov’s field constituted an additional positive feedback on hypoxia, as it has been identified as an important generator of oxygen at depths of 20–60 m (Zaitsev, 1997). Zernov’s field is sustaining an ecosystem known as the Phyllophora biocenosis, offering habitat and spawning grounds to 47 species of fish, 110 species of invertebrates and other living organisms, among which 9 species are listed in the Red Book of Ukraine (Kostylev et al., 2010). Since recruits from this area disperse outward from the seaweed, the ecological importance of this field, and thus the damaging effect of hypoxia, extends beyond its actual boundaries.

The main aims of this study are (1) to understand and identify the drivers of hypoxia at seasonal and interannual scales, (2) to propose a statistical model to predict the interannual variability of hypoxia and to quantify the contributions of the identified drivers to this variability, (3) to assess the timescale of recovery of the system submitted to eutrophication due to the sediment inertia, and (4) to give some recommendations for the monitoring of hypoxia on the Black Sea NWS.

Since the numerical model presented here has the ambition to be used for the prediction of hypoxia in answer to management strategies, several error metrics, issued from the comparison of model results and in situ observations, are combined to illustrate the model performances regarding different aspects of the oxygen dynamics.

The paper is structured as follows. The 3-D coupled model is presented in Sect. 2, along with the data and metrics used for the validation. Section 3 reviews the key processes driving the dynamics of oxygen in the Black Sea NWS and details the mechanisms which lead to the seasonal occurrence of hypoxia. Section 4 evaluates the model performance by comparing the variabilities of the oxygen distribution resolved by the model to those pictured from in situ data. Based on the previous description of the oxygen dynamics, Sect. 5 evaluates the interannual variability of hypoxia in response to eutrophication and meteorological external pressures. Section 6 discusses the practical implications of this study in relation notably to the implementation of the European Marine Strategy Framework Directive (Cardoso et al., 2010). Finally, a summary of the new findings provided by this study and some recommendations are given in Sect. 7

2 Materials and method

2.1 The coupled model

The physical model is the GeoHydrodynamic and Environmental Research (GHER) 3-D hydrodynamical model described in, e.g., Beckers (1991) and Delhez (1996) and used in the particular case of the Black Sea in Grégoire et al. (1998, 2004), Stanev and Beckers

(1999), and Beckers et al. (2002). It resolves the currents and the physical state of the sea, which are temperature, salinity, internal mixing and surface elevation. The implementation used in the frame of these simulations is described in Capet et al. (2012), and validated in detail with satellite sea surface temperature (SST) and sea level elevation data.

The biogeochemical model simulates oxygen, nitrogen, phosphorus, silicate and carbon cycling and explicitly represents processes in anoxic and suboxic conditions. It is described in detail in Grégoire et al. (2008). Compared to Grégoire et al. (2008), the model has been coupled (online) in 3-D with the GHER 3-D hydrodynamic model and extended with a dynamic representation of the benthic compartment (in Grégoire et al. (2008), a reflective boundary condition was used for describing benthic degradation). This representation is based on the comparative analysis performed by Soetaert et al. (2000) on the representation of benthic processes that is both reliable and tractable for long-term simulations in a 3-D ocean model. Hence, the benthic compartment is described by a semi-empirical model whose state variables are 2-D variables (vertically integrated C and N content with two degrees of lability). From these 2-D stock variables, the fluxes of solutes are estimated using bulk parameters (i.e., the fraction of organic matter degraded by denitrification and anaerobic oxidation, oxygen consumption in nitrification). As in Soetaert et al. (2000), these bulk parameters are estimated from Monte Carlo simulations performed with an existing 1-D diagenetic model of the Black Sea sediments developed and validated by Wijsman et al. (1999). The organic matter accumulated in the sediment stocks is subjected to resuspension from the action of wave- and current-induced bottom stress, which is modeled using the setting presented in Stanev and Kandilarov (2012).

The coupling between the three components of the model (hydrodynamic, biogeochemical, benthic) is fully online. For instance, the transport of biogeochemical variables is determined at each time step from the advection and diffusion fields computed by the hydrodynamical model. Additionally, the rate of each biogeochemical process depends on the temperature field, and the oxygen solubility is also dependent on the salinity. On the other hand, the penetration of solar radiation, which governs the heating of the upper layer, is influenced by the vertical distribution of phytoplankton and organic matter computed by the biogeochemical model. Similarly the benthic component receives from the overlaying waters the export of detritus and diatoms and provides the flux of solutes issued from sediment degradation. The dynamics of benthic detritus depends on environmental conditions of bottom waters (temperature, currents including waves, oxygen, nitrate and ammonium). The coupling between the benthic and pelagic compartment is described in details in a companion paper in which the modeled benthic fluxes of oxygen, nitrate, ammonium, silicate and phosphate are compared with available observations.

The model domain covers the whole Black Sea, on a 15 km Arakawa-C grid, with 31 vertical levels using double sigma coordinates. Riverine water flows and nutrients' (NO_x , PO_4 , SiO_2) monthly loads are issued from Ludwig et al. (2009) and the Black Sea commission data (after 2000). The total Black Sea riverine discharge is delivered through the 6 main rivers: Danube, Dniester, Dnieper, Rioni, Kizilirmak and Sakarya (the first three flowing directly on the NWS, Fig. 7.1). Averaged and constant atmospheric deposits of nitrate and phosphate are imposed all over the basin (NO_x : $0.78 \text{ g m}^{-2} \text{ yr}^{-1}$; PO_4 : $0.7 \text{ mg m}^{-2} \text{ yr}^{-1}$; Kanakidou et al. (2012)), which represents 3 Gmol N yr^{-1} for the NWS

(Fig. 7.1). Average concentrations of nitrogen organic forms are estimated for the three shelf rivers (Cauwet et al., 2002; Reschke et al., 2002; Walling and Fang, 2003). When multiplied by the considered discharges, this leads to a total load of $10.1 \text{ Gmol N yr}^{-1}$ (7, 0.8 and 2.3 for Danube, Dnieper and Dniester, respectively).

Atmospheric forcings are issued from the ERA-Interim reanalysis provided by the ECMWF data center¹ with a 6 h and 0.75° resolution.

2.2 Data sets

A total of 14 123 oxygen measurements, available in the NOAA World Ocean Database² (WOD), are retrieved for the area of investigation (Fig. 7.1) for 1980 to 2000. Additional data reported to the Black Sea Commission (BSC) are included in the data set, making it possible to cover the years 2000–2010 (636 points). Since hypoxia on the NWS usually occurs on the bottom of stratified areas at the end of summer, the assessment of the occurrence of hypoxia requires data collected below the mixed layer, during the summer months (August–October). Additionally, to quantify the intensity of the hypoxic event in term of spatial extension, a sufficient spatial coverage over the bathymetric gradient is required. While a satisfactory part of the WOD data meets these criteria (Table 7.1), a major proportion of BSC data are located in very coastal areas, and are usually not available for the period of hypoxia development. This means that basically no observation is available to assess the potential recovery of the Black Sea NWS from hypoxia after 2000. The data located in very coastal areas (i.e., bathymetry, Z , $< 17 \text{ m}$; see Table 7.1) are not considered for the validation procedure because of the higher relative importance of processes unresolved by the model (e.g., small-scale hydrodynamics, benthic flora and fauna)

2.3 Model skill metrics

The data described in Sect. 2.2 (Table 7.1) are used to assess the model ability to resolve the dynamics of oxygen using a point-to-point approach: each observation is compared with the model predictions at the data point (model results which are weekly averages are interpolated in time and space to obtain a value corresponding to the position and time of sampling). This level of validation is penalizing, as it requires perfect matches in space and time, but avoids the problem of representativity occurring when deriving volume averages from two samples with contrasted distribution, i.e., the sparse and strongly irregular distribution of observations, and the dense and regular distribution of model values (see also the discussion in Sect. 5.6).

The following metrics are combined to address distinct aspects of the comparison between model and observations, according to the recommendations of Allen et al. (2007) and Stow et al. (2009). Besides, these can be compared with well-accepted reference values, allowing the performances of the model to be judged in a more objective way. The mean and standard deviation of a variable X are noted $\bar{X}$ and σ_X , respectively.

¹European Center for Medium-Range Weather Forecasts (<http://www.ecmwf.int/>)

²<http://www.nodc.noaa.gov/OC5/SELECT/dbsearch/dbsearch.html>

Table 7.1: Number of observations available from the World Ocean Database (WOD) and Black Sea Commission (BSC) data sets. The second column considers all the data, while the next columns only consider subsets selected the following hypoxia-related criteria (see the text for details): data collected away from the coast (total water depth, Z , < 17 m; 3rd column), below the summer mixed layer (observation depth $z > 15$ m, 4th column) and during the months of strongest hypoxia (Aug-Sept-Oct) (second line of each data set). Bold number indicates the data used for validation in Sect. 4.

Selection criteria	All data	$Z > 17$	$Z > 17$ $z > 15$
WOD (1981–2001)	14 123	14 088	7670
Aug-Sep-Oct	3850	3847	2108
BSC (2000–2009)	636	382	86
Aug-Sep-Oct	113	57	8

- The percentage bias compares the mean value of observations (O) and predictions (P), and expresses the average bias as a percentage value of the observations average, $PB = \frac{\bar{P}-\bar{O}}{\bar{O}} \cdot 100$. It indicates a global overestimation (underestimation) when positive (negative) and the model is considered as excellent (in that regard) when $|PB| < 10 \%$ (Allen et al., 2007).
- The standard deviation ratio, $r_\sigma = \frac{\sigma_O}{\sigma_P}$, compares the distribution of observations and predictions around their respective average. It indicates a larger variability in the observation (the predictions) when $r_\sigma > 1$ ($r_\sigma < 1$).
- The Nash–Sutcliffe efficiency, $N-S = 1 - \frac{\sum(O-P)^2}{(\sum(O-\bar{O}))^2}$, relates the model errors to the variability in the observations. The squaring increases the weight of big errors. Allen et al. (2007) classify the performance levels as > 0.65 being excellent; $[0.65, 0.5]$ being very good; $[0.5, 0.2]$ being good; and < 0.2 being poor.
- The widely used Pearson correlation coefficient, ρ , indicates how the variations of P and O around their respective mean are related. Significant correlations ($p < 0.01$, two-tailed distributions) can be concluded for $\rho > 0.71$ and 0.47 for data sets of respectively 12 and 29 elements, which correspond to the number of months and years considered in Sect. 4.

3 Seasonal hypoxia in a stratified shelf: key processes

In order to detail the seasonal mechanisms leading to the establishment of hypoxia, this section analyzes a climatological year reconstructed from three years of model run (1991–1993), exploring the contribution of the physical and biogeochemical factors involved in the dynamics of the oxygen budget. Unless specified otherwise, averages and budgets are considered for the investigation area depicted in Fig. 7.1

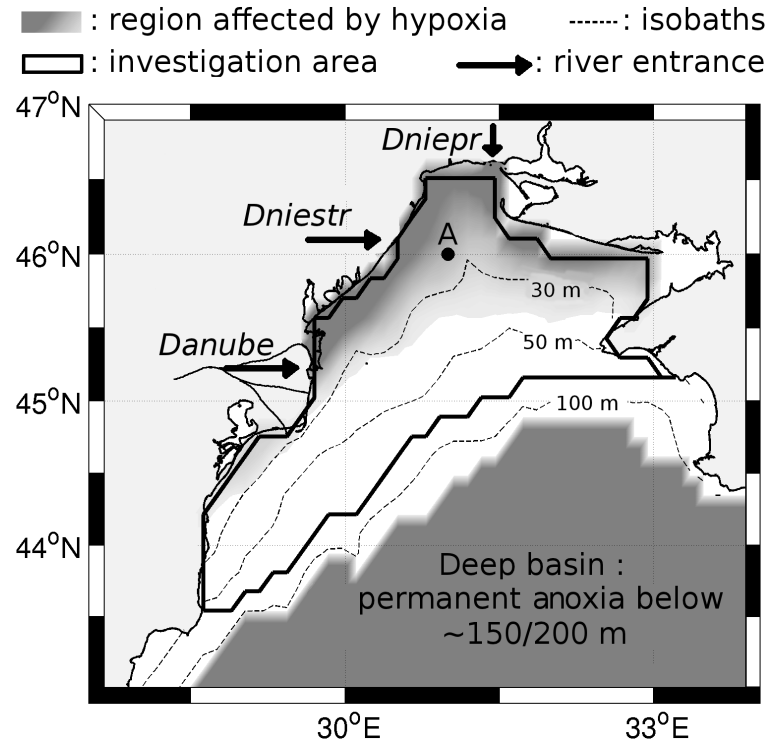


Figure 7.1: This map shows the area of investigation over which spatial averages are computed, the area in which the model predicts hypoxia and anoxia for water depth $> 120\text{--}150\text{ m}$ (averaged situation for the period 1981–2009), and the entrances of the rivers considered in the model. The three distributaries of the Danube are also indicated (from north to south: Chilia, Sulina and Saint George). The dot (A) locates the profile presented in Fig. 7.2.

3.1 Temperature and Stratification

Figure 7.2 illustrates the seasonal evolution of a vertical oxygen profile simulated at an arbitrary site affected by seasonal hypoxia (point A in Fig. 7.1). The figure shows how stratification allows the settlement of bottom hypoxic conditions by preventing the bottom oxygen-depleted waters from mixing with the surface ventilated waters.

The water column in this region is permanently stratified. The potential energy anomaly, i.e., the volume-specific difference in potential energy between the stratified and mixed state of the water column, is defined by

$$\phi = \frac{g}{Z} \cdot \int_0^Z z \cdot [\rho(T, S) - \rho(\bar{T}, \bar{S})] dz \quad (7.1)$$

where g is the gravity constant, Z the total water depth and ρ the density computed for the given value of temperature, T , and salinity, S . The thermal (ϕ_T) and haline (ϕ_S) contributions to the stratification can be computed by

$$\phi_T = \frac{g}{Z} \cdot \int_0^Z z \cdot [\rho(T, \bar{S}) - \rho(\bar{T}, \bar{S})] dz \quad (7.2)$$

$$\phi_S = \phi - \phi_T. \quad (7.3)$$

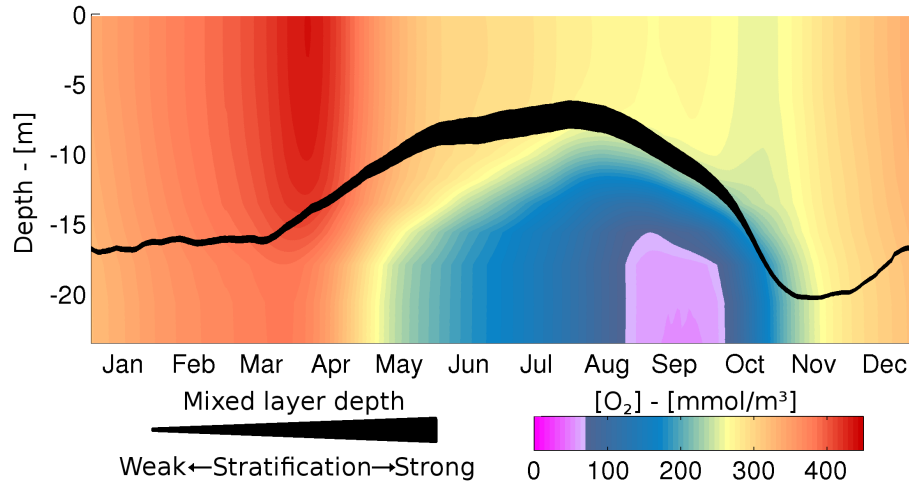


Figure 7.2: Typical seasonal evolution of the oxygen vertical profile in the northern part of the Black Sea NWS (point A in Fig. 7.1). Hypoxic conditions (i.e., oxygen concentrations below the threshold of 62 mmol m^{-3}) are underlined by the color scale. The mixed layer depth is represented by the position of the black line and the intensity of the stratification, as estimated by the Brunt–Vaïasala frequency, by the line thickness.

Haline stratification is present during the whole year and peaks in May, when river discharges are maximum, while the warming of surface waters enhances the stratification from the beginning of spring (early April) until mid-fall (mid-October) (Fig. 7.3).

The duration of this enhanced stratification period varies from year to year and is a key factor in determining the severity of bottom hypoxia. For further use, we define the stratification and mixing periods (Fig. 7.3) by using a criterion on the maximum value of the Brunt–Vaasala frequency along the vertical: $\max_{z=0}^Z \sqrt{-g \frac{\delta \rho(z)}{\rho(z)}} \geq$ and $< 0.05 \text{ s}^{-1}$ for stratification and mixing period, respectively. The mixed layer depth, z_ρ , is defined as the depth where a density difference, $\Delta \rho$, compared to the 3m density reaches a threshold of 0.0125 kg m^{-3} as proposed for the Black Sea by Kara et al. (2009). z_ρ reaches $\sim 10 \text{ m}$ on average during the stratification period.

During the stratification period, bottom waters are virtually separated from surface waters. This clearly appears when looking at the differences between surface and bottom temperature (Fig. 7.4). The low-rising curve of bottom temperature indicates a limited warming of the bottom layer by the surface layer, which has the consequence that the average summer bottom temperature is determined by the winter/spring SST rather than by the summer SST. This is important since summer bottom temperature acts on the metabolic and respiration rates below the mixed layer depth and on the benthic diagenesis, hence directly on the intensity of the consumption of the oxygen pool locked below the thermocline. Obviously, the absence of tidal currents over the bottom also leads to less mixing.

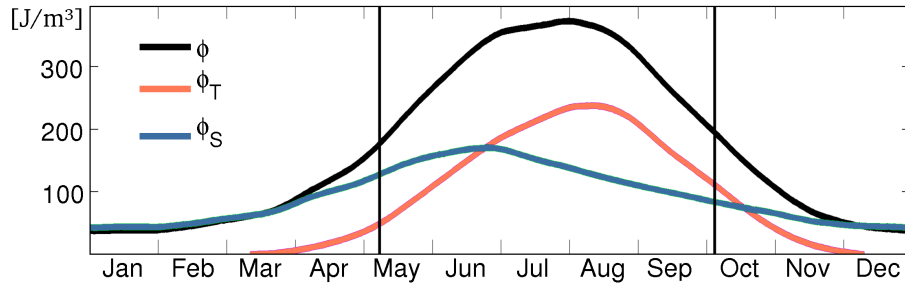


Figure 7.3: Seasonal evolution of the vertical stratification as appraised by the potential energy anomaly (Eq. 7.1), i.e., the volume-specific difference in potential energy between stratified and mixed state of the water column. The red and blue lines depict the thermal and haline contributions to the potential energy anomaly (Eqs. 7.2 and 7.3). Averages are computed over the investigation area presented in Fig. 1. Vertical lines indicate the beginning and the end of the stratification period defined by a criterion on the Brunt–Väisälä frequency (Sect. 4.1).

3.2 Oxygen solubility and surface fluxes

The surface oxygen concentration is constantly regulated by the air–sea fluxes (Fig. 7.4), which tend to bring the surface concentration towards the saturation value. This saturation value depends on the oxygen solubility, which is mainly determined by the SST. Therefore, the seasonal SST signal explains the larger part of the surface concentration variability: the seasonal variations of the spatially averaged difference, $[O_2]_{\text{surf}} - [O_2]_{\text{surf,sat}}$, is less than half of that of $[O_2]_{\text{surf}}$ ($\sigma = 13$ and 30 mmol m^{-3} , respectively).

In spring and summer, surface waters are oversaturated in oxygen due to enhanced photosynthesis and to the decreased solubility of oxygen as SST increases. This leads to a release of oxygen towards the atmosphere (Fig. 7.4). In fall, the oxygen saturation increases as SST decreases, and the oxygen content of surface waters decreases as a result of the vertical mixing with the underlying oxygen-depleted waters. Surface waters are thus undersaturated and oxygen is taken up from the atmosphere. This ventilation of surface waters lasts until the next spring.

The exchanges of oxygen with the atmosphere of the investigated area are almost balanced over the year: the total annual uptake of 372 Gmol yr^{-1} is compensated by a release of 407 Gmol yr^{-1} , resulting in an annual net release of 35 Gmol yr^{-1} (Fig. 7.5). This annual net surface flux is variable and averages to an uptake of 2 Gmol yr^{-1} when the average is computed over the 1981–2009 period. While atmospheric fluxes have a marginal contribution to the annual oxygen budget, these play a crucial role in the seasonal mechanism of hypoxia as the intensity of the winter/spring ventilation fixes the initial concentration of oxygen in the bottom waters before their occlusion by the thermocline.

3.3 Biogeochemical processes and annual oxygen budget

Figure 7.5 presents the contribution of biogeochemical processes (budgets integrated over the whole shelf) to the simulated oxygen budget for the mixed and stratified period (distinguishing in this last case the layers above and below z_ρ for the vertical integration).

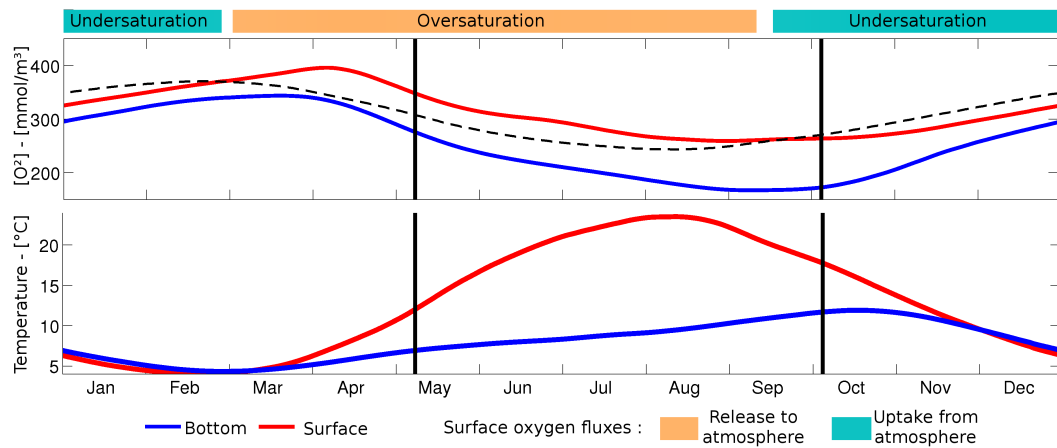


Figure 7.4: Upper panel: seasonal cycle of the surface and bottom oxygen concentration and of the surface saturation value determined by the sea surface temperature. During periods of oversaturation (i.e., the sea surface oxygen concentration is higher than the saturation value), the air–sea oxygen flux is directed to the atmosphere, while in the case of undersaturation this flux is directed to the sea. Lower panel: seasonal cycle of the surface and bottom temperature.

Of the amount of oxygen produced by the (net) photosynthesis of autotrophs, 85 % is consumed for the remineralization of organic matter (in the water column and sediments), 8 % is consumed for the oxidation of ammonium and of the reduced substances released by the benthic layer, 4 % is exported laterally and 3 % is delivered to the atmosphere. About one-third of the organic matter degradation occurs in the sediments, but this number may vary according to the equilibrium status of the sediments compared to the nutrient load, as detailed in Sect. 5.3.

Both processes are thus intensified in summer, but more markedly for the respiration, which shifts the summer balance towards oxygen consumption.

More importantly, at that time, we simulate different vertical distribution of autotrophs and heterotrophs: photosynthesis mainly occurs in the surface mixed layer (74 % of summer production), where light is available, while respiration of the sinking organic matter occurs principally below the mixed layer depth (66 % including benthic diagenesis). Additionally, 80 % of the summer chemical consumption occurs below the mixed layer depth.

These different distributions explain the summer depletion of oxygen below the mixed layer.

Finally, the concentration of oxygen in the bottom waters at the end of the stratification period is determined by the content of oxygen before stratification, which is fixed by winter ventilation (and hence the SST during this period), by the amount of oxygen consumed during the stratified period essentially through the heterotrophs respiration in the water column and the sediments, and by the duration of the stratified period. The importance of these factors is confirmed by the statistical analysis of the interannual variability described in Sect. 5.

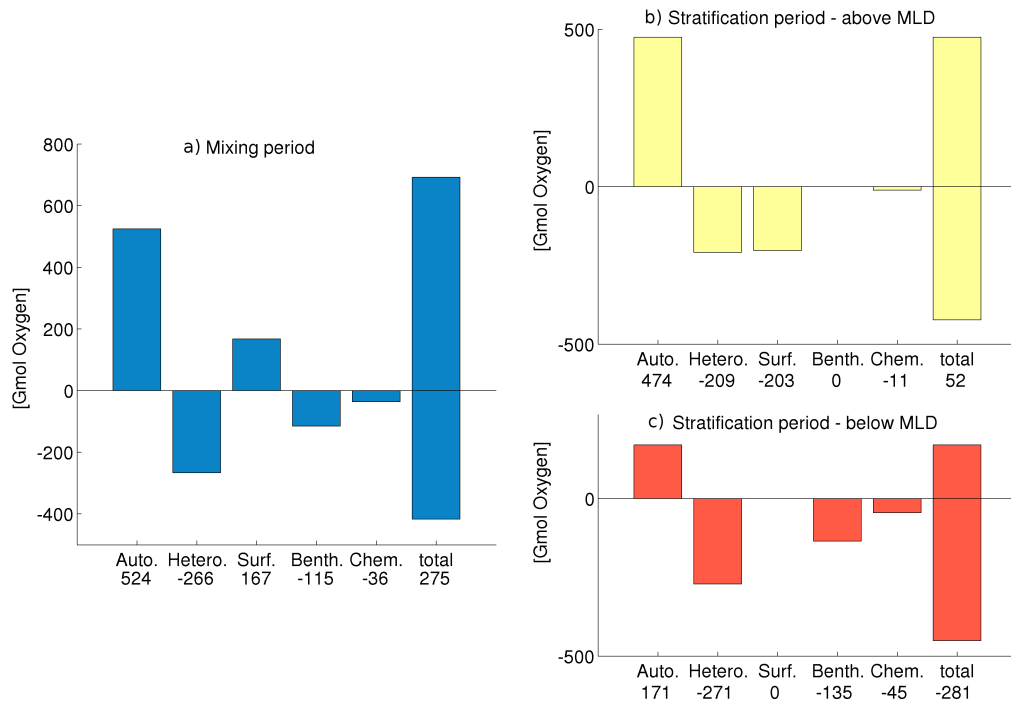


Figure 7.5: Contribution of biogeochemical processes to the oxygen budget for the mixing and stratification period (left and right respectively). For the mixing period (**a**), processes are integrated over the whole water column, while during the stratified period the integration is performed separately above (**b**) and below (**c**) the mixed layer depth. The following processes are considered: net photosynthesis (Auto., including oxygen production associated with nitrate reduction); heterotroph respiration (Hetero.); the oxygen air-sea fluxes (Surf., counted positive when directed towards the sea); benthic diagenesis (Benth.); and oxygen consumption in chemical reactions (Chem., including nitrification and the oxidation of reduced substances).

4 Model validation

Since the present study is centered on the understanding and predictions of hypoxic events, the validation exercise is concentrated on the assessment of model performances in simulating the oxygen dynamics. The validation of the simulated physical variables is described in Capet et al. (2012) where the interannual variability (1960–2000) of the model-simulated SST and sea surface elevation is compared with satellite observations. This validation exercise demonstrates the model ability to correctly reproduce the interannual variability of SST and associated hydrodynamical fields such as the dynamics of the mixed layer. This means that the model has the ability to simulate the dynamics of water ventilation and resulting oxygenation, which is an important factor governing the oxygen dynamics (see Sect. 3). The simulated benthic fluxes of oxygen (as well as nitrate, ammonium, silicate and phosphate) have recently been compared (not shown) with all the data sets available on the Black Sea NWS (Friedl et al., 1998; Friedrich et al., 2002) and unpublished data kindly provided by I. Akoumianaki (EU Sesame project data set) and A. Lichtschlag (EU HYPOX project data set). This means that a good representation of the oxygen distribution and its variations in time and space by the model suggests a good representation of the pelagic sources and sinks of oxygen (e.g., photosynthesis, respiration, chemical reactions).

Table 7.2: Model skill statistics obtained when considering all the observation/model prediction pairs (Global), annual medians (Years, m), annual number of hypoxic events (Years, n_H), monthly medians (Months, m), monthly number of hypoxic events (Months, n_H). Error metrics are defined in Sect. 2.3: ρ : Pearson correlation; N-S: Nash–Sutcliffe efficiency; and r_σ : standard deviation ratio. The numbers in parentheses are obtained when only considering the WOD database (Sect. 2.2).

Metrics	Global	Years		Months	
		m	n_H	m	n_H
ρ	0.67	0.62 (0.84)	0.96	0.89 (0.97)	0.99
N-S	0.39	0.35 (0.64)	0.91	0.75 (0.93)	0.95
r_σ	1.08	1.26 (1.20)		0.94 (0.95)	

In the following, we first present the global model skills in simulating oxygen. Then, the validation procedure is focused on answering the following questions:

1. Is the model able to represent the seasonal cycle of oxygen?
2. Is the model able to represent the interannual variability of oxygen?
3. Is the model able to represent the location of oxygen-depleted waters?
4. Is the model able to resolve the threshold of hypoxia?

The skill metrics are given in Table 7.2.

Global assessment of model performances

The global (i.e., considering all the data) percentage bias is virtually nul (0.03%), indicating that the model resolves the oxygen dynamics without a persistent bias. The standard deviation ratio is higher than one, indicating a higher variability in the observations. This is expected since model results correspond to weekly averages, estimated on a $15\text{ km} \times 15\text{ km}$ grid, while observed values are precisely located in space and time, and are therefore subject to small-scale variabilities which are either unresolved by the model (e.g., small-scale physical structure) or smoothed by the weekly averaging (e.g., the diurnal cycle of surface photosynthesis). The global N–S statistic is penalized by the large errors (Fig. 7.7c) associated with point-to-point validation, but still qualifies the model as “good” (Sect. 2.3).

Is the model able to represent the seasonal cycle of oxygen?

Figure 7.6 shows the monthly distribution (median, percentiles) of the oxygen concentration deduced from observations and model results as well as the associated distribution of bias and percentage of hypoxic records. Model skill statistics are then computed on the medians obtained for each month (Table 7.2). These indicate excellent skill of the model regarding the timing and the range of seasonal variability. However, a seasonal

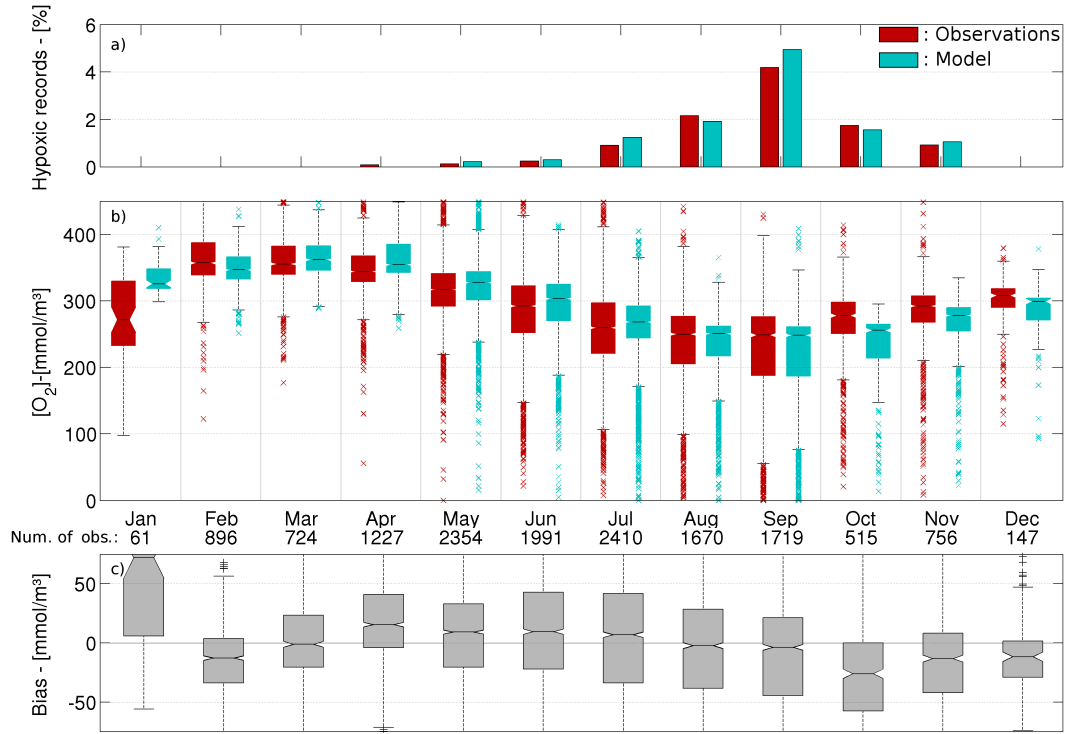


Figure 7.6: The ability of the model to resolve the seasonal cycle of oxygen concentration is addressed by merging observations and predictions by month. For this comparison, model results are interpolated at the location and time of data sampling. (a) Proportion of records below the hypoxic threshold ($[O_2] < 62 \text{ mmol m}^{-3}$). (b) Distribution (median, percentile) by month of the oxygen concentrations: the central bars indicate the medians, the filled areas extend to the 0.25 and 0.75 percentile (respectively, Q_{25} and Q_{75}), the dotted bars indicate the $1.5 \cdot (Q_{75} - Q_{25})$ range, and the extreme values are marked by an “x”. (c) Distributions of biases: positive (negative) bias correspond to overestimation (underestimation) by the model.

signal can be seen in the monthly biases (Fig. 7.6c), which is very close to that of the oxygen saturation in surface waters (Fig. 7.4). The overestimation of the surface oxygen concentration in spring and the underestimation in fall occur when the surface waters are oversaturated and undersaturated, respectively. This suggests an underestimation of the air–sea fluxes intensity, possibly due to the use of averaged wind speed (hence of lower magnitude) to compute the exchange coefficients appearing in the formulation of the air–sea flux (Ho et al., 2006). This also explains the slightly larger seasonal variability in the model reflected by the standard deviation ratio.

Is the model able to represent the interannual variability of oxygen content?

Following the same approach, observations and predictions are gathered by years (Fig. 7.7), discarding the years with less than 10 available observations.

The error metrics reveal an excellent ability of the model to represent the interannual variability present in the WOD data, but this ability is considered as good when including the BSC data in the computation. It should be noted, however, that the very sparse distribution of data after 2000 prevents a reliable estimate of the model skill during this

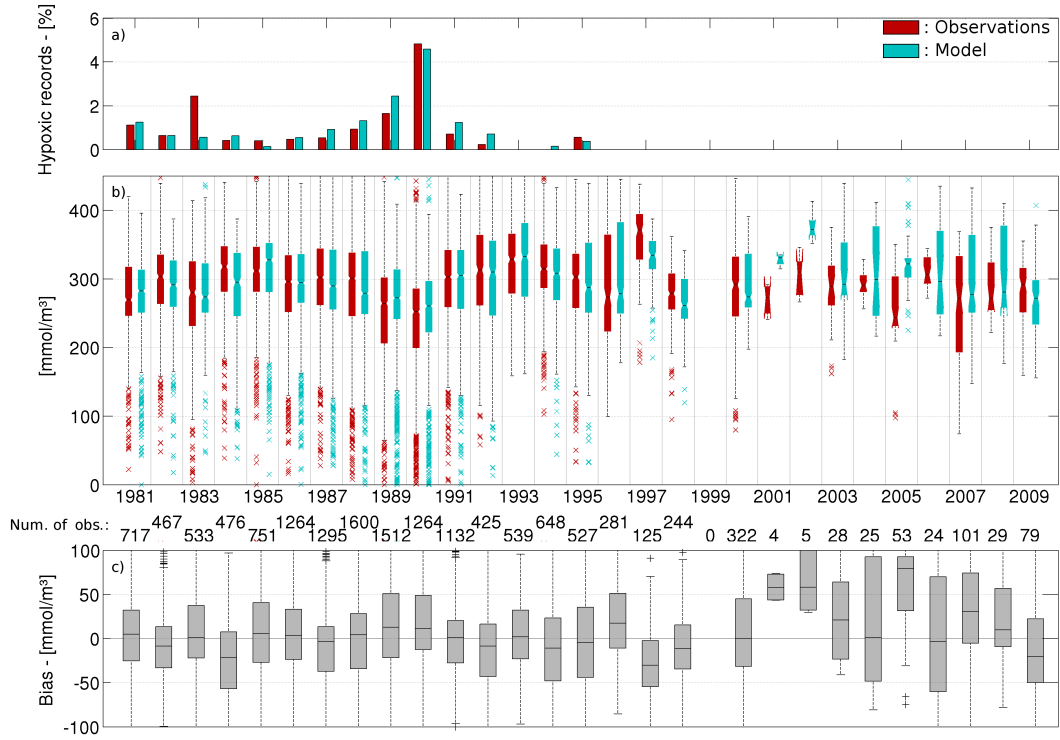


Figure 7.7: The ability of the model to resolve the interannual variability of oxygen concentration is addressed by merging observations and predictions by year. For this comparison, model results are interpolated at the location and time of data sampling. (a) Proportion of records below the hypoxic threshold ($[O_2] < \text{mmol m}^{-3}$). (b) Distribution (median, percentile) by year of the oxygen concentrations: the central bars indicate the medians, the filled areas extend to the 0.25 and 0.75 percentile (respectively, Q_{25} and Q_{75}), the dotted bars indicate the $1.5 \cdot (Q_{75} - Q_{25})$ range, and the extreme values are marked by an “x”. (c) Distributions of biases: positive (negative) bias correspond to overestimation (underestimation) by the model.

period.

The standard deviation ratio indicates a slightly wider range of interannual variability in the observations, reflecting that some of the complexity of the oxygen dynamics (Sect. 1) is not represented by the model.

Is the model able to represent the location of oxygen depleted waters?

The distribution of observed and simulated vertical oxygen profiles along the bathymetric axis (Figs. 7.8 a and b respectively) indicates a zone of low oxygen content along the bottom between approximately the 15 m and the 45 m isobaths in both cases. In waters deeper than 45 m, hypoxic conditions still appear at some sites in the data but not anymore in the model, while the model predicts hypoxia in the very coastal area (total water depth, Z , < 20 m) contrary to the data. The disagreement between model and data along the coast may be explained by several factors, such as the misrepresentation of coastal small-scale hydrodynamic features due to the insufficient horizontal resolution of the model and of the atmospheric forcings, and also the ignorance in the model of the role of the benthic flora (e.g., the seagrass *Zostera*) as oxygenator of the water.

A first mapping of the area of hypoxia over the NWS was proposed by Zaitsev (1997) (redrawn in Fig. 7.9a), who located bottom hypoxic waters near the rivers mouths, mainly north of the St. George Danube entrance, extending until the Ukrainian coast in some cases and, to a smaller extent, along the Romanian coast. Unfortunately Zaitsev (1997) did not mention how this mapping was derived (e.g., oxygen concentration, *Phyllophora* extent), but we can note that the horizontal extent of hypoxia predicted by the model based on an oxygen threshold agrees quite well with that estimated from Zaitsev (1997) as shown by the comparison of Fig. 7.9a and c.

The reduction of the southeastern extension of the area of hypoxia in the model compared to the mapping proposed by Zaitsev (1997) can be explained by the absence of distinction of the different branches of the Danube in the model. In the model, all the Danube discharges occur through the northernmost Chilia branch, which is the most important one (Fig. 7.1). It is noteworthy, however, that the model predicts hypoxia in the bay of Constanta in agreement with Zaitsev (1997) without the direct inputs of the southernmost St. George branch.

Is the model able to represent the threshold of hypoxia?

To address this question the number of hypoxic records ($[O_2] < 62 \text{ mmol m}^{-3}$) are compared along their seasonal (Fig. 7.6a) and interannual (Fig. 7.7a) distributions. It should be noted that only a few observations are below that threshold (174 measurements in total, none in the BSC database). Meanwhile, the error statistics reported in Table 7.2 indicate that the distribution of hypoxic records among the different months and years is very well reproduced by the model.

5 Interannual variability of bottom hypoxia

5.1 An index to quantify the annual intensity of hypoxia

The repercussion of hypoxia in a given region depends not only on the spatial extension of the hypoxic event but also on its duration in time, which is a critical factor for the mortality of living organisms (Vaquer-Sunyer and Duarte, 2008). An index of the severity of hypoxia should thus merge these two characteristics of spatial extension and time duration. This information is rarely available from local observations since they usually provide either a snapshot view of the status of hypoxia (e.g., field cruise) or a local assessment (e.g., time series obtained at a fixed station). In some cases, spatial maps of areas affected by low oxygen concentrations are obtained by merging non-synoptic data sets.

In the present case, the model resolves both the spatial and temporal aspects of hypoxia, which allows appraising the temporal variability of the simulated benthic hypoxia area. Figure 7.11a presents examples of this seasonal variations for selected years, illustrating the limitation of defining hypoxia by a snapshot map.

In order to take into account temporal dynamics, we quantify the annual intensity of

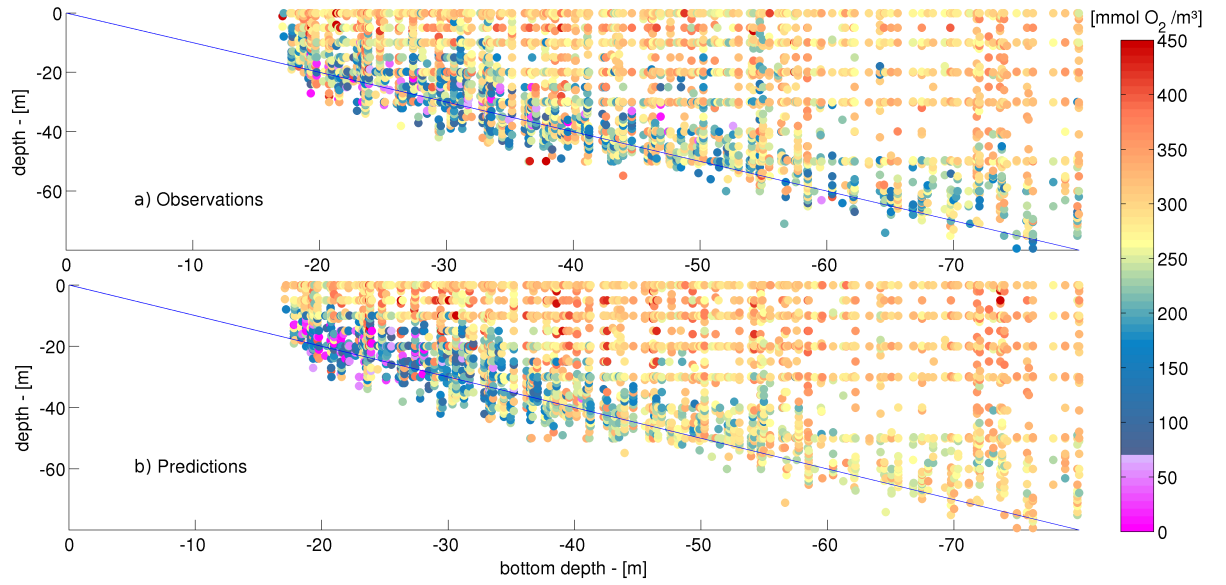


Figure 7.8: (a) Observed and (b) predicted vertical distribution of oxygen concentrations along the bathymetric axis.

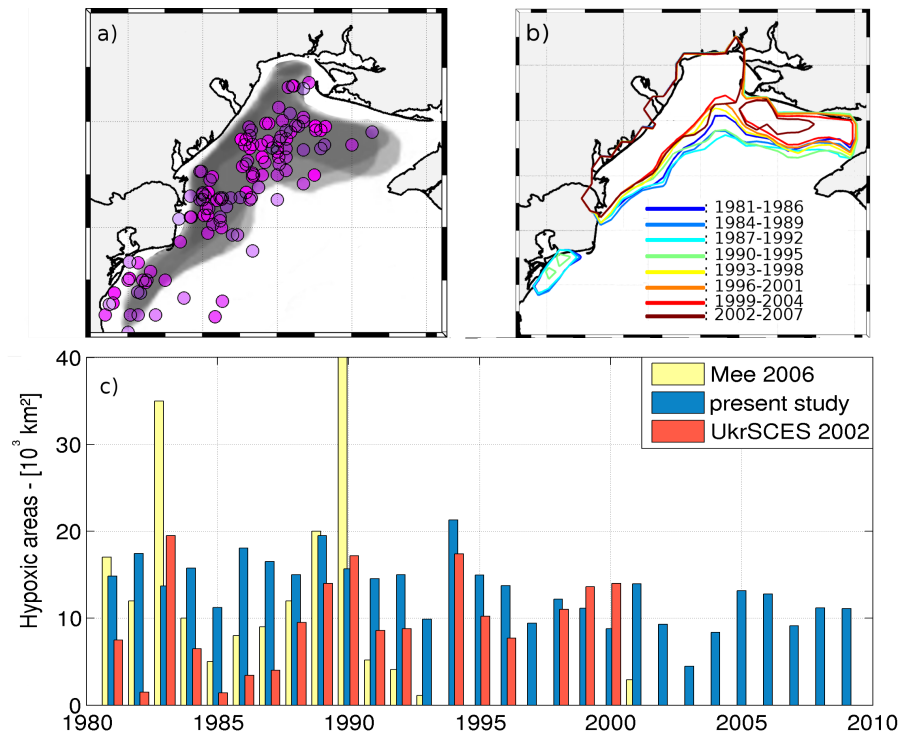


Figure 7.9: (a) Area affected by hypoxia, redrawn from Zaitsev (1997), and locations of hypoxic records from the WOD database. (b) Spatial extension of the area over which the model predicts hypoxia lasting more than one month. Variability due to meteorological effects is filtered out by averaging the results over 6 yr periods. (c) Extension of the surface affected by bottom hypoxia, as reported in the literature (Mee, 2006; UkrSCES, 2002) and simulated by the 3-D model.

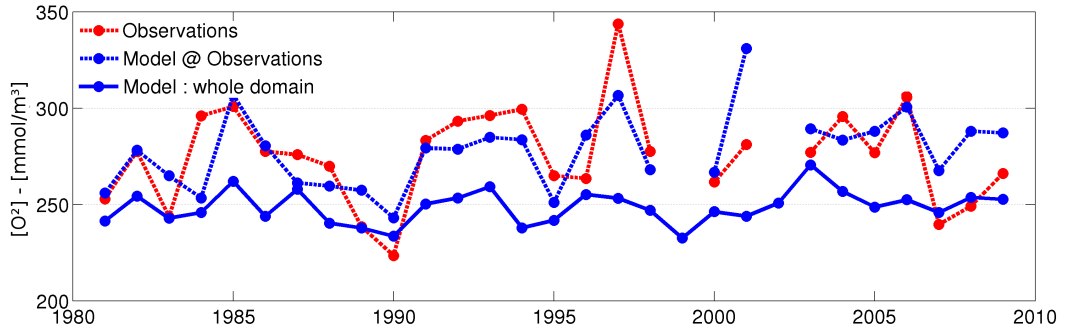


Figure 7.10: Interannual evolution of the summer (average July–August) oxygen concentration computed by averaging available observations (dotted red line), model predictions at observation points (in dotted blue line) and 3-D model results (solid blue line) over the investigation area (Fig. 7.1). The comparison of the solid and dotted blue lines clearly illustrates that the interpretation of oxygen variability may be biased by the spatial heterogeneity of data distribution among the years.

hypoxia with the index H defined by

$$H = \frac{1}{\bar{D}} \int_{\text{year}} A(t) dt \quad (7.4)$$

$$D = \frac{1}{\max A(t)} \int_{\text{year}} A(t) dt, \quad (7.5)$$

in which $A(t)$ is the area affected by bottom hypoxia at time t , D is the timescale of the hypoxic event, and $\bar{D}$ its average computed over the simulation period (102 days). D corresponds roughly to the time during which hypoxia occurs over a surface larger than half of the maximal area (see Fig. 7.11a).

The normalization of the integral by $\bar{D}$ gives to H the units of an area. Eqs. (7.4) and (7.5) imply that H is equivalent to the maximal hypoxic area, $\max A(t)$, if $D = \bar{D}$ for this year, and higher (lower) if D is larger (smaller) than $\bar{D}$, i.e., if the timescale of the hypoxic event is larger (shorter) than its average value. These formulations provide an easy algebraic relationship between H , D and $\max A(t)$, graphically illustrated in Fig. 7.11b. This figure highlights that H integrates both temporal and spatial aspects in its definition since high values of H are obtained for either large $\max A(t)$ or for large D .

5.2 Empiric linear models

Several studies use empirical models (e.g., linear or multiple linear regressions) to link the interannual variability of hypoxia to a selection of external drivers (Conley et al., 2007, 2009; Turner et al., 2012). These studies used observations and selected the potential drivers among available data, according to the current understanding of hypoxia.

In our case the process of hypoxia is completely and explicitly resolved by the model, and all potential drivers and processes may be extracted from the model results and forcings. Using this ideal “data set”, we propose deriving an empirical relationship linking the intensity of hypoxia, represented by the H index (Sect. 5.1), to its drivers.

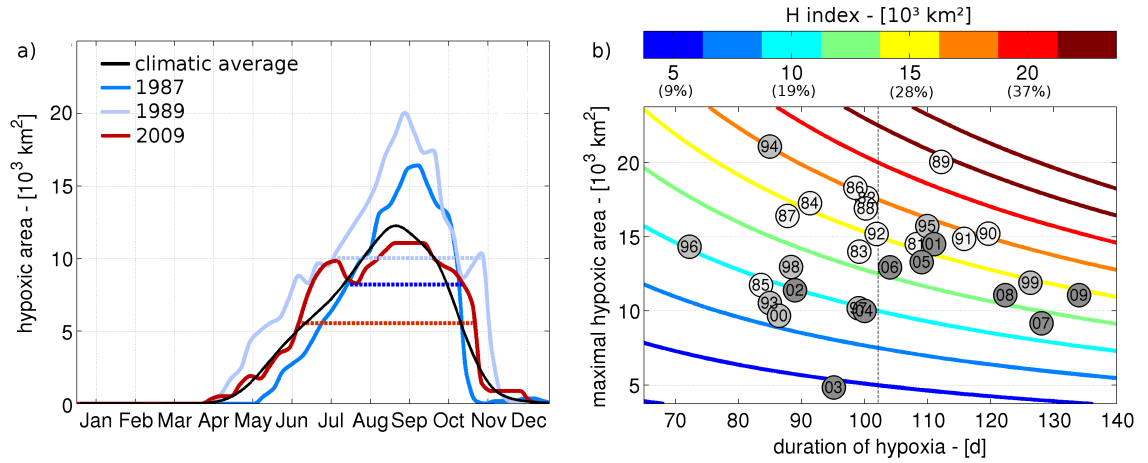


Figure 7.11: (a) Seasonal dynamics of the hypoxic area, $A(t)$, for selected years (colored solid lines) and climatological average (black solid line). The dotted lines indicate the time during which hypoxia covers more than half of the maximal area simulated during the considered year (i.e., the timescale of hypoxia, D , defined by Eq. 7.4). (b) The H index (colored lines) represents the annual intensity of hypoxia as an environmental stressor and combines the aspects of spatial and temporal extension of the hypoxic event. Its definition (Eq. 7.4) allows this graphical representation of the relationship between H , $\text{max} A(t)$, and D . The circles locate the hypoxic events simulated for each year (1981–1991: light gray; 1992–2000: mid-gray; and 2001–2009: dark gray). Their distribution shows the variability between the years and the lack of relationship between $\text{max} A(t)$ and D . In order to compare the case of the Black Sea NWS with other sites affected by hypoxia, the percentages given below the colored scale correspond to a scaling of H by the whole NWS area, depicted in Fig. 7.1.

This empirical relationship is not based on a mechanistic description of the processes but has the following advantages:

1. It requires a reduced number of data for the prediction of hypoxia.
2. It is more easily comparable to studies addressing other areas, for instance by comparing the regression parameters of similar drivers among sites. This would allow deriving a relationship between these parameters and the characteristics (e.g., geomorphology) of the sites, extending the scope of hypoxia understanding across the global coastal areas.
3. It provides an easy way to identify the drivers and to assess their respective weight in governing the variability of hypoxia, differentiating for instance eutrophication from atmospheric impact.

However, even if the drivers involved in this regression analysis are assumed to have a causal link with hypoxia, we should be careful when using this formulation for making predictions in a range of conditions for which the model has not been fitted. This is an inherent limitation of statistical models.

A multiple linear regression procedure (e.g., Legendre and Legendre, 1998) consists in deriving a regression equation expressing the response variable Y as a linear combination

of a set of predictors (or explanatory variables) $X_1, \dots, X_N$:

$$Y' = a_0 + a_1 X_1 + \dots + a_N X_N \quad (7.6)$$

where Y' is the estimated value of Y and the coefficients $a_1, \dots, a_N$ are computed automatically in order to minimize the residuals $(Y' - Y)^2$.

The predictors may be selected arbitrarily based on a priori assumptions, or selected automatically using statistic metrics. Here, we use a stepwise regression procedure (backward elimination based on $p = 0.01$ significance threshold) to identify among a preselected set of potential predictors issued from the model (i.e., winter SST; mean summer SST; late summer SST (Aug-Sept-Oct); March SST; mean winter organic carbon stock in the sediments; average summer winds: magnitude, zonal and meridional components; minimum summer average Brunt-Väisälä frequency; water and nutrients riverine discharge) an optimal subset of predictors such that no additional predictor would increase significantly the coefficient of determination of the regression, R (computed as the ratio of the variance of the response explained by the predictors and the true variance of Y) (Legendre and Legendre, 1998).

The stepwise procedure indicates that H can be retrieved from a linear combination of the annual nitrate load (N), the winter sediment organic content (C), March SST (T_s), and late summer SST (T_f , averaged for Aug-Sept-Oct) (Fig. 7.12). In its standardized forms, the regression equation is writes as follows:

$$H^* = a_0 + a_N \cdot N^* + a_C \cdot C^* + a_{T_s} \cdot T_s^* + a_{T_f} \cdot T_f^* \quad (7.7)$$

with $X^* = \frac{X - \mu_X}{\sigma_X}$.

This regression equation explains 82 % ($R^2 = 0.82$) of the variability of H . The use of standardized predictors allows comparing the standard regression coefficients, a_i , to measure the relative impacts of the different predictors on the variability of H . However, the confidence intervals associated with these coefficients (shown in Fig. 7.12) must be considered to ascertain within satisfying probabilities the preponderant role of a variable over another.

Climatic and eutrophication impacts on hypoxia may be distinguished by performing partial regressions, i.e., estimating how much of the variation of hypoxia can be attributed exclusively to climate (eutrophic) drivers once the effect of eutrophication (climate) has been taken into account. This analysis indicates that both factors have a similar impact, with eutrophication-related variables (N, C) explaining slightly more ($R^2 = 0.36$) than the climatic related predictors (T_s, T_f , $R^2 = 0.27$).

A higher part of the H variance is attributed to climatic drivers when reducing the number of years considered for the partial regression. This indicates that climatic drivers mostly drive a shorter timescale variability while eutrophication drivers act on a longer term. Interestingly, the role of temperature introduces an oscillation in the interannual variations of hypoxia, which is related to the East Asia/West Russia atmospheric teleconnection pattern (Capet et al., 2012).

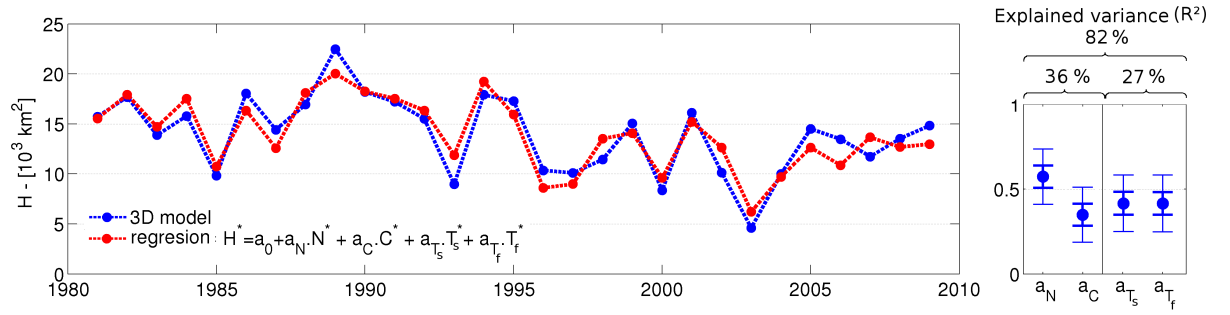


Figure 7.12: Interannual variations of the annual hypoxic index, H (Eq. 7.4), diagnosed from the results of the 3-D coupled model and computed from the regression Eq. (7.7). The standardized regression coefficients on the right panel indicate the relative role of each predictor in explaining the variability of H , with error bars indicating the $p = 0.5$ and 0.9 confidence intervals. Partial regressions assign a comparable part of the variance of H to eutrophication (N , C) and climate (T , D) drivers.

Interpretation of the selected predictors

A proper interpretation of regression coefficients requires that the selected predictors are not significantly correlated (Legendre and Legendre, 1998). Here, the predictors selected by the stepwise regression are each related to different processes, and their relation to hypoxia may be interpreted as follows.

Nitrate load is the main fuel of eutrophication. Model results show that N is significantly correlated to the maximum surface oxygen concentration simulated during the spring bloom ($\rho = 0.7$) and to the range of bottom oxygen decrease from spring to autumn ($\rho = 0.86$).

March SST, T_s , is a better predictor of bottom hypoxia than the summer or winter SST. This important role of the SST in March has already been discussed in Sect. 3 and is due to two main reasons:

1. The March SST fixes the temperature of bottom waters for the duration of the stratification period (correlation between March SST and bottom summer temperature is $\rho = 0.82$) and hence affects the summer rates of organic matter respiration.
2. The March SST controls oxygen solubility and hence the intensity of oxygenation before the stratification period. Therefore, it fixes the oxygen content of bottom waters in spring ($\rho = 0.85$), before their occlusion by the thermocline.

The late summer SST, T_f , plays an important role in determining the duration of the stratified period. As the lowest oxygen concentrations are reached at the end of summer, an anomalous extension of the stratification period causes increased damages to the ecosystem. In particular, T_f is related to the annual release of reduced compounds from the sediments ($\rho = 0.67$), including H_2S (UkrSCES, 2002).

While a part of the sediment organic matter is labile and remineralized within a timescale of months, a part of the sediment organic stock is more refractory (semi-labile) and requires more time for its remineralization. During years of high nutrient loads, the semi-

labile stock accumulates year after year and continues to cause oxygen consumption several years after high-riverine-load events. The predictor C , the amount of organic matter in the sediments computed for the winter season, reflects this semi-labile component, as the labile fraction of organic matter is almost entirely remineralized in summer or resuspended at the begin of winter. The mean summer benthic oxygen demand is significantly correlated to C ($\rho = 0.82$), indicating the important role of this accumulated stock in benthic diagenesis.

5.3 Impact of sediment inertia on the timescale of recovery

The fact that the accumulation of organic matter in the sediments keeps record of the nutrient load history and may significantly intensify hypoxia is an important mechanism which has to be considered when addressing the long-term variability of hypoxia in response to a given regime of nutrient load. In the case of decreasing load (which has been the case in study area since the early 1990s) the sediment introduces an inertia in the process of recovery. In the case of a maintained or increasing level of nutrient load, this mechanism causes an increase of the response ratio “hypoxic area / annual nutrient load”, as illustrated in the Gulf of Mexico by [Turner et al. \(2008\)](#)

The evolution of C as a function of the annual nitrate load history can be reproduced by a parametric model using, in addition to N , the March SST (as a proxy of bottom temperature, Sect. 3) and the history of the silicate-to-nitrate ratio (i.e., Si : N) of riverine load:

$$C(y+1) = C(y)(1 - \beta(y)) + \alpha(y) \cdot N(y) \quad (7.8)$$

$$\beta(y) = \beta_0 \cdot Q^{T_s^*(y)} \quad (7.9)$$

$$\alpha(y) = \alpha_0 + \alpha_{\text{Si:N}} \cdot (\text{Si}(y) : \text{N}(y)) \quad (7.10)$$

in which y represents any particular year. β_0 can be seen as a bulk parameter representing the natural decrease rate of C due to resuspension, diagenesis and burial (i.e., for $N = 0$ and $T^*=0$ we have $C(y) = C(0) \exp^{-\beta_0 y}$); β has the same interpretation as β_0 but additionally considers the effect of temperature through a Q_{10} formulation; and α represents the part of riverine load that feeds C , and depends on the ratio Si : N. This ratio is a proxy of the proportion of diatoms in phytoplankton which conditions the amount of organic matter sinking to the sediment (this effect has been found important to represent the evolution of C after 2002 when the Si : N ratio of riverine nutrients increases substantially and modifies the composition of phytoplankton communities).

Using the interannual evolution of C simulated by the 3-D coupled model, parameters α_0 , β_0 , Q_{10} and $\alpha_{\text{Si:N}}$ are estimated using a non-linear fitting procedure. The reconstruction of C history from the initial condition, C_0 , using Eq. (7.8) and the fitted parameters provides a coefficient of determination $R^2 = 0.95$ (Fig. 7.13).

The timescale of sediment memory after a high-load period can be estimated from the parameter β_0 which reaches a value of $0.16(\pm 0.02, p > 0.1)$, corresponding to a characteristic timescale of $1/\beta = 9.3$ yr.

Important information that can be derived from Eq. (7.8) is the value of the stock of semi-labile benthic carbon reached at equilibrium (noted C_{eq}) for a given value of N (noted N_{eq}). To derive an estimation for the values $C_{eq}(N_{eq})$, Eq. (7.8) is integrated for 10 yr using a value of N that increases linearly from its value reached in 2009 to the selected N_{eq} (imposing typical temperature and Si conditions). Then, the integration is continued for 10 additional years while maintaining a constant load level ($N = N_{eq}$). Fig. 7.13 shows the levels of C_{eq} reached for different values of N_{eq} . It can be seen that in some cases 10 yr of integration is not long enough to reach steady state in the sediments.

5.4 Assimilation capacity

The main motivation for studying hypoxia is to derive management strategies (e.g., river loading restriction policies) to avoid it, or at least to keep hypoxia intensity below a threshold, H_0 , that ensures healthy functioning of the coastal and marine ecosystem, as defined by the Marine Strategy Framework Directive (MSFD) established by the European Union (Cardoso et al., 2010).

As N is the only driver identified in Sect. 5.2 that can eventually be regulated, we propose focusing on the dependence of H as a function of N , by taking a closer look at the distribution $H(N)$.

Obviously, the original time series H does not only depend on N , but is also affected by the specific effects of unbalanced sediment and climatic anomalies. Using the time series of these drivers and the coefficients obtained in Sect. 5.2, we can rewrite Eq. 7.7 to obtain H_{eq} , the intensity of hypoxia that correspond to the particular situation of average atmospheric conditions (i.e., climatic drivers equal to their average for 1981–2009) and sediment stock in equilibrium with the river nitrogen load.

$$H_{eq} = H - \sigma_H \cdot \left(a_C \cdot \frac{(C - C_{eq})}{\sigma_C} - a_{T_s} \cdot T_s^* - a_{T_f} \cdot T_f^* \right) \quad (7.11)$$

in which the values C_{eq} corresponding to various values of N are estimated from Sect. 5.3 (Fig. 7.13). H_{eq} is now only depending on N and may thus be used to assess the value of H reached for a given nitrogen discharge (N_{eq}) under climate conditions typical of the last 30 yr and with a sediment in equilibrium with N_{eq} .

The resulting distribution, $H_{eq}(N_{eq})$, can be described by a power law ($H_{eq} = a \cdot (N_{eq} - N_0)^b$; $R^2 = 0.90$; Fig. 7.14). Unlike the linear relationship, implicitly assumed within Sect. 5.2, the use of a power law, in addition to resulting in slightly enhanced R^2 , also presents the conceptual advantage of allowing $H_{eq}(N_0) = 0$ for $N_0 > 0$, whether a linear relationship would result in $H_{eq}(N = 0) > 0$, which makes no sense.

Atmospheric drivers have an impact on H which compares to that of eutrophication (Sect. 5.2). This is shown in Fig. 7.14 by indicating the effect on H_{eq} of one standard deviation of the atmospheric drivers around their average value (i.e., $H_{eq} \pm [a_{T_s} + a_{T_f}] \cdot \sigma_H$). This important effect of the climatic drivers underlines that, even in the framework of pertinent nutrient management, the system is not free of risk of hypoxia occurrence due to atmospheric variability.

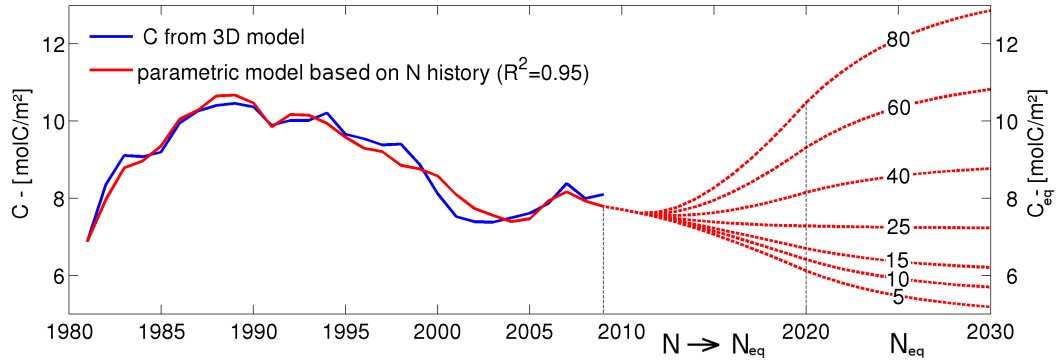


Figure 7.13: Interannual variations of the sediment organic content in winter, C , simulated by the 3-D coupled model and by the parametric model described by Eq. (7.8). After 2009, the parametric model is integrated for 10 yr using a value of N that linearly increases from its value reached in 2009 to different levels of N_{eq} . Then, the integration is continued for 10 additional years, maintaining constant the level of nitrate load ($N = N_{eq}$).

5.5 Practical relationship

We have shown and explained the role of the different predictors appearing in the formulation of H , and in particular the importance of the accumulation of organic matter in the sediments. However, as the predictor C can not be easily estimated without a model, we propose for practical purposes a relationship that directly links the value of H , corresponding to equilibrated organic sediment content, to accessible predictors:

$$H = a \cdot (N - N_0)^b + A_{T_s} \cdot (T_s - 4.6) + A_{T_f} \cdot (T_f - 20.26) \quad (7.12)$$

with $a = 2.64 \pm 2.21$, $b = 0.48 \pm 0.19$, $N_0 = 8.38 \pm 8.8$, $A_{T_s} = 1.07 \pm 0.44$, $A_{T_f} = 2.05 \pm 0.75$. The parameters are obtained by a regular fitting procedure to match the time series provided by $H - \sigma_H \cdot a_C \cdot \frac{(C^* - C_{eq})}{\sigma_C}$, i.e., H corrected from the effect of unbalanced sediment contents. The confidence intervals are computed for $p < 0.1$.

5.6 The recovery process: representativity of monitoring coverage

There are different and contradictory ideas about the recovery process from hypoxia on the Black Sea NWS after eutrophication in the 1990s and 2000s. For instance, the study of Mee (2006), which is cited in number of reviews (e.g., Diaz, 2001; Diaz and Rosenberg, 2008; Kemp et al., 2009; Rabalais et al., 2010), finds a clear recovery during the 1992–2000 period, closely following the reduction of nitrate load.

A quite different picture of the trend of hypoxia during the last decades is presented in the Ukrainian national report (UkrSCES, 2002). More specifically, Fig. 7.9 compares the interannual variability of the extent of hypoxic areas provided by these two studies (and additionally by the model presented in this paper) and evidences two main important differences:

1. The maximum surface is 2 times smaller in UkrSCES (2002) (20 000 km², in 1983).

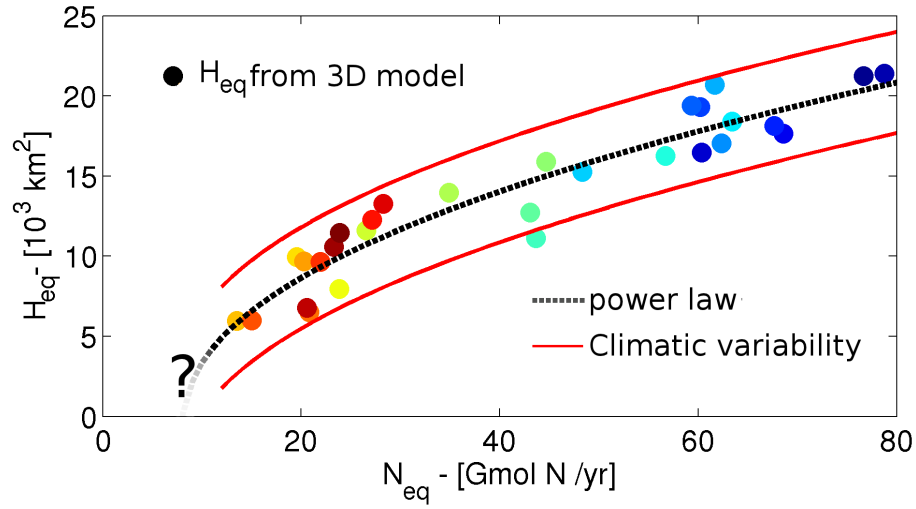


Figure 7.14: Level of hypoxia, H_{eq} , reached at “equilibrium” for a range of nitrate riverine load, N_{eq} . By equilibrium we mean that the atmospheric variables remain at averaged conditions (1981–2009) and that the sediment is in equilibrium with the nitrate load (Sect. 5.3). The colored dots indicate the distribution of H_{eq} obtained from the 3-D model results (Eq. 7.11). This distribution can be described by a non-linear relationship between H_{eq} and N_{eq} ($R^2 = 0.90$). The effect of climatic variability is illustrated by adding (subtracting) the effect of one standard deviation for the two climatic predictors to the central line of H_{eq} .

2. The surface in 1999 and 2000 is similar to that of 1989 (14 000 km²) in UkrSCES (2002), suggesting no recovery, contrary to Mee (2006).

We can note that the model estimations are closer to the Ukrainian report concerning the recovery of the system from hypoxia during the 1990s. These different interpretations of the same phenomenon may come from the use of different data sets by the authors. Unfortunately, we were not able to find details about the data and the methods used to estimate the extent of hypoxia in the study of Mee (2006). We only find that the presented values before 1993 match those presented by Zaitsev (1993), in which no more information is given concerning data coverage and computation methods.

To illustrate how sensitive the conclusions concerning hypoxia and its recovery are to the distribution of data, Fig. 7.10 compares the interannual evolution of the summer (July–August) oxygen concentration as obtained from the available data, from the model outputs restricted to data locations and from the model outputs averaged over the whole area (Fig. 7.1).

The months July and August were chosen because

1. those are the months with the highest number of observations, with data for almost every year (Fig. 7.6),
2. the model bias is minimal for these months (Fig. 7.6c),
3. and bottom hypoxic events are frequent.

Observations and model results obtained at observation locations both indicate a rise of the average summer oxygen concentrations during the 1990s. However, this trend is

not visible anymore when the model results are considered over the whole area, which indicates that a part of this apparent recovery may be non-factual and rather results from the inhomogeneity of monitoring after the mid-1990s.

Similarly, Fig. 7.7 shows that there is a significant correlation ($\rho = 0.63$, $p < 0.01$) between the total number of observations performed during a given year and the percentage of hypoxic events revealed by these data. As an example, no hypoxic event is recorded between 1995 and 2000, but a careful look at the data distribution during this period reveals that no measurement has been made north of $45^{\circ}30'$ where hypoxia usually occurs. This suggests that the observation coverage does not always allow appraising the “real” interannual variability of hypoxia and biased the interpretation of its potential recovery.

Rather than the consensual picture of a recovery from hypoxia closely following the decrease in nutrient load in the Black Sea NWS, the present study indicates a delayed recovery, attributed to the sediment’s memory of eutrophication events (Sect. 5.2). This slower recovery may explain why biological signs of recovery only started to be visible in the 2000 decade (Mee et al., 2005; Langmead et al., 2009; Kostylev et al., 2010). Furthermore, the present-day occurrence of hypoxia is supported directly by in situ observations (Friedrich et al. (2002); J. Friedrich, personal communication, 2010; M. E. Mihailov, personal communication, 2010) and indirectly by the occurrences of massive fish mortality (D. Banaru, personal communication, 2012).

6 Discussion

The present study shows that over the whole period (1981–2009) the impact of atmospheric drivers on hypoxia is commensurate with that of eutrophication (Sect. 5.2). It is interesting to remark that, while the eutrophication predictors generally have lower values in the last decade, the climatic predictors have larger values (not shown) and are thus mainly responsible for the high values of H occurring in the last decade (2000–2009). This stresses that a possible climate change will complicate the management of hypoxia through riverine load restriction policies. It must be noted that in Sect. 5 the effect of temperature is interpreted as a natural variability, which, while indicative, may not reflect the long-term effect of a firm warming trend on the system. It can be seen in Fig. 7.11 that the high H indexes in the last decade are mainly due to longer temporal extension of hypoxia, while high indexes in the eutrophication period were related to larger spatial extension. Because of these different temporal dynamics, the eutrophication- and climate-driven hypoxia may bear a distinct impact on the ecosystem.

Lethal and non-lethal effects of low oxygen concentrations on living organisms strongly depend on the tolerance of the considered species, of the low level of oxygen concentration and of the duration of the hypoxic event (Vaquer-Sunyer and Duarte, 2008). In particular, the damaging effect of hypoxia on a given ecosystem is not expected to vary linearly with the index H defined in Sect. 5.1. H is rather defined as an index to quantify the importance of hypoxia as an environmental stressor. The choice of a sustainable level of H that meets the requirements of good environmental status (GES), as defined by the European Marine Strategy Directive (Cardoso et al., 2010), is therefore a very delicate issue which requires the combination of appropriate tools, as well as dedicated and site-

specific studies.

The response of H to eutrophication and climatic variations given in Sect. 5 may not be valid when using values of the drivers (predictors) far out of the range covered by the present hindcast model experiment. For instance, we suspect that for low nutrient load conditions – not encountered during the period 1981–2009 and, hence, for which the model could not have been validated – the effect of benthic macro-biota could play an important role in regulating hypoxia. Nevertheless, Sect. 5 gives useful indications of the sensitivity of hypoxia to the riverine nitrate load. These can be used to construct scenarios of river load restrictions to be tested with further modeling experiments in order to give an estimation of the maximum nitrate load which would allow the Black Sea NWS to fully recover from hypoxia. To be realistic, these scenario model experiments should be forced with realistic climatic scenario.

7 Conclusions

The Black Sea NWS has been affected by seasonal bottom hypoxia for decades. In the worst cases, the hypoxic zone covers all of the shelf north of 45.5°N and extends along the Romanian coast in the bay of Constanta. The oxygen-depleted waters are located at the bottom between the coast and the 45 m isobaths.

These hypoxic events have a dramatic impact on the benthic biota and have been linked to the almost disappearance of the mussel *Mytilus Galloprovincialis* in the 1980s, the reduction of the surface of Zernov’s Phyllophora field and the loss of important commercial fish stocks. Bottom hypoxia alters the health of the ecosystem and is a serious barrier for reaching GES in the Black Sea. However, its understanding, mapping and mitigation still require tools able to address its temporal and spatial scales of variability and to incorporate its various drivers.

In this paper, we use a combination of mechanistic modeling and statistical tools to address the complexity of hypoxia. A 3-D coupled hydrodynamical–biogeochemical model is used to represent the oxygen dynamics during the 1981–2009 period in response to the physical and biogeochemical processes submitted to the historical nutrient load and atmospheric variability.

The ability of the coupled model to simulate the dynamics of oxygen, at seasonal and interannual scales as well as its spatial variations, is asserted from the computation of various error metrics between model results and in situ measurements gathered from the WOD (18 735 points, 1980–2000) and from the BSC (733 points, 2000–2009). In particular, the comparison of the observed and simulated number of occurrence of hypoxic points ($[\text{O}_2] < 62\text{ mmol m}^{-3}$) for each month and year indicates that the model is able to render this particular threshold.

The mapping of the surface of hypoxia from punctual measurements is a delicate issue that may lead to discrepancies between sources (e.g., Mee, 2006; UkrSCES, 2002) due to different spatial coverage of the data. The spatial heterogeneity of the data among years could lead to biased conclusions on the status of hypoxia. For instance, a concentration of observations south of the typical hypoxia area leads in some cases to the conclusion

that a recovery occurred after the early 1990s, shortly after the reduction of nutrient load. This quick recovery is not reflected by the model results, which rather depict a recovery delayed by the inertia of the sediment layer and mitigated by the important role of atmospheric conditions (see below). There is thus an urgent need for dedicated oxygen-monitoring efforts concentrated on the sites and periods of hypoxia occurrence as well as an integration of the collected data sets in an internationally accessible database. For instance, almost no observations are available during the periods and in the regions of seasonal hypoxia occurrence after 2000.

The coupled model has been used to understand the dynamics of hypoxia at seasonal scales and in particular its driving factors. Seasonal hypoxia occurs because stratification, resulting first from river discharge (April) and then from the warming of surface waters (May), isolates bottom waters from the surface, with the consequence that oxygen depletion caused by the respiration of sinking organic matter can not be balanced by turbulent re-oxygenation. Just before the onset of stratification, March SST significantly impacts the intensity of hypoxia by

1. controlling the oxygen solubility in the last period of vertical mixing, and hence the oxygen concentration of bottom waters before their occlusion,
2. and setting the temperature of bottom waters for the stratification period, and hence affecting the summer rates of organic matter respiration.

Pelagic respiration and benthic diagenesis cause the decrease of oxygen concentrations in the bottom waters until the end of the stratified period (October). While pelagic respiration is mostly related to nitrate load, benthic diagenesis of accumulated organic sediments introduces a memory of eutrophication with a typical timescale estimated at 9.3yr, which contributes to maintain hypoxia after high-nutrient-load events.

The lowest oxygen concentrations are reached at the end of the stratification period. An anomalously long duration of the stratification, due to anomalously high SST in late summer, decreases the bottom oxygen level to very low values and sustains the release of reduced substances to the overlaying waters such as hydrogen sulfide with potentially dramatic consequences for the benthic ecosystem.

The intensity of hypoxia, as an environmental stressor, is quantified for each year by an index H , defined to account both for the spatial and temporal extension of the hypoxic event, as both these aspects matter regarding the repercussions of hypoxia on the living organisms.

Using the results of the 3-D model and the external forcings as an ideal “data set”, long time series (1981–2009) of physical and biogeochemical variables serve as predictors in a multiple regression model representing the interannual variations of H .

Within this large set, a stepwise regression procedure isolates four driving predictors: the annual load of nitrate, the semi-labile carbon content in the sediments, the SST in March and the SST in the late summer. These four predictors allow reconstructing 82 % of the hypoxia intensity interannual variability. Partial regressions show that the drivers linked to eutrophication (i.e., nitrate load, sediment organic content) explain a

slightly larger part (36 %) of the interannual variability in hypoxia intensity than climate predictors (March SST, late summer SST, 27 %).

From this regression we derive a non-linear relationship that links H to the riverine nitrogen load for the particular conditions of sediments in equilibrium with the river nitrogen load and for a typical present climate. This relationship has the advantage of simplicity but should be used with care outside its conditions of derivation (e.g., a different climate, low levels of nitrate load not encountered during the period 1981–2009).

Finally, this relationship could be used to identify the level of the riverine nitrate load that is critical in terms of hypoxia generation and to link these with management strategies of river discharges that integrate socio-economic aspects. This is an important step towards reaching the GES of marine waters as defined by the European Marine Strategy Framework Directive ([Cardoso et al., 2010](#)).

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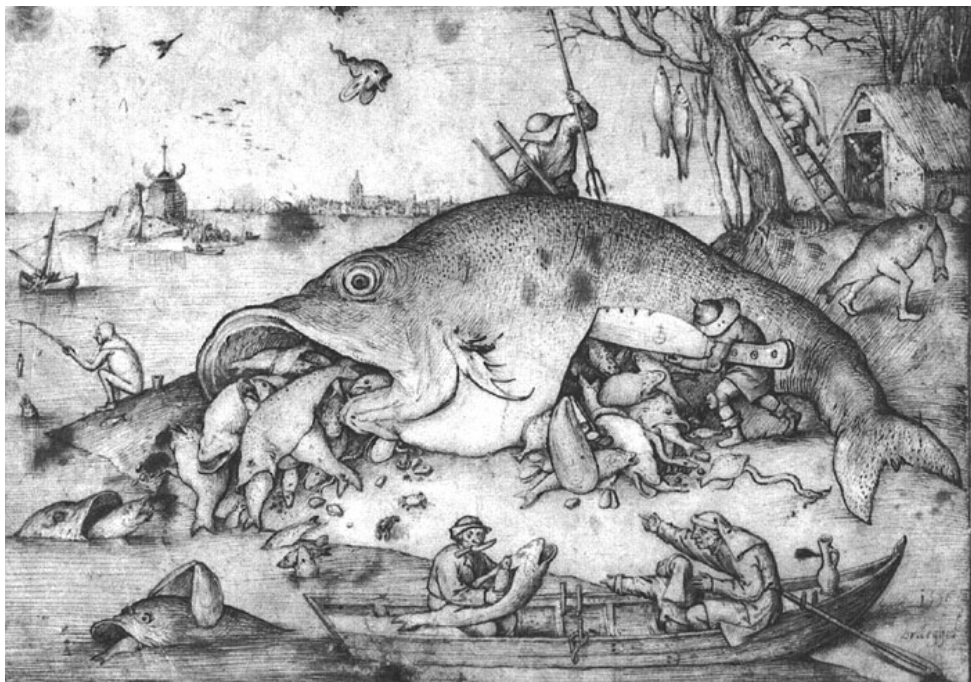
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Chapter 8

Conclusions and Perspectives



De grote vissen eten de kleine, Pieter Bruegel, 1556

1 Conclusions

The work achieved during this thesis mainly consisted in setting up a powerful tool to study the biogeochemical cycles in the Black Sea. This tool has been applied to two specific issues: the multivariate sensitivity of hydrodynamic structure to atmospheric patterns, and the dynamics of hypoxia on the northwestern shelf. These issues merely constitute punctual examples of the large range of investigations for which the model can be used. Hereafter we review the main conclusions established during this thesis and propose a series of investigation perspectives, either that can be directly addressed by the model in its present state or that require identified developments.

The interannual variability of Black Sea hydrodynamic structure was first investigated on the basis of in-situ observations, by computing vertical properties from vertical profiles: the mixed layer depth and the cold content of the Black Sea's Cold Intermediate Layer (CIL). A methodology using the DIVA interpolating software was proposed to distinguish the spatial and temporal (seasonal and interannual) variations of these properties from the unevenly distributed datasets extracted from the World Ocean Database.

By this methodology we could obtain unbiased monthly spatial climatologies for the mixed layer depth and CIL cold content, as well as seasonal and interannual trends over the period 1960-2010. Multilinear regressions offered a first appreciation of the influence of atmospheric conditions on the interannual variability of these properties. This analysis proved to be particularly relevant in the case of the CIL cold content for which 88% of the variability could be explained by past winter air temperature anomalies. The cumulative impact of winter air temperature anomalies on the CIL indicates that its dynamics involves interannual accumulation and feedback mechanisms and in particular allows to use past winter air temperature anomalies to provide a range of expectations for the CIL cold content of the following year.

The general methodology is suitable to address other types of representativity errors, for instance by grouping data according to the observation method, the hours of the day or database origins, instead of grouping them by months and years as was done presently. A number of precautions related to the interpretations of the results were presented. The main approximation lies in the fact that the trends associated with the different groups are assumed to be additive, spatially coherent, and independent of the other groups. For instance, one may expect the seasonal variability to differ between strongly contrasting year. Appropriately, the detrending tool presented in this study provides, along with the climatological product, the temporal information needed to address this question. For instance one may choose to disaggregate the original dataset into sub-periods of persistent anomalies and recompute the seasonal anomalies for these sub-periods.

The following step was to investigate the sensitivity of the Black Sea hydrodynamic structure to atmospheric conditions through the implementation of the GHER hydrodynamic model on the Black Sea domain. The GHER model has been implemented for the Black Sea basin using two resolutions, of approximately 5 and 15 km. In-depth assessment of the model skills indicates to which extent the model is able to reproduce the mechanisms driving the response of the Black Sea hydrodynamic system to external forcings. While exact matches were not expected from these unconstrained simulations,

i.e. without resorting to data assimilation or automatic relaxation towards imposed climatologies, spatial, seasonal and interannual variabilities were generally well reproduced and free of systematic drift.

The major imperfections of the model lie in the fine scale circulation on the northwestern shelf, impacted by the spatial resolution of the wind forcings, and the overestimated winter mixing that results from the absence of a convective scheme to resolve the sinking of CIL waters formed in the vicinity of the shelf break. Underestimation of the basin wide Rim current has also been indicated. Refining the model's spatial resolution does not significantly enhance these specific issues, which means that the mathematical formulations of convective sinking and forcing data have to be enhanced prior to proceed to finer resolution model setups.

A statistical review of the regional atmospheric anomalies over the period 1960-2000 has provided a convenient way to classify the recurrent atmospheric patterns and to relate these to large scale and well-studied teleconnection systems. We underlined the contrasting time scales of the influence of the North Atlantic Oscillation (NAO) and the East Asia/West Russia (EA/WR) oscillations on the air temperature over the Black Sea, and consequently on the sea surface temperature. The NAO impacts on the signature of air masses west of the Black Sea and exerts a long term (> 5 years) influence on air temperature. The EA/WR oscillation directly controls the meridional component of the Black Sea wind field, and therefore is more closely related to air temperature on short time scales (< 5 years), as southerly (resp. northerly) winds bring warmer (resp. colder) air masses over the Black Sea.

By identifying, in a 40 year simulation multivariate modes of variability of the Black sea hydrodynamical structure we evidenced the prominent role of the Rim current as a regulating factor buffering the sensitivity of the Black Sea to atmospheric variations. It has been found that an increasing persistence of atmospheric anomalies during the 1960-2000 period brought the Black Sea system further from its equilibrium, as was illustrated by the enhancement of the Rim current at the end of the 80s, consequence of a persistent cyclonic wind anomaly.

While this study was restricted to the four last decades of the 20th century, it provide a baseline to better appreciate the alteration of the Black Sea structure in the context of the foreseen global warming.

The biogeochemical modelling investigation relied on a model developed previously in one dimension and adapted to the open region of the Black Sea. Transposing this model into a tridimensional environment required to refine the relationship between physics and biogeochemistry and to adapt it in order to adequately address the strong environmental gradients of the Black Sea, both horizontal and vertical. The model was extended to integrate the dynamics of phosphorus and completed with a detailed light penetration model that accounts for the specific inherent optical properties of various components of the sea water.

Biogeochemical cycles on the wide and shallow northwestern shelf are largely impacted by exchanges between the benthic and pelagic layer, whose representation in biogeochemical models had generally been oversimplified. The development and implementation of an efficient approach to this problematic issue allowed us to inquire the important spatial

and temporal variability of these coupling mechanisms. Rather than opting for a full vertical resolution of the sediment layers, we favored a meta-modelling approach which considerably reduces the computational requirements, hence preserves the practical use of the model for long term investigations.

The enhanced model has proved able to reproduce the spatial and seasonal variability indicated by in situ benthic fluxes estimates. From 30 years of coupled simulations, we proposed new values for the contribution of sedimentary diagenesis to biogeochemical cycles in the NWS, in particular regarding the importance of benthic denitrification which removes about half of the terrestrial input of nitrogen.

The implications of this study regarding benthic-pelagic coupling extend beyond the scope of the present Black Sea implementation. Notably, we evidence the importance of resolving the physical transport of sediments through bottom stress effects to accurately reproduce the horizontal distribution of benthic fluxes and the lateral export to the open sea or, more essentially, to resolve the biogeochemical role of the continental shelves.

On a larger scale, the model skill assessment procedures indicate a matching representation of the main biogeochemical cycles with the qualitative resolution of horizontal and vertical distribution of nutrients and oxygen. The winter over-mixing reported previously hindered the accurate quantitative resolution of the vertical profiles in the open sea. Additional factors are certainly involved in the mismatch, as for instance the absence of dinitrogen fixation processes, but we advise that the physical aspects should be solved prior to considering more complex biological issues.

On the northwestern shelf the model presents limitations in resolving the very fast absorption of river-borne nutrients depicted by in situ observations. However, river mouth and sea-side levels of nutrient match the observations, which points towards unresolved fine scale biogeochemical processes. It is suspected that unaccounted benthic ecosystems play an important role in this fast absorption of terrestrial nutrients inputs.

The direct implications of resolving the benthic-pelagic coupling in the Black Sea NWS is that it allows for a comprehensive analysis of the dynamics of hypoxia.

The investigation of hypoxia dynamics over the period 1980-2009 from in situ observations and from model results revealed that, due to the spatial and temporal variability of hypoxia, an extensive monitoring is needed to provide a satisfactory assessment of the hypoxia status from in situ observations alone. We illustrated that the absence of observational evidence supporting the presence of hypoxia has misleadingly been used in previous studies, concluding to the absence of hypoxia after the mid-90s. The result is that numerous publications comparing the dynamics of hypoxia in several sites around the globe systematically address the Black Sea as a case of a marked recovery (e.g. [Steckbauer et al., 2011](#); [Kemp et al., 2009](#)). Here, the model successfully resolve the variability reproduced by observations but also indicates hypoxic occurrences in places where no data are available.

We suggest that a reconsideration of the Black Sea hypoxia dynamics should be included in global studies, and that a specific monitoring plan should be set up, focused on the area and period of the year where hypoxia is known to prevail. Eventually, this mechanistic model study provides the knowledge needed to focus this monitoring, hence permitting

substantial savings in future operational surveys. Monitoring should thus be focused on Ukrainian waters, from July to October, and in near-bottom waters.

The damaging impact of hypoxia on marine living resources is quantified by an index H accounting for both spatial and temporal extension of the seasonal event. By a comprehensive analysis of the mechanisms underlying the seasonal evolution of the vertical oxygen profiles we were able to identify four factors controlling the annual intensity of hypoxia, represented through the H -index diagnosed from the 3D modelling results. These four drivers include two related to eutrophication (nitrogen riverine loads, and sedimentary organic content) and two related to climatic conditions (March, and late summer sea surface temperature). Partial regression analysis indicated that climate factors impact almost as much as eutrophication factors, driving a shorter term variability by controlling the ventilation processes.

High nitrogen loads trigger higher organic matter sinking fluxes, hence increase the respiration processes in the bottom waters and in the sediments where it can not be balanced neither by photosynthesis nor by ventilation. This was the main driver during the 80s. Sedimentary organic content keeps track of the past history of eutrophication, when high organic matter sinking fluxes exceed the mineralization rates in the sediments, hence accumulate over the years in the sediment layers. The resulting benthic oxygen demand introduces an inertial component in the relationship between eutrophication and hypoxia. This process sustained hypoxia during the 1990s after riverine nutrients loads have been reduced drastically and suddenly.

March SST has two indirect influences in the mechanism of hypoxia. First, high SST in March reduces the solubility of oxygen in sea water during the last mixing days of the water column. Therefore it relates to the initial inventory of oxygen below the mixed layer depth when the thermocline sets on. Second and for the same reason, March SST sets the temperature of bottom waters for the whole summer period. High temperature triggers high metabolic rates, hence increase the respiration processes and therefore the consumption of oxygen.

Finally late summer temperature are related to the timing of the thermocline breakdown. High SST in August-September delay the ventilation process at the time when oxygen concentrations are at their lowest, hence may significantly increase the damaging impact of hypoxia. In the 2000-2010 decade, climatic factors gradually took the lead in driving hypoxia with warmer summers inducing a longer temporal extension of the hypoxic events of smaller extension but longer duration. This major conclusion is a further urge to consider global warming in the construction of sound marine resources management policies as it underlines that ecosystem sensitivity to anthropogenic pressures (in that case eutrophication) differs under contrasting climatic regimes. To enforce the model representation of hypoxia for a wider range of stressors and for larger time scales, we recommend to further develop the representation of the specific dynamics of phosphate in the sediments, in particular the formation and decomposition of ferrous complexes under various oxygenation levels, and to include the functional roles of benthic ecosystems.

2 Perspectives

2.1 Scenarios

We have presented the model's ability to resolve the main aspects of hydrodynamical variability at basin scale and at time scales from seasonal to multi-decadal. As the model has always been used without nudging or data assimilation, it can be used in its current state to address scenario and long-term projection studies. The validation procedure achieved in this thesis can be exploited to identify the most critical parameters, i.e. those associated with the largest error sources. By perturbing these parameters to generate ensemble simulations, one could derive the error associated with projected model results and provide expectation ranges for the most relevant characteristics.

Projections studies however, are strongly conditioned by the provision of reliable forcing datasets of riverine discharges and atmospheric conditions for the future. While such a scenario exists at global scale, fine resolution local products for the Black Sea are currently not satisfactory. These products are often impacted by a flawed representation of the oceanic component in the atmospheric model, and an underestimation of the orographic constraints on Black Sea's local atmospheric dynamics. This may result for instance in important bias for the air temperature. Such bias are corrected for past and present forcings sets by data assimilation (e.g. ECMWF reanalysis), but can obviously not be corrected for future conditions.

Projection studies should therefore carefully compare reanalysis products with unconditioned forcing sets, computed without data assimilation for the past years. Without this comparison, differences between projections and hind cast simulations could wrongly be interpreted as symptomatic of climate change where they would in fact just be induced by uncorrected biases in the future forcing data.

2.2 Interannual variability of the biogeochemical cycles

The biogeochemical model is still impacted by the absence of a convective sinking scheme resolving the sinking of dense water formed near the shelf break, and over-mixing in the open sea preventing an accurate representation of the subsurface maxima of nutrients (the maxima are resolved, but underestimated).

While it can be said that the model resolves a fair part of the biogeochemical structure, this issue may pose a problem to study the long-term trends with accuracy, and in particular the effect of projected forcing modifications on the Black Sea's biogeochemical structure.

Addressing these issues would allow to apply multivariate analysis similar to that presented in Chapter 4 for biogeochemical variables. This would considerably strengthen our knowledge on how the connections operate between climatic large scale variations and, first, the biogeochemical Black Sea structure, and then, marine goods and services in the Black Sea.

2.3 Hypoxia

The problem of coastal hypoxia is foreseen to increase worldwide, due to the increase of both temperature and nutrients loads associated with population growth. Therefore it constitutes one of the most urging challenges addressed to the marine scientific community.

Both the specific Black Sea model implementation and the general methodology proposed in chapter 7 constitute unique approaches to the issue of hypoxia. The implementation of such detailed mechanistic approaches in different sites would allow to appreciate how the geomorphology of these sites impacts on the specific sensitivity of hypoxia to its driving factors. In particular, the H-index proposed in this work is a good candidate to compare objectively the severity of hypoxia across different sites. As we underlined such mechanistic studies should consider the important role of benthic-pelagic coupling to resolve adequately the inertial relationship between hypoxia and eutrophication. The efficient modelling approach proposed in chapter 6 constitute maybe the best actual methodology to integrate benthic-pelagic coupling for long term simulations. A post-doctoral project is scheduled to apply these tools and to enforce the statistical description of hypoxic events in the northern Adriatic sea. We hope that working out the portability of these tools will allow for a coordinated consideration of marine hypoxia around the world and a sound scientific message to address to political entities.

A main task remains to be addressed in that regard : to quantify the H index in terms of damaging impact on marine resources, both in terms of exploitable populations, and of key ecological functions sustained by the benthic ecosystems.

Researches have been initiated in this direction. They compare the spatial distribution of macrobenthos species and their functional traits to the spatial distribution of oxygen dynamics characteristics. This is a promising and exciting research line that will certainly show its relevance in the coming years.

2.4 Fisheries

The management of fishery resources is one of the most important objectives of oceanographic studies. Unfortunately, this question is very difficult to address in mechanistic terms because of the poor reliability of traditional data sets, impacted by important political and economical stakes (e.g. [Watson and Pauly, 2001](#)), and because of the large range of physical scales that have to be considered to cover exhaustively the processes affecting the dynamics of fish stocks.

It remains unclear how stressors of different natures (e.g. atmospheric shifts, fishing pressure) affect fish stocks and how these impacts propagate across trophic levels. In particular it is difficult to evaluate at which trophic levels top-down and bottom-up controls prevail.

For instance trophic cascade is proposed as a mechanism having propagated the impact of overfishing on planktonic and even nutrients dynamics ([Llope et al., 2011](#)). On the other hand, strong atmospheric shifts coincide in time with the impressive reported drop-down of important fish stocks and are therefore also suspected to have a controlling impact on

fish populations (Oguz et al., 2006). End-to-end modelling aims to integrate these various scales in a single modelling system.

The Ecopath-with-Ecosim approach

The Ecopath-with-Ecosim (EwE) approach (Christensen and Walters, 2004) is a data-driven, basically non-dimensional approach to fish stock assessment allowing for temporal and spatial variations around baseline trophic equilibrium. This approach allows one to consider a high number of species and to investigate the effects of various type of fishing gears.

Originally, planktonic populations in EwE are not considered, or only constrained by top-down predatory relationships. A coupling approach proposed by Libralato and Solidoro (2009) allows the authors to introduce, at least partially, the bottom-up control that climate and riverine loads exert on planktonic populations. In collaboration with Georgi Daskalov (Bulgarian Academy of Science) this method was implemented in the Black Sea, exploiting the model presented in this work and a preexisting EwE Black Sea implementation (Daskalov, 2002).

Further development of this research line should identify additional physical or biogeochemical processes constraining high trophic levels dynamics. These processes would then be considered as forcing function to condition the population growth and mortality and predatory interactions in the EwE model. For instance, considering the impact of hypoxic conditions on high trophic levels survival and predatory behavior, in particular regarding benthic populations, could derive the economical cost of hypoxia events by assessing its impact on fishery stocks. Providing the means to balance the cost of nutrient loads managements against the risk of affecting fishery resources would constitute a very valuable tool to design sustainable coastal management policies.

The Lagrangian approach

The alteration of larval retention conditions under various hydrodynamical regimes constitutes a candidate explanation for the hydrodynamic impacts on fish stocks dynamics. Related hypotheses may be tested by exploiting Lagrangian particle tracking algorithms, eventually completed by growth models to represent the evolution of fish larvae until their recruitment.

Such aspect have been investigated using the off-line particle-tracking software ICHTIYOP (Lett et al., 2008). However, the need for a very fine resolution (ideally less than 2 km) to resolve adequately meso-scale circulation features, and the overambitious objective to include results from the biogeochemical model to force the larval growth model prevented us from reaching convincing conclusions. A sound continuation of this research line should consider an on-line coupling with a Fortran particle tracking software (e.g. TRACMASS, <http://tracmass.org/>), allowing for a finer temporal resolution, and to explore the feasibility of considering a finer physical model with a coarser biogeochemical model, or to combine on-line and off-line coupling for the physical and biogeochemical models, respectively.

2.5 Benthic ecosystems

To widen the application field of the biogeochemical model in the coastal area, the most urging development concerns the ecological functions of the benthic ecosystems, whose implications range from basin-wide biogeochemistry to fishery resources. As stated previously, the non-consideration of benthic ecosystems is suspected to hamper the model aptitude to resolve the very fast absorption of the high nutrient levels depicted by measurements in the direct vicinity of river mouths.

While the benthic model component described in Chapter 6 is a first step in that direction, it does not account for the contribution of living benthic and epibenthic communities to biogeochemical cycles, be they floral or faunal. For instance, the Black Sea NWS hosts a very large aggregation of the agarophyte *Phyllophora*, the Zernov Field (Zaitsev, 1997), which is known to act as a significant oxygenator and to offer habitat to many endangered fish populations (Kostylev et al., 2010). It would be very surprising that a sound resolution of the Black Sea ecosystem considering high trophic level could be achieved without a refined representation of such biotopes.

Of course sediment cores or in situ incubations used as observational basis to the present work, do not account for epibenthic contributions. Further observational data have to be assembled and collected to provide the basic material on which the modelling approach can be developed. Automatized optical and acoustic characterization of benthic habitats on large scales, and integrated fluxes as provided by eddy-covariance measurements are part of the technical development that would allow one to exploit the notion of habitat (Diaz et al., 2004), and functional trait analysis (Bremner et al., 2006) as a link between the environmental aspect, resolved now by the 3D GHER-BAMHBI model, and the functional role of benthic populations.

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