



1 **Dynamics and Ecological impacts of dissolved Iron on the Ross Sea Continental Shelf:**

2 **Machine Learning Reconstruction**

3 Ruobing Cao¹, Walker Smith^{1,2}, Enhui Liao¹, Ziang Li^{1,3}, Shuangling Chen⁴, and Yuncong Ge¹

4 1. School of Oceanography, Shanghai Jiao Tong University, Shanghai, China

5 2. Key Laboratory of Polar Ecosystem and Climate Change, Shanghai, China

6 3. National Oceanography Centre, University of Southampton, Southampton, United

7 Kingdom

8 4. State Key Laboratory of Satellite Ocean Environment Dynamics, Second Institute of

9 Oceanography, Ministry of Natural Resources, Hangzhou, China

10

11 Corresponding authors:

12 Walker Smith, wos@vims.edu

13 Enhui Liao, ehliao@sjtu.edu.cn



Abstract

Dissolved iron (dFe) availability is a key factor regulating phytoplankton productivity over the Ross Sea continental shelf, yet its spatial and temporal distributions remain poorly constrained because of sparse observations. We reconstructed monthly three-dimensional dFe distributions from 2005 to 2019 at $0.5^\circ \times 0.184^\circ$ resolution on the Ross Sea continental shelf with XGBoost model trained by historical dFe observations and paired environmental variables and continuous fields produced by MOM6. The reconstruction demonstrated the spatial features of dFe, including elevated concentrations along the western coast and north of Franklin Island and widespread surface dFe depletion ($<0.1 \text{ nmol L}^{-1}$) across the central Ross Sea from late spring with an overall R^2 of 0.79 and a mean absolute error of 0.29 in ln-transformed dFe. Based on our results, the pronounced regional differences of surface dFe could be explained by seasonal relationship between the ferricline and mixed layer. In winter, the mixed layer extended below the ferricline in the western Ross Sea and Ross Sea Polynya but generally remained shallower in the eastern Ross Sea. This pattern was consistent with regional differences in spring bloom development, suggesting that winter access to subsurface Fe contributed to bloom preconditioning. In summer, the relatively small separation between the mixed layer and ferricline in the western Ross Sea potentially favored continued vertical Fe supply and sustained high chlorophyll concentrations during the open-water period. Overall, this product provides accurate estimates of the regional dFe-phytoplankton coupled dynamics in the Ross Sea.



35 **Short summary**

36 Iron is an essential nutrient for marine microalgae, but in the Ross Sea, observations are too
37 sparse to show the temporal and spatial changes. We used historical measurements, model-
38 produced data, and machine learning algorithm to reconstruct iron conditions from 2005 to
39 2019. We found strong differences linked to how iron-rich deeper waters are accessible to the
40 surface by vertical mixing or diffusion, helping explain where and when algal blooms develop.
41 This helps explain variations of biomass in time and space.

42



43 1. Introduction

44 The Ross Sea continental shelf is an Antarctic marginal sea with complex bathymetry,
45 including islands, banks, and troughs, and is influenced by numerous glaciers and ice sheets. It
46 is also impacted by seasonal sea ice and is extensively covered by sea ice for ca. six months
47 each year. It also has persistent latent heat polynyas that are maintained by katabatic winds
48 (Falco et al., 2024). Consequently, the iron supply is supported by multiple local processes,
49 including vertical mixing, sediment resuspension, aerosol inputs, and glacial, sea ice and ice
50 shelf melting. Removal processes (phytoplankton uptake and particle scavenging) greatly
51 reduce surface levels during austral spring and summer (Sedwick et al., 2000; Dinniman et al.,
52 2020). These complex physical and biogeochemical processes differ among subregions. It is
53 challenging to describe the spatial heterogeneity of iron distributions and evaluate its ecological
54 impact in the Ross Sea without a comprehensive data set with extensive time and space
55 coverage.

56 Phytoplankton biomass and biogeochemical variables on the Ross Sea continental shelf
57 vary substantially on seasonal time scales. Iron concentrations are elevated in autumn and
58 winter (ca. 1.0 nM) but are reduced substantially in spring and summer by phytoplankton
59 growth, reaching ca. 0.06 nM (Sedwick et al. 2011), a concentration sufficiently low to impose
60 Fe limitation on phytoplankton growth (Timmermans et al., 2004). The low concentrations
61 appeared to regulate phytoplankton composition and result in elevated particulate organic
62 carbon to chlorophyll ratios (Smith & Kaufman, 2018). The role of iron in controlling
63 phytoplankton growth has been demonstrated repeatedly in iron addition experiments (Martin
64 et al., 1994; Coale et al., 1996; Boyd et al., 2000). Despite its importance, the lack of
65 observational data that delineate the spatial and temporal variations in the region restricts our
66 understanding of the association between iron availability and biogeochemical traits.

67 In past decades, observational efforts to measure trace metal concentrations in this region
68 have extended both spatial and temporal coverage. Despite this, most observations have been
69 collected in spring and summer, and no information is available in winter. In 2017 Sedwick et
70 al. (2022) conducted the first autumn trace metal observations in the Ross Sea and documented
71 iron concentrations beneath sea ice and within the Terra Nova Bay polynya. Despite these
72 advances, current data coverage remains sparse relative to the vast extent of the Ross Sea.



73 Individual cruise expeditions can only sample a limited number of stations, leaving substantial
74 gaps in observational coverage.

75 Numerical simulations and oceanic biogeochemical (BGC) models have been widely used
76 to predict the distributions of BGC variables with broader spatial coverage and greater temporal
77 resolution. Although the model outputs represent estimated rather than directly measured values,
78 they serve a critical role in filling observational gaps, enabling the construction of spatially and
79 temporally continuous fields. However, the performance of these numerical simulation-based
80 reconstructions strongly depends on the accurate parameterization of oceanic processes, which
81 remains challenging for some biogeochemical variables such as trace metals. Tagliabue et al.
82 (2016) evaluated global dissolved iron (dFe) distributions in 13 global ocean biogeochemistry
83 models, and compared the results with observed dFe profiles from the GEOTRACES project.
84 Their results suggested that models exhibited substantial errors in reproducing global dFe,
85 likely due to the inaccurate representation of key processes and parameters (e.g., dFe residence
86 time).

87 Alternatively, data-driven reconstructions, represented by machine learning algorithms,
88 infer spatial and temporal distributions from related environmental predictors by learning the
89 distribution patterns and statistical correlations between selected variables in an observational
90 data set, avoiding the difficulty of parameterizing highly complex oceanic processes. These
91 methods have been used in oceanography for the reconstruction of physical parameters such as
92 temperature, capturing seasonal anomalies successfully (Su et al., 2019). They have also been
93 applied to biogeochemical variables, including dissolved oxygen concentrations (Ito et al., 2024)
94 and surface pCO₂ (Chau et al., 2022; Wu et al., 2025) across different spatial scales. Despite
95 fewer observations of trace metal concentrations, machine learning has been used to reconstruct
96 trace metal distributions. Huang et al. (2022) produced a global monthly climatology of dFe at
97 1° spatial resolution and with 31 vertical levels iron distributions through the use of a Random
98 Forest model. Jiang et al. (2025) reconstructed global dissolved Cd (dCd) to explain the
99 relationship between dCd and phosphate. Both studies demonstrated the potential of machine-
100 learning approaches for trace metal analysis.

101 Nevertheless, existing global-scale machine-learning products have limited applicability
102 to Antarctic marginal seas. For example, the product developed by Huang et al. (2022) covered



only between 72°S and 72°N, excluding most Antarctic marginal seas from its spatial domain despite their importance to biogeochemical cycles. In addition, because the dominant sources and sinks of dissolved iron vary substantially among oceanic regions, relationships derived from global datasets may not adequately capture region-specific controls, thereby reducing reconstruction accuracy at regional scales. Previous studies using machine learning models for biogeochemical parameter reconstructions have emphasized the importance of scale-dependent and region-specific modeling approaches (Wu et al., 2025).

We developed a machine-learning framework to reconstruct dissolved iron (dFe) over the Ross Sea continental shelf (water depth < 1500 m) to resolve its spatial variability and seasonal evolution. Given the sparse coverage of both dFe and its environmental predictors, we further examined whether relationships derived from observations could be transferred to environmental fields from numerical models. This field-driven machine learning reconstruction generated spatially and temporally continuous dFe distributions which appeared consistent with the field data and superior to those generated by the numerical models. The reconstructed dFe fields were subsequently used to characterize its spatial and seasonal variability and to investigate the biogeochemical influence of iron.

119

120 **2. Data and methods**

121 **2.1 Data sources and preprocessing**

Dissolved iron (dFe) concentrations data derived using trace metal clean techniques in the Ross Sea were compiled from a number of cruises conducted between 2006 to 2019 (Table S1) (<https://www.bco-dmo.org>). The data include over 1300 dFe measurement from 127 profiles located on the continental shelf (Fig. 1a). Most samples were collected in the western Ross Sea, as well as dense coverage near the Ross Sea Ice Shelf (Fig.1). Temporally, the data covered from November to the end of May, with no data in March (Fig. 1e). Only one cruise provided dFe data during ice-covered autumn (sea ice concentration >85%). There also are no winter observations (June – October). Despite the heterogeneous spatial and temporal sampling distribution, these cruise observations spanned most subregions of the Ross Sea continental shelf and covered a wide range of sea ice concentrations (0-100%).

Multiple parameters related to physical characteristics [temperature, salinity, potential



density anomaly (σ_0), biogeochemical variables [(nitrate (NO_3^-), phosphate (PO_4^{3-}), silicate (Si), dissolved oxygen (DO), Chlorophyll a (chl a), particulate organic carbon (POC)], geological conditions (bathymetry), atmospheric processes [wind speed, direction and aerosol optical depth (AOD)] were utilized as potential predictors for dFe reconstruction. In addition, as seasonal variations of sea ice and ice shelf impacts also play important roles in this region, distance from the ice edge was also included. The oceanographic and BGC parameters used for model training were primarily taken from ship-based measurements from the same cruise. Due to the pronounced seasonal cycles, the date variable was encoded with sine and cosine transformations (Huang et al., 2022). Wind data were taken from ERA5 and processed through Google Earth Engine platform (<https://earthengine.google.com/>). The specific products for each variable are listed in Table S2. Sea ice information was obtained from AWI/IUP Bremen sea ice product (<https://data.seaice.uni-bremen.de/>). Sea ice edge distances were defined as the signed distance from each point to the 15% sea ice concentration, as well as indicating whether the point was inside or outside the sea ice coverage.

The MOM6-COBALT2 model (MOM6 hereafter) (Liao et al., 2020), which integrates modular ocean model version 6, sea ice simulator version 2, carbon ocean biogeochemistry, and lower trophics version 2 (Adcroft et al., 2019; Stock et al., 2020), was used to provide spatially and temporally continuous fields of oceanographic variables, including potential temperature (θ), salinity, σ_0 , DO, NO_3^- , and PO_4^{3-} , for dFe reconstruction. The model setup followed Liao et al. (2020).

2.2 Model design

The workflow for model development and dFe reconstruction occurred in steps (Fig. 2). First, the predictor variables and dFe observations were matched to the native grid of MOM6 to construct a unified data set. During the model development, dFe observations served as the prediction target for the machine learning algorithm. 10% of the complete data from isolated cruise profile were isolated as an independent validation set. The remaining 90% of the data were divided into 4 folds according to their sampling location, with all observations from the same profile assigned to a single fold. This block based 4-fold cross validation was then applied to develop XGBoost model to avoid the over-fitness caused by spatial autocorrelation (Stock,



163 2025).

164 Bayesian optimization was employed for hyperparameter selection. XGBoost is a learning
165 algorithm based on gradient-boosted decision trees (Friedman, 2002) developed by Chen &
166 Guestrin (2016). Compared with traditional gradient boosting decision tree algorithms, a
167 regularized learning objective, sparsity-aware learning and a weighted approximate quantile
168 sketch were introduced into XGBoost (Chen & Guestrin, 2016) to reduce overfitting and
169 promote generalization, especially for sparse data sets. Model performance was evaluated for
170 both the four-fold cross-validation and the independent validation dataset by comparing
171 predicted and observed dFe concentrations using root mean square error (RMSE), mean
172 absolute error (MAE), coefficient of determination (R^2), and Spearman's rank correlation
173 coefficient (ρ).

174 A stepwise algorithm simplified from Zhong et al. (2022) was constructed to select
175 efficient combinations for dFe prediction. At the beginning of stepwise predictor selection, only
176 grid information (latitude, longitude, depth, and time) was initially used as the predictor set for
177 dFe values. For each subsequent step, one candidate variable at a time was added to the
178 predictor pool, and the corresponding MAE was calculated for each addition. The variable
179 producing the greatest reduction in MAE was temporarily retained in the predictor set. The
180 above step was repeated based on the updated predictor set, until the addition of any remaining
181 candidate variable did not improve predictive performance (defined as the decrease of MAE
182 < 0.003 compared with the previous step). Thereafter, these variables were removed individually
183 from the predictor pool. Variables whose exclusion increased MAE by less than 0.0002 were
184 discarded. This step was intended to reduce redundancy caused by variable intercorrelations
185 and improved model performance.

186 To assess model transferability, the observation-trained XGBoost model was directly
187 applied to corresponding MOM6-derived predictors without retraining. The predicted dFe was
188 then compared with observations to evaluate whether the relationships learned from
189 observational data remained valid when transferred to numerical model fields. Its performance
190 was further compared with the dFe directly simulated by MOM6.

191

192 2.3 Interpretation analysis



Two approaches were used to estimate the effects of different environmental variables on dFe distributions. First, Spearman correlation coefficients (ρ) were calculated between measured dFe and each selected environmental variable. Spearman correlation coefficients were calculated to estimate the monotonic correlation between two quantitative variables without restricting the relationship to a linear association. Spearman correlation is suitable for variables exhibiting non-normal distributions (Miot, 2018) and is less sensitive to extreme values; it is widely used for indicate associations among environmental factors (Ciavatta et al. 2016; Hyder et al., 2018).

Second, the SHapley Additive exPlanations (SHAP) approach was applied to identify the key factors affecting dFe predictions. SHAP was developed for enhancing the interpretability of machine learning models (Lundberg & Lee, 2017), and is grounded in cooperative game theory (Shapley, 1953). SHAP computes Shapley values to attribute the contribution of each explanatory variable to a model's prediction. Within the machine-learning framework, Shapley values can quantify the contribution of each variable on dFe concentration. By integrating these two statistical approaches for subset layers, the potential mechanisms affecting dFe concentrations at different depths can be explored.

2.4 Ferricline calculation and chlorophyll *a* estimation

The reconstructed dFe fields were first vertically interpolated to 1-m intervals. The ferricline depth was then calculated as the depth at which the vertical dFe gradient ($\partial \text{dFe} / \partial z$) exceeds 0.0008 nM m^{-1} . Climatological chl *a* concentrations were derived from satellite observations using a locally developed Ross Sea-specific algorithm, which has improved sensitivity for quantifying phytoplankton blooms in this region (Chen et al., 2022).

3. Result

3.1 Model performance and transferability

The performance of trained XGboost algorithm was evaluated using R^2 , and Spearman correlation coefficients (ρ) in cross-validation (Fig. 3a). Predictive performance was also evaluated for the independent validation profiles (Fig. 3b). When the observation-trained model was applied directly to MOM6-derived environmental predictors without retraining, the



reconstructed dFe remained highly correlated with observations with MAE=0.29, RMSE=0.37, $\rho=0.89$, and $R^2=0.79$, (Fig. 3c). However, because the dFe observations used for evaluation of MOM6-driven recontraction were also included in model training, these results reflect the agreement between the reconstruction and historical observations, but may overestimate independent predictive skill. Since the model was trained and evaluated on ln-scaled values, an MAE of 0.30 corresponds approximately to a relative error on the order of 30% on the original scale. This result was markedly improved compared with dFe simulated directly by MOM6 (Fig. S1).

For both observation validation and MOM6-driven dFe reconstructions, high dFe concentrations tended to be underestimated, whereas low concentrations were slightly overestimated, with relatively large errors at the lower end of the concentration range (Fig. 3d). Vertically, relative errors in the independent validation were generally larger in the upper water column and decreased with depth. In contrast, after transferring the model to MOM6-derived fields, relative errors remained relatively uniform through most of the water column and decreased only below ~900 m, apart from several extreme values near the surface (Fig. 3e). In the surface layer (0–50 m), where relative errors were largest, reconstructed dFe was still significantly correlated with in situ dFe ($\rho = 0.81$, $p < 0.001$), indicating that the model reproduced the relative spatial ordering of dFe even though absolute concentrations were less well constrained.

3.2 Depth-dependent factors influencing dFe prediction

Dissolved Fe distribution was associated with multiple environmental processes, as reflected by the SHAP interpretation analysis and Spearman correlation coefficients (ρ), with clear variations among depth layers (Fig. 4). Salinity was consistently among the most influential predictors across all three depth layers, and its contribution was more pronounced in deep water than in the surface and subsurface layers (Fig. 4a). Following salinity, distance to bottom (D_{bot}) also showed large SHAP importance in deep water. Moreover, it exhibited the highest absolute ρ (−0.60) in this layer, indicating that dFe tended to increase closer to the seafloor. Similar to deep water, D_{bot} was also relatively important in the subsurface layer, although its absolute SHAP value was smaller. However, the relatively low ρ indicated that the



relationship between D_{bot} and dFe was not strongly monotonic. In contrast, NO_3^- and PO_4^{3-} showed relatively high values in both SHAP importance and ρ , indicating broadly consistent variations between these macronutrients and dFe.

In surface waters, both the SHAP contributions and the absolute Spearman correlation coefficients were generally smaller than those in the subsurface and deep layers, suggesting the absence of a single dominant environmental factor associated with dFe variability. However, compared with the deeper layers, the relative importance of sea ice-related variables increased, with $\rho_{\text{SIC}} = 0.31$ and $\rho_{\text{Dsic}} = -0.19$. The relationship between D_{bot} and predicted dFe was nonlinear and was influenced by the location of water layer, with positive SHAP contributions at small distances from the seafloor that decreased rapidly as D_{bot} increased. In waters shallower than 200 m, the influence of benthic processes is negligible. (Fig. 4c).

3.3 Spatial and vertical dFe distributions during open water periods

The reconstructed fields captured pronounced spatial variations in the mean vertical distribution of dFe during the open water period (November–February) (Fig. 5). Along the zonal transect at 74.8°S, extending from the coastal region of Terra Nova Bay (TNB) toward the shelf break, elevated near-bottom dFe was mainly observed in areas with relatively deep bathymetry, including the Drygalski Trough within TNB and the depression between Crary Bank and Pennell Bank (Fig. 5a). In the TNB region, the sediment-associated high-dFe signal extended relatively close to the surface, resulting in comparatively high dFe concentrations throughout much of the water column. In contrast, although elevated benthic dFe was also evident between Crary Bank and Pennell Bank, this signal was largely restricted within ca. 150 m of the seafloor, and no clear enhancement in the surface or subsurface layers was noted. Near the shelf break, a relatively large dFe signal was also observed at intermediate depths, potentially corresponding to the intrusion of CDW through the Glomar Challenger Trough. A similar enhancement of dFe over a depression was observed along the meridional transect at 178°E from the Ross Ice Shelf front to the shelf break (Fig. 5b). In this region, however, the bottom-associated dFe enhancement was mainly confined to ~100 m above the seafloor, while surface and subsurface waters remained relatively depleted in dFe.

Regional mean profiles for the western Ross Sea coastal region (WRS), the central Ross



Ice Shelf Polynya (RISP), and the eastern Ross Sea (ERS) all showed relatively depleted dFe in the surface homogeneous layer followed by increasing concentrations with depth (Fig. 5c). Maximum mean dFe concentrations occurred at approximately 600–700 m. In the upper layer, mean dFe concentrations in the RISP and ERS were below 0.1 nM and significantly lower than those in the WRS ($p < 0.05$). In contrast, within the deep dFe maximum layer, concentrations were comparable between the WRS and RISP and were higher than those in the ERS (Fig. 5c).

3.4 Ferricline and vertical mixing

Ferricline depths (Z_{dFe}) exhibited pronounced spatial and seasonal variability across the Ross Sea continental shelf (Fig. 6). The ferricline was defined as the depth at which the vertical dFe gradient deviates from zero, representing the upper boundary rather than the center of the iron maximum (Tagliabue et al., 2014). Seasonally, Z_{dFe} generally followed changes in stratification, with deeper ferriclins in winter (Fig. 6c) and shallower ferriclins in summer (Fig. 6a, b). However, the spatial relationship between Z_{dFe} and mixed layer depth (MLD) was not uniform across the shelf. During summer, MLDs were generally shallow throughout the Ross Sea shelf, except north of Franklin Island, whereas Z_{dFe} remained substantially shallower in the western Ross Sea than in the eastern region.

The monthly position of the ferricline and mixed layer showed a clear regional pattern across the Ross Sea shelf (Fig. 6g-i). In most of the eastern Ross Sea, Z_{dFe} remained deeper than the MLD throughout the year. A similar pattern occurred near the shelf break and extended southward onto the continental shelf along the Joides Trough. In contrast, the MLD generally extended below or close to Z_{dFe} in the western Ross Sea. The Ross Ice Shelf Polynya showed a more pronounced seasonal transition, particularly near the southwestern Ross Ice Shelf front, where the MLD extended below the ferricline during winter but became shallower than Z_{dFe} during summer.

3.5 Spatial and temporal variations of surface dFe and chlorophyll *a*

The climatological (2005-2014) dFe reconstruction in the upper 50 m indicated depleted dFe at the surface in the Ross Sea continental shelf during the open water period (November to February), with dFe ranged from 0.04 to 0.40 nM (mean = 0.11 nM) (Fig. 7a-d). After



November low-dFe water (<0.1 nM) appeared in the central and eastern Ross Sea, including most of the Ross Sea Polynya, and then expanded across almost the entire Ross Sea continental shelf in the following months. In spring and summer, dFe concentrations >0.15 nM were found around Franklin Island and in the coastal zone of the western Ross Sea. Although these concentrations and area decreased seasonally, they remained above 0.1 nM throughout summer. This iron plume around Franklin Island is mainly found north of the island. Such elevated coastal values did not occur in McMurdo Sound.

Satellite-derived climatological Chl *a* concentrations also showed pronounced spatial heterogeneity during the open water period (Fig. 7d-g). Elevated Chl *a* first emerged along the western Ross Ice Shelf in November and became more widespread in the following months. Through spring and summer, Chl *a* remained high in the southwestern Ross Sea except for McMurdo Sound, with monthly average concentrations exceeding 8 mg m^{-3} . Across the shelf, however, the spatial relationship between dFe and Chl *a* did not follow a simple monotonic pattern. Classification based on the upper and lower quartiles of dFe and Chl *a* further revealed distinct spatial combinations (Fig. 7h-k). In November, high dFe-high Chl *a* (HFeHC) conditions occurred mainly in the coastal western Ross Sea, whereas low dFe high Chl *a* (LFeHC) conditions appeared in the Ross Ice Shelf Polynya. During the subsequent months, the spatial extent of HFeHC conditions gradually increased, while LFeHC areas contracted and became largely restricted to the western margin of the Ross Ice Shelf. In contrast, Chl *a* remained relatively low near the shelf break, where high dFe low Chl *a* conditions were maintained around the Joides Trough.

4. Discussion

By integrating observational constraints, machine learning-derived relationships between dFe and environmental variables, and the continuous environmental fields provided by the MOM6 numerical model, we generated a three-dimensional, monthly resolved dFe reconstruction for the Ross Sea continental shelf. Prediction uncertainties varied with depth, with relatively larger errors occurring in the upper ocean. This may partly reflect the greater complexity of surface dFe variability, which previous studies have suggested can be influenced by multiple physical, biological, and biogeochemical processes (Mack et al., 2017; Marsay et



al., 2017). Such relatively large prediction errors in shallow waters have also been reported in global machine learning reconstructions of dFe (Huang et al., 2022). Moreover, our model was developed specifically for the Ross Sea using locally relevant observations and environmental relationships, rather than attempting to represent globally heterogeneous controls on dFe within a single framework. Despite the remaining uncertainties, the XGBoost predictions showed a significant Spearman correlation with observations, indicating that the model captured a substantial fraction of the observed relative variability in dFe concentrations.

Our reconstruction reproduced several characteristic features of dFe distributions previously observed across the Ross Sea continental shelf: including relatively high surface dFe concentrations along the western coastal region, elevated dFe near the seafloor, particularly within the major trough systems, and the development of an extensive low-dFe (<0.1 nM) region across the central Ross Sea shelf during the open water season (Marsay et al., 2017; Sedwick et al., 2022; Gerringa et al., 2020). Accordingly, the reconstruction provides a useful basis for examining regional-scale spatial contrasts and seasonal-to-interannual variability in dFe across the Ross Sea.

4.1 Contrasting controls on dFe across the Ross Sea

Machine learning model training, together with the subsequent SHAP analysis, provides an effective data-driven approach for exploring the environmental factors associated with the observed variability of dFe in the Ross Sea. By combining oceanographic features, SHAP dependence patterns, and Spearman correlations, our analyses identified the environmental variables most strongly associated with dFe variations (Lundberg & Lee, 2017) and further characterized whether these relationships were monotonic throughout the water column. These statistical associations should not be interpreted as direct evidence of causality, but when interpreted together with established knowledge of iron cycling in the Ross Sea (Marsay et al., 2017; McGillicuddy et al., 2015; Sedwick et al., 2011, 2022), these relationships provide useful insights into the processes that may regulate dFe supply and removal.

Salinity ranked first in the SHAP approach for all layers. This variable together with potential temperature (θ) and potential density anomaly referenced to 0 dbar (σ_0) is generally used to separate different water masses. The ρ of salinity, θ , and σ_0 in surface and subsurface



373 indicated that decreased potential temperature and, elevated density and salinity tended to result
 374 in elevated dFe, which represent the features of Shelf Water (Orsi & Wiederwohl, 2009).
 375 However, this association does not mean the dFe was added from Shelf Water directly but is
 376 likely due to the enhancement of vertical mixing during Shelf Water formation.

377 Distance to the bottom (D_{bot}) was the strongest predictor of dFe below 200 m and showed
 378 a significant negative correlation with dFe ($\rho = -0.60$, $p < 0.05$). This pattern is consistent with
 379 previous studies identifying benthic inputs as an important source of dFe to the Ross Sea
 380 continental shelf (McGillicuddy et al., 2015). Benthic Fe is supplied largely through sediment
 381 resuspension and subsequent release of dissolved Fe into bottom waters (Fitzwater et al., 2000),
 382 resulting in elevated dFe concentrations near the seafloor (Sedwick et al., 2022). In contrast,
 383 the predictive importance of D_{bot} decreased markedly in the subsurface and surface layers,
 384 suggesting that the influence of sediment sourced Fe is progressively attenuated away from the
 385 seafloor. This vertical weakening implies that only part of the benthic Fe signal is effectively
 386 transferred to the upper ocean or their influence was masked by other Fe removal and
 387 transformation processes.

388 In addition to the predictors discussed above, NO_3^- and PO_4^{3-} were also associated with
 389 dFe variability in the subsurface layer, showing broadly consistent relationships with dFe. This
 390 pattern may reflect the concurrent regeneration of macronutrients and Fe during organic matter
 391 remineralization between 50-200 m (Gerringa et al., 2020). On the Ross Sea continental shelf,
 392 a substantial fraction of sinking organic matter is remineralized within the upper 200 m (Meyer
 393 et al., 2022; Cao et al., 2025), potentially providing an internal source of regenerated dFe.
 394 However, the relatively modest correlations between dFe and macronutrients ($\rho = \text{ca. } 0.3$)
 395 suggest that this coupling is limited. Unlike macronutrients, regenerated Fe is strongly modified
 396 by scavenging and particle partitioning, which can decouple dFe distributions from those of
 397 macronutrients (Tagliabue et al., 2019). As reported by Sedwick et al., (2011), the depths
 398 between ferricline and nitricline can be over 30 m in the Ross Sea.

399 Sea ice melt has been widely regarded as an important seasonal source of dFe to Ross Sea
 400 surface waters (Sedwick et al., 2011; Salmon et al., 2020). However, sea ice-related predictors
 401 showed only limited importance in our analysis, although their absolute ρ values increased
 402 toward the surface, consistent with a process primarily affecting the upper ocean. The Spearman



correlation between D_{ice} and surface dFe was only -0.19 , indicating no monotonic relationship between the two variables. This weak relationship may reflect the way in which sea ice effects are expressed in surface dFe variability rather than implying a negligible role of sea ice. During early spring, sea ice retreat reduces surface albedo, while meltwater promotes the formation of a shallow and strongly stratified surface layer. These changes create optimal irradiance conditions for phytoplankton growth (Smith & Nelson, 1985). The marginal ice zone is therefore become the activate region for phytoplankton growth in the Ross Sea (Smith & Nelson, 1985).

As phytoplankton blooms are coupled with sea ice melt, Fe released from melting ice may be rapidly draw down by the developing bloom rather than accumulating as elevated dFe. Sea ice-derived Fe supply and biological removal may therefore partially offset one another, leaving only a weak residual relationship between sea ice conditions and observed dFe concentrations. In addition, part of the biological response associated with sea ice retreat may already be represented by other predictors such as macronutrients, thereby reducing the apparent contribution assigned to sea ice variables by SHAP. Surface dFe thus appears to reflect the combined influence of several processes of comparable importance, rather than a single dominant process as observed for sediment-related influences in deeper waters. This interpretation is also consistent with the generally smaller mean absolute SHAP values in the surface and subsurface layers.

422

4.2 Vertical mixing and regionally different dFe supplements

Iron availability is widely recognized as one of the major factors controlling phytoplankton growth in the Ross Sea (Smith et al., 2014). It interacts with vertical mixing and sea ice conditions to regulate phytoplankton development and further shape regional biogeochemical characteristics (Smith & Kaufman, 2018). Phytoplankton dynamics are not uniform across the Ross Sea continental shelf, and different subregions exhibit distinct phytoplankton composition. This reconstructed dFe data set provides an opportunity to explore how regional differences in Fe supply and vertical accessibility contribute to these contrasting phytoplankton dynamics.

The relative positions of the ferricline and mixed layer influence the potential for subsurface dFe to be supplied to surface waters (Tagliabue et al., 2014). In the SO, deep winter



433 mixing can entrain a relatively large subsurface Fe reservoir into the upper ocean, whereas
434 diffusive dFe supply contributes no more than 10% of the surface Fe inventory (Tagliabue et
435 al., 2014). Mixed layer depths in the Ross Sea undergo strong seasonal evolution and also vary
436 among regions (Porter et al., 2019; Cao et al., 2025). In the southwestern Ross Sea, deep winter
437 mixing can entrain a relatively large subsurface Fe reservoir into the upper ocean
438 (McGillicuddy et al., 2015). However, vertical Fe supply during the growing season should not
439 be neglected. Vertical dFe fluxes across the Ross Sea shelf can vary by approximately three
440 orders of magnitude (Gerringa et al., 2015), and in some regions summer Fe supply may be
441 sufficient to sustain continued phytoplankton growth. Therefore, during the open water period,
442 the size of the upper ocean dFe pool reflected the balance between Fe inputs and removal. Fe
443 inputs include the inventory established by deep winter mixing and continued Fe supply during
444 the growing season, the relative importance of which can be qualitatively assessed from the
445 seasonal evolution of mixed-layer and ferricline depths. Meanwhile, dFe can be taken up by
446 phytoplankton and transferred into the particulate Fe pool, or removed from surface waters
447 through particle sinking.

448 The seasonal relationship between MLD and ferricline depth differed substantially within
449 the Ross Sea, indicating regional differences in the potential accessibility of subsurface Fe to
450 the surface layer. Such differences in vertical Fe accessibility provide a physical framework for
451 interpreting the contrasting seasonal patterns of surface dFe and phytoplankton biomass. In the
452 WRS, the persistent overlap between the mixed layer and ferricline suggests that subsurface Fe
453 remained relatively accessible to the upper ocean throughout the seasonal cycle. Such coupling
454 is consistent with previous studies emphasizing the importance of vertical entrainment and deep
455 mixing for replenishing surface Fe in the Ross Sea (McGillicuddy et al., 2015). In contrast, the
456 seasonal separation between the mixed layer and ferricline in the RISP implies a progressive
457 reduction in direct access to the subsurface Fe reservoir as stratification develops. Under these
458 conditions, phytoplankton growth would increasingly depend on Fe accumulated earlier in the
459 season, together with internal recycling during summer (Marsay et al., 2017). Nevertheless,
460 localized vertical Fe supply may persist where bathymetry enhances tidal and turbulent mixing.
461 Ross Bank provides an example, where topographically intensified mixing can facilitate the
462 upward transport of benthic Fe, although the relative importance varies seasonally (Greenan et



al., 2025). This interpretation is consistent with observations of rapid seasonal dFe drawdown in the Ross Sea Polynya, although localized vertical Fe fluxes may remain important during summer (Sedwick et al., 2011; Gerringa et al., 2015, Greenan et al., 2025).

When the seasonal differences in vertical Fe accessibility are considered together with the contrasting dFe-Chl *a* states during the growing season, the regional patterns can be interpreted in terms of different balances between Fe supply and biological demand. The WRS was characterized predominantly by a high dFe-high Chl *a* state. In addition to relatively persistent access to subsurface Fe, this region receives Fe from multiple sources, including the large winter Fe inventory, coastal inputs, and sea ice melt (McGillicuddy et al., 2015; Marsay et al., 2017). Although some of these processes are not explicitly represented by the predictors used in our reconstruction, their combined contribution may help maintain relatively high ambient dFe even under strong biological demand, resulting in a more supply supported Fe regime in the WRS.

In contrast, the RISP more frequently developed a low dFe-high Chl *a* state as the Fe inventory established by deep winter mixing can support the early algal bloom and biomass accumulation, but rapid phytoplankton uptake subsequently depletes surface dFe. (Sedwick et al., 2011; McGillicuddy et al., 2015). As this initially accumulated Fe is depleted, recycling of biogenic Fe within the upper ocean can sustain regenerated production later in the season (Marsay et al., 2017). The major phytoplankton group shift from *Phaeocystis* to diatom may also support comparable biomass with lower Fe requirement (Smith et al., 2014; Zhang et al., 2023). Thus, although both the WRS and RISP exhibited substantial phytoplankton biomass, the supporting mechanism may differ: the WRS appears to receive more persistent and diverse external Fe inputs, whereas the RISP relies on an initially accumulated Fe inventory followed by recycling and field stoichiometric change (Smith & Kaufman, 2018). Different Fe supply pathways may deliver Fe with contrasting chemical forms and bioavailability (Fourquez et al., 2022). For example, Fe-siderophore complexes have been proved to stimulate the biomass increase in phytoplankton dominated by diatoms (Kustka et al., 2015). Such differences arise because biological recycling modifies Fe speciation and its association with organic ligands, which can strongly influence Fe uptake by phytoplankton (Hassler et al., 2011; Nuester et al., 2014). Therefore, these differences may contribute to the seasonal phytoplankton composition



shifts (Smith et al., 2014). Although species-specific Fe-ligands complexes utilization variations were not observed among different diatoms by Kustka et al., 2015), which was excepted exist between diatom and *Phaeocystis*.

4.3 Potential for interpreting annual changes

Antarctic sea ice increased modestly over much of the satellite era, but this pattern reversed after 2014–2015, followed by a rapid decline in sea ice extent (Parkinson, 2019; Smith & Meyer, 2026), raising questions about how long-term changes in sea ice conditions may affect upper-ocean Fe supply and availability. The Ross Sea provides a useful region in which to examine this linkage because of its strong interannual and decadal sea ice variability. Sea ice coverage in the Ross Sea increased substantially from 1979 to approximately 2014, at an average rate of $13.7 \times 10^3 \text{ km}^2 \text{ yr}^{-1}$ (Hobbs et al., 2016), with particularly pronounced increases in the western Ross Sea. This long-term increase subsequently ceased and was followed by a period of rapid sea ice decline and enhanced interannual variability (Parkinson, 2019). How such changes are reflected in the upper-ocean Fe inventory remain poorly understood. Our reconstructed dFe fields from 2005–2019 provide a statistical perspective on this question. Before 2014, subsurface dFe declined significantly across the Ross Sea (Fig. 8a), while a corresponding surface decline occurred only in the WRS and RISP and was strongest in the WRS (Fig. 8b), coinciding with the more pronounced increase in sea ice in this region; however, the subsequent reversal in sea ice trends was not accompanied by a corresponding recovery in surface dFe, suggesting that upper ocean dFe does not respond linearly or immediately to sea ice variability but reflects the balance between physical Fe supply and biological drawdown. This is consistent with model projections showing that future sea ice loss may enhance upper-ocean Fe supply while simultaneously stimulating biological Fe consumption; hence, surface dFe concentrations would not necessarily increase (Krumhardt et al., 2022).

4.4 Limitations of machine learning analysis

This XGBoost-M6 dFe reconstruction for the Ross Sea resolved subregional variability in dFe and identified the major factors driving these variations. However, because of the unique characteristics of the region, the model still has several limitations in both training and



523 application, which may introduce errors into the results. These errors come from several sources.
524 First, the data used for model training itself contain substantial gaps. After stepwise predictor
525 selection, neither chlorophyll a nor POC were included in the final model training, because
526 cross-validation showed that adding these variables did not improve model performance.
527 However, this does not mean that phytoplankton growth has little influence on surface dFe.
528 More likely, it reflects the limited coverage of chlorophyll a and POC in the original training
529 data, which results from sampling gaps, detection limits and data quality filtration. These
530 missing data could not be supplemented with satellite products. This absence of data will also
531 influence the data used for construction, because extensive cloud cover strongly constrains
532 ocean color retrievals in this region (Meyer et al., 2025).

533 The atmospheric predictors did not improve predictive performance sufficiently to be
534 retained in the final model, which is consistent with suggestions that atmospheric iron
535 deposition is a minor contributor to iron concentrations (Sedwick et al., 2011; Marsay et al.,
536 2014). However, the effects of atmospheric processes on oceanic iron supply often occur with
537 a temporal lag (Lim et al., 2022). These lagged responses were not included in the predictor-
538 matching process, and temporal mismatches may have reduced the model's ability to exploit
539 atmospheric variables for improved model performance. Although atmospheric influence is
540 limited across the Ross Sea, specific regions may be influenced by dust from the McMurdo Dry
541 Valleys and atmospheric inputs might be locally enhanced (Sedwick et al., 2011; Winton et al.,
542 2016).

543

544 **5. Conclusion**

545 We developed an observation-based XGBoost model to characterize the relationships
546 between dFe and environmental variables over the Ross Sea continental shelf, and successfully
547 transferred these relationships to MOM6-derived environmental fields to generate spatially and
548 temporally continuous monthly 3-dimensional dFe reconstructions. By combining XGBoost
549 with SHAP analysis, we identified pronounced depth-dependent environmental associations
550 with dFe. Below 200 m, proximity to the seafloor became increasingly important, indicating a
551 strong bottom-associated influence on deep dFe distributions, whereas surface dFe was
552 associated with multiple environmental factors without a single dominant control. The



reconstructed fields further revealed marked spatial heterogeneity in dFe, with elevated concentrations near the seafloor over deep troughs and basin-like topographic features, while the western Ross Sea maintained relatively high upper-ocean dFe during the growing season. The relative position of the ferricline and mixed layer also exhibited distinct regional and seasonal patterns, suggesting differences in the vertical accessibility of subsurface iron among shelf regions. These contrasts in iron availability likely contribute to the heterogeneous patterns of phytoplankton biomass accumulation observed across the Ross Sea shelf.

Data availability

The reconstructed dFe data are available as a NetCDF file at <https://doi.org/10.5281/zenodo.23339459> (Cao et al., 2026, v1).

Author contributions

RC conducted the main analyses, developed the code, and performed the experiments. WS conceived the original idea of the study, acquired funding, and provided continuous guidance. EL provided guidance on the development and implementation of the machine-learning framework, the application of MOM6 model outputs, and the integration of related analytical approaches. ZL assisted with the MLD analysis. SC assisted with the chlorophyll *a* analysis. YG contributed to dFe data curation and analysis. RC drafted the manuscript with critical feedback and revisions from WS and EL. All authors contributed to and approved the final version of the manuscript.

Conflict of Interest

The authors declare there are no conflicts of interest for this manuscript.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (NSFC) project to WOS (W2431033). The authors thank many research groups that collected the field data, and the GEE platform (<https://earthengine.google.com/>) for maintaining and providing the data used in this study. We thank Xueying Zhang for her help in MOM6 data processing.



583

584 **References**

- 585 Adcroft, A., Anderson, W., Balaji, V., Blanton, C., Bushuk, M., Dufour, C. O., Dunne, J. P.,
586 Griffies, S. M., Hallberg, R., Harrison, M. J., Held, I. M., Jansen, M. F., John, J. G.,
587 Krasting, J. P., Langenhorst, A. R., Legg, S., Liang, Z., McHugh, C., Radhakrishnan, A.,
588 Reichl, B. G., Rosati, T., Samuels, B. L., Shao, A., Stouffer, R., Winton, M., Wittenberg,
589 A. T., Xiang, B., Zadeh, N., & Zhang R. (2019). The GFDL global ocean and sea ice model
590 OM4.0: Model description and simulation features. *Journal of Advances in Modeling*
591 *Earth Systems*, 11, 3167–3211. <https://doi.org/10.1029/2019MS001726>
- 592 Boyd, P. W., Watson, A. J., Law, C. S., Abraham, E. R., Trull, T., Murdoch, Bakker, R., D. C.
593 E., Bowie, A. R., Buesseler, K. O., Chang, H., Charette, M., Croot, P., Downing, K., Frew,
594 R., Gall, M., Hadfield, M., Hall, J., Harvey, M., Jameson, G., LaRoche, J., Liddicoat, M.,
595 Ling, R., T. M., Michael McKay, M. R., Nodder, S., Pickmere, S., Pridmore, R., Rintoul,
596 S., Safi, K., Sutton, Strzepek, P., R., Tanneberger, K., Turner, S., Waite, A., & Zeldis J.,
597 (2000). A mesoscale phytoplankton bloom in the polar Southern Ocean stimulated by iron
598 fertilization. *Nature*, 407(6805), 695-702. <https://doi.org/10.1038/35037500>
- 599 Cao, R., Smith Jr, W. O., Zhong, Y., Riser, S., Johnson, K. S., & Talley, L. (2025). The seasonal
600 patterns of hydrographic and biogeochemical variables in the Ross Sea: A BGC-Argo
601 analysis. *Deep Sea Research Part II: Topical Studies in Oceanography*, 219, 105436.
602 [10.1016/j.dsr2.2024.105436](https://doi.org/10.1016/j.dsr2.2024.105436). <https://doi.org/10.1016/j.dsr2.2024.105436>
- 603 Chen, S., Smith, W. O. Jr., & Yu, X. (2021). Revisiting the ocean color algorithms for particulate
604 organic carbon and chlorophyll-a concentrations in the Ross Sea. *Journal of Geophysical*
605 *Research: Oceans*, 126, e2021JC017749. <https://doi.org/10.1029/2021JC017749>
- 606 Chau, T. T. T., Gehlen, M., & Chevallier, F. (2022). Global ocean surface carbon product
607 (Doctoral dissertation, Le Laboratoire des Sciences du Climat et de l'Environnement).
608 DOI : 10.48670/moi-00047
- 609 Chen, T., & Guestrin, C. (2016). Xgboost: A scalable tree boosting system. In: *Proceedings of*
610 *the 22nd acm sigkdd international conference on knowledge discovery and data mining*,
611 *ACM, New York City*. pp 785–794. <https://doi.org/10.1145/2939672.2939785>
- 612 Ciavatta, S., S. Kay, S. Saux-Picart, M. Butenschön, and J. I. Allen (2016), Decadal reanalysis



-
- 613 of biogeochemical indicators and fluxes in the North West European shelf-sea ecosystem.
 614 Journal of Geophysical Research: Oceans, 121, 1824–1845, doi:10.1002/2015JC011496.
 615 Coale, K. H., Johnson, K. S., Fitzwater, S. E., Gordon, R. M., Tanner, S., Chavez, F. P., Ferioli,
 616 L., Sakamoto, C., Rogers, P., Millero, F., Steinberg, P., Nightingale, P., Cooper, D.,
 617 Cochlan, W. P., Landry, M. R., Constantinou, J., Rollwagen, G., Trasvina A., & Kudela R.
 618 (1996). A massive phytoplankton bloom induced by an ecosystem-scale iron fertilization
 619 experiment in the equatorial Pacific Ocean. Nature, 383(6600), 495-501.
 620 <https://doi.org/10.1038/383495a>
 621 Dinniman, M. S., St-Laurent, P., Arrigo, K. R., Hofmann, E. E., & van Dijken, G. L. (2020).
 622 Analysis of iron sources in Antarctic continental shelf waters. Journal of Geophysical
 623 Research: Oceans, 125, e2019JC015736. <https://doi.org/10.1029/2019JC015736>
 624 Falco, P., Krauzig, N., Castagno, P., Garzia, A., Martellucci, R., Cotroneo, Y., Flocco, D.,
 625 Menna, M., Pirro, A., Mauri, E., Memmola, F., Solidoro, C., Pacciaroni, M., Notarstefano,
 626 G., Budillon G., & Zambianchi E. (2024). Winter thermohaline evolution along and below
 627 the Ross Ice Shelf. Nature Communications, 15(1), 10581.
 628 <https://doi.org/10.1038/s41467-024-54751-8>
 629 Fitzwater, S. E., Johnson, K. S., Gordon, R. M., Coale, K. H., & Smith Jr, W. O. (2000). Trace
 630 metal concentrations in the Ross Sea and their relationship with nutrients and
 631 phytoplankton growth. Deep Sea Research Part II: Topical Studies in Oceanography,
 632 47(15-16), 3159-3179. 10.1016/S0967-0645(00)00063-1.
 633 Fourquez, M., Janssen, D. J., Conway, T. M., Cabanes, D., Ellwood, M. J., Sieber, M., Trimbom,
 634 S., Hassler, C. (2023). Chasing iron bioavailability in the Southern Ocean: Insights from
 635 *Phaeocystis antarctica* and iron speciation. Science Advances, 9(26), eadf9696.
 636 DOI:10.1126/sciadv.adf9696
 637 Friedman, J. H. (2002). Stochastic gradient boosting. Computational statistics & data analysis,
 638 38(4), 367-378.
 639 Gerringa, L. J., Alderkamp, A. C., Van Dijken, G., Laan, P., Middag, R., & Arrigo, K. R. (2020).
 640 Dissolved trace metals in the Ross Sea. Frontiers in Marine Science, 7, 577098.
 641 <https://doi.org/10.3389/fmars.2020.577098>
 642 Greenan, B. J., Dinniman, M. S., McGillicuddy Jr, D. J., Sedwick, P. N., Mack, S. L., & Smith



-
- 643 Jr, W. O. (2025). The relative contribution of deep and shallow benthic sources to iron
644 supply in the Ross Sea, with specific emphasis on Ross Bank. *Deep Sea Research Part II:*
645 *Topical Studies in Oceanography*, 219, 105450.
646 <https://doi.org/10.1016/j.dsr2.2024.105450>
- 647 Hassler, C. S., Schoemann, V., Nichols, C. M., Butler, E. C., & Boyd, P. W. (2011). Saccharides
648 enhance iron bioavailability to Southern Ocean phytoplankton. *Proceedings of the*
649 *National Academy of Sciences*, 108(3), 1076-1081.
650 <https://doi.org/10.1073/pnas.1010963108>
- 651 Hobbs, W. R., Massom, R., Stammerjohn, S., Reid, P., Williams, G., & Meier, W. (2016). A
652 review of recent changes in Southern Ocean sea ice, their drivers and forcings. *Global and*
653 *Planetary Change*, 143, 228-250. <https://doi.org/10.1016/j.gloplacha.2016.06.008>
- 654 Huang Y, Tagliabue A and Cassar N (2022) Data-Driven Modeling of Dissolved Iron in the
655 Global Ocean. *Frontiers in Marine Science*, 9:837183. doi: 10.3389/fmars.2022.837183
- 656 Hyder, P., Edwards, J. M., Allan, R. P., Hewitt, H. T., Bracegirdle, T. J., Gregory, J. M., Wood,
657 R. A., Meijers, A. J. S., Mulcahy, J., Field, P., Furtado, K., Bodas-Salcedo, A., Williams,
658 K. D., Copsey, D., Josey, S. A., Liu, C., Roberts, C. D., Sanchez, C., Ridley, J., Thorpe, L.,
659 Hardiman, S. C., Mayer, M., Berry D. I., & Belcher, S. E. (2018). Critical Southern Ocean
660 climate model biases traced to atmospheric model cloud errors. *Nature Communications*,
661 9(1), 3625. <https://doi.org/10.1038/s41467-018-05634-2>
- 662 Ito, T., Cervania, A., Cross, K., Ainchwar, S., & Delawalla, S. (2024). Mapping dissolved
663 oxygen concentrations by combining shipboard and Argo observations using machine
664 learning algorithms. *Journal of Geophysical Research: Machine Learning and*
665 *Computation*, 1(3), e2024JH000272. <https://doi.org/10.1029/2024JH000272>
- 666 Krumhardt, K. M., Long, M. C., Sylvester, Z. T., & Petrik, C. M. (2022). Climate drivers of
667 Southern Ocean phytoplankton community composition and potential impacts on higher
668 trophic levels. *Frontiers in Marine Science*, 9, 916140.
669 <https://doi.org/10.3389/fmars.2022.916140>
- 670 Liao, E., Resplandy, L., Liu, J., & Bowman, K. W. (2020). Amplification of the ocean carbon
671 sink during El Niños: Role of poleward Ekman transport and influence on atmospheric
672 CO₂. *Global Biogeochemical Cycles*, 34, e2020GB006574.



-
- 673 <https://doi.org/10.1029/2020GB006574>
- 674 Lundberg, S. M., & Lee, S. I. (2017). A unified approach to interpreting model predictions. 31st
 675 International Conference on Neural Information Processing Systems (NIPS'17).
- 676 Mack, S. L., Dinniman, M. S., McGillicuddy Jr, D. J., Sedwick, P. N., & Klinck, J. M. (2017).
 677 Dissolved iron transport pathways in the Ross Sea: Influence of tides and horizontal
 678 resolution in a regional ocean model. *Journal of Marine Systems*, 166, 73-86.
 679 10.1016/j.jmarsys.2016.10.008
- 680 Marsay, C. M., P. M. Barrett, D. J. McGillicuddy, and P. N. Sedwick (2017), Distributions,
 681 sources, and transformations of dissolved and particulate iron on the Ross Sea continental
 682 shelf during summer, *Journal of Geophysical Research: Oceans*, 122, 6371–6393,
 683 doi:10.1002/2017JC013068.
- 684 Marsay, C. M., P. N. Sedwick, M. S. Dinniman, P. M. Barrett, S. L. Mack, and D. J.
 685 McGillicuddy Jr. (2014), Estimating the benthic efflux of dissolved iron on the Ross Sea
 686 continental shelf, *Geophysical Research Letters*, 41, 7576–7583,
 687 doi:10.1002/2014GL061684.
- 688 Martin, J. H., Coale, K. H., Johnson, K. S., Fitzwater, S. E., Gordon, R. M., Tanner, S. J., ... &
 689 Tindale, N. W. (1994). Testing the iron hypothesis in ecosystems of the equatorial Pacific
 690 Ocean. *Nature*, 371(6493), 123-129. <https://doi.org/10.1038/371123a0>
- 691 McGillicuddy Jr., D. J., P. N. Sedwick, M. S. Dinniman, K. R. Arrigo, T. S. Bibby, B. J. W.
 692 Greenan, E. E. Hofmann, J. M. Klinck, W. O. Jr. Smith, S. L. Mack, et al. (2015), Iron
 693 supply and demand in an Antarctic shelf ecosystem, *Geophysical Research Letters*, 42,
 694 8088–8097, doi:10.1002/2015GL065727.
- 695 Meyer, M. G., Portela, E., Smith, W. O. Jr., & Heywood, K. J. (2025). Critical uncoupling
 696 between biogeochemical stocks and rates in Ross Sea springtime production–export
 697 dynamics. *Ocean Science*, 21, 1223–1236. <https://doi.org/10.5194/os-21-1223-2025>
- 698 Meyer, M. G., Jones, R. M., & Smith, W. O. Jr. (2022). Quantifying seasonal particulate organic
 699 carbon concentrations and export potential in the southwestern Ross Sea using
 700 autonomous gliders. *Journal of Geophysical Research: Oceans*, 127, e2022JC018798.
 701 <https://doi.org/10.1029/2022JC018798>
- 702 Miot, H. A. (2018). Correlation analysis in clinical and experimental studies. *Jornal vascular*



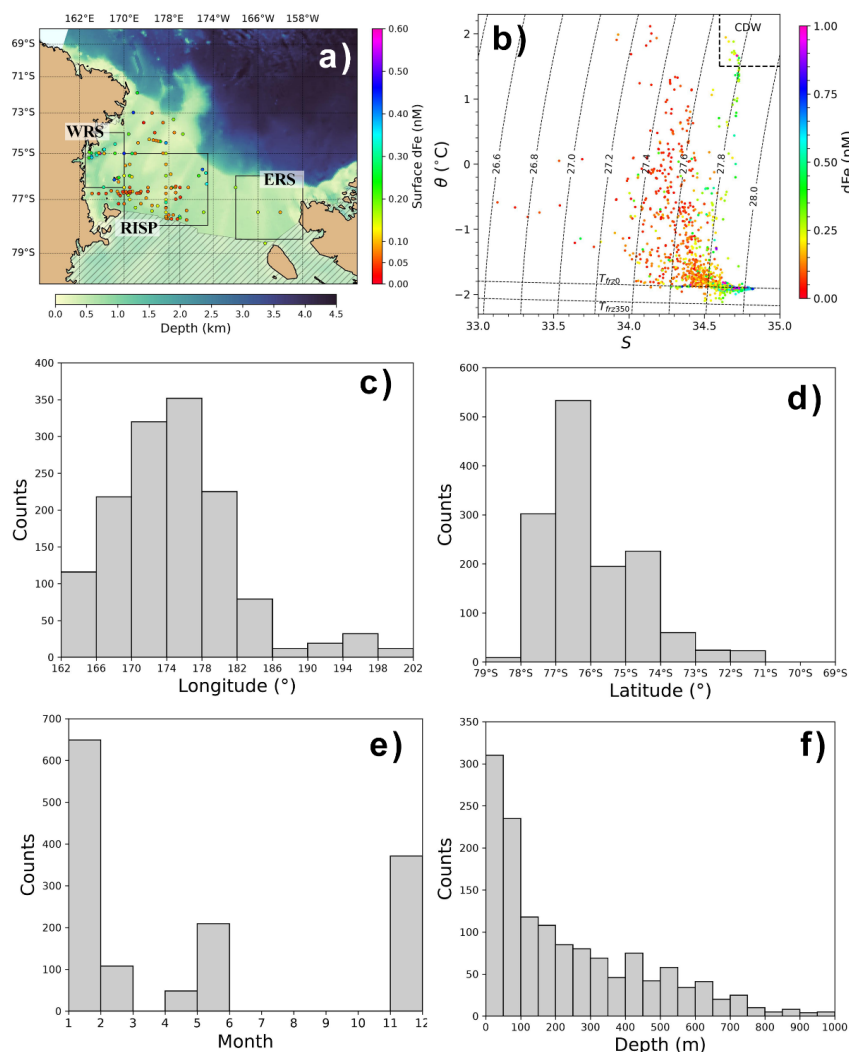
-
- 703 brasileiro, 17, 275-279. <https://doi.org/10.1590/1677-5449.174118>
- 704 Nuester, J., Shema, S., Vermont, A., Fields, D. M., & Twining, B. S. (2014). The regeneration
 705 of highly bioavailable iron by meso- and microzooplankton. *Limnology and oceanography*,
 706 59(4), 1399-1409. doi: 10.4319/lo.2014.59.4.1399.
- 707 Orsi, A. H., & Wiederwohl, C. L. (2009). A recount of Ross Sea waters. *Deep Sea Research*
 708 Part II: Topical Studies in Oceanography, 56(13-14), 778-795. 10.1016/j.dsr2.2008.10.033
- 709 Parkinson, C. L. (2019). A 40-y record reveals gradual Antarctic sea ice increases followed by
 710 decreases at rates far exceeding the rates seen in the Arctic. *Proceedings of the National*
 711 *Academy of Sciences*, 116(29), 14414-14423. <https://doi.org/10.1073/pnas.1906556116>
- 712 Porter, D. F., Springer, S. R., Padman, L., Fricker, H. A., Tinto, K. J., Riser, S. C., et al. (2019).
 713 Evolution of the seasonal surface mixed layer of the Ross Sea, Antarctica, observed with
 714 autonomous profiling floats. *Journal of Geophysical Research: Oceans*, 124, 4934–4953.
 715 <https://doi.org/10.1029/2018JC014683>
- 716 Salmon, E., Hofmann, E. E., Dinniman, M. S., & Smith Jr, W. O. (2020). Evaluation of iron
 717 sources in the Ross Sea. *Journal of Marine Systems*, 212, 103429.
 718 10.1016/j.jmarsys.2020.103429
- 719 Sedwick, P. N., Marsay, C. M., Sohst, B. M., Aguilar-Islas, A. M., Lohan, M. C., Long, M. C.,
 720 Arrigo K. R., Dunbar R. B., Saito M. A., Smith, W., & DiTullio, G. R. (2011). Early season
 721 depletion of dissolved iron in the Ross Sea polynya: Implications for iron dynamics on the
 722 Antarctic continental shelf. *Journal of Geophysical Research: Oceans*, 116(C12).
 723 <https://doi.org/10.1029/2010JC006553>
- 724 Sedwick, P. N., DiTullio, G. R., & Mackey, D. J. (2000). Iron and manganese in the Ross Sea,
 725 Antarctica: Seasonal iron limitation in Antarctic shelf waters. *Journal of Geophysical*
 726 *Research: Oceans*, 105(C5), 11321-11336. <https://doi.org/10.1029/2000JC000256>
- 727 Sedwick, P. N., Sohst, B. M., O'Hara, C., Stammerjohn, S. E., Loose, B., Dinniman, M. S., et
 728 al. (2022). Seasonal dynamics of dissolved iron on the Antarctic continental shelf: Late-
 729 fall observations from the Terra Nova Bay and Ross Ice Shelf polynyas. *Journal of*
 730 *Geophysical Research: Oceans*, 127, e2022JC018999.
 731 <https://doi.org/10.1029/2022JC018999>
- 732 Shapley L. S. (1953) A value for n-person games. *Contribution to the Theory of Games*. 1953;



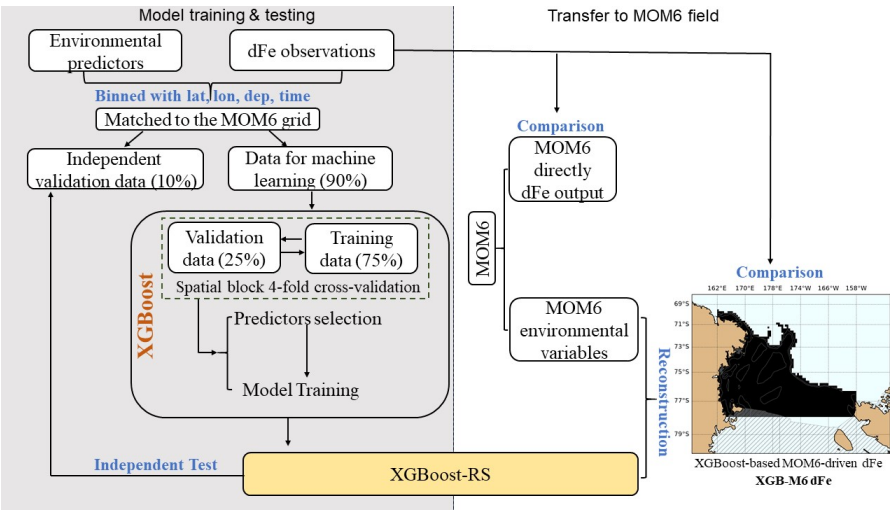
-
- 733 2: 307-318.
- 734 Smith Jr, W. O., Ainley, D. G., Arrigo, K. R., & Dinniman, M. S. (2014). The oceanography
 735 and ecology of the Ross Sea. *Annual Review of Marine Science*, 6(1), 469-487.
 736 <https://doi.org/10.1146/annurev-marine-010213-135114>
- 737 Smith Jr, W. O., & Kaufman, D. E. (2018). Climatological temporal and spatial distributions of
 738 nutrients and particulate matter in the Ross Sea. *Progress in Oceanography*, 168, 182-195.
 739 <https://doi.org/10.1016/j.poccean.2018.10.003>
- 740 Smith Jr, W. O., & Meyer, M.G. (2026). Marine plankton of open Antarctic Seas. In
 741 *Encyclopedia of the World's Biomes, Third Edition* (M.I. Goldstein, L. Suring and S.
 742 Breck, eds.). Elsevier, Amsterdam (in press).
- 743 Smith Jr, W. O., & Nelson, D. M. (1985). Phytoplankton bloom produced by a receding ice
 744 edge in the Ross Sea: Spatial coherence with the density field. *Science*, 227, 163–166.
 745 DOI: 10.1126/science.227.4683.163
- 746 Stock, A. (2025). Choosing blocks for spatial cross-validation: lessons from a marine remote
 747 sensing case study. *Frontiers in Remote Sensing*, 6, 1531097.
 748 <https://doi.org/10.3389/frsen.2025.1531097>
- 749 Stock, C. A., Dunne, J. P., Fan, S., Ginoux, P., John, J., Krasting, J. P., Laufkötter, C., Paulot,
 750 F., & Zadeh N., (2020). Ocean biogeochemistry in GFDL's Earth System Model 4.1 and
 751 its response to increasing atmospheric CO₂. *Journal of Advances in Modeling Earth*
 752 *Systems*, 12, e2019MS002043. <https://doi.org/10.1029/2019MS002043>
- 753 Su, H., Yang, X., Lu, W., & Yan, X.-H. (2019). Estimating subsurface thermohaline structure
 754 of the global ocean using surface remote sensing observations. *Remote Sensing*, 11(13),
 755 1598. <https://doi.org/10.3390/rs11131598>
- 756 Tagliabue, A., Aumont, O., DeAth, R., Dunne, J. P., Dutkiewicz, S., Galbraith, E., Misumi, K.,
 757 Moore, J. K., Ridgwell, A., Sherman, E., Stock C., Vichi, M., Völker, C., & Yool, A (2016),
 758 How well do global ocean biogeochemistry models simulate dissolved iron distributions?
 759 *Global Biogeochemical Cycles*, 30, 149–174, doi:10.1002/2015GB005289.
- 760 Tagliabue, A., Bowie, A. R., DeVries, T., Ellwood, M. J., Landing, W. M., Milne, A., ... & Boyd,
 761 P. W. (2019). The interplay between regeneration and scavenging fluxes drives ocean iron
 762 cycling. *Nature Communications*, 10(1), 4960. <https://doi.org/10.1038/s41467-019->



-
- 763 [12775-5](#)
- 764 Taylor, M. H., M. Losch, and A. Bracher (2013), On the drivers of phytoplankton blooms in the
- 765 Antarctic marginal ice zone: A modeling approach, *Journal of Geophysical Research:*
- 766 *Oceans*, 118, 63–75, doi:10.1029/2012JC008418.
- 767 Winton, V. H. L., Dunbar, G. B., Atkins, C. B., Bertler, N. A. N., Delmonte, B., Andersson, P.
- 768 S., Bowie, A., & Edwards, R (2016). The origin of lithogenic sediment in the south-
- 769 western Ross Sea and implications for iron fertilization. *Antarctic Science*, 28(4), 250–
- 770 260. doi:10.1017/S095410201600002X
- 771 Timmermans Klaas R., van der Wagt Bas, de Baar Hein J. W. (2004), Growth rates, half-
- 772 saturation constants, and silicate, nitrate, and phosphate depletion in relation to iron
- 773 availability of four large, open-ocean diatoms from the Southern Ocean, *Limnology and*
- 774 *Oceanography*, 6, doi: 10.4319/lo.2004.49.6.2141.
- 775 Wu, Z., Lu, W., Roobaert, A., Song, L., Yan, X. H., & Cai, W. J. (2025). A machine-learning
- 776 reconstruction of sea surface p CO₂ in the North American Atlantic coastal ocean margin
- 777 from 1993 to 2021. *Earth System Science Data*, 17(1), 43–63.
- 778 <https://doi.org/10.5281/zenodo.14038561>
- 779 Jiang, Z., Liao, E., Li, Z., & Zhang, R. (2025). Modeling the global ocean distribution of
- 780 dissolved cadmium based on machine learning—SHAP algorithm. *Science of the Total*
- 781 *Environment*, 958, 177951. <https://doi.org/10.1016/j.scitotenv.2024.177951>
- 782 Zhang, Y., Zhao, W., Wei, H., Yang, W., & Luo, X. (2023). Iron limitation and uneven grazing
- 783 pressure on phytoplankton co-lead the seasonal species succession in the Ross Ice Shelf
- 784 Polynya. *Journal of Geophysical Research: Oceans*, 128, e2022JC019026.
- 785 <https://doi.org/10.1029/2022JC019026>
- 786 Zhong, G., Li, X., Song, J., Qu, B., Wang, F., Wang, Y., Wang, Y., Zhang, B., Sun, X., Zhang,
- 787 W., Wang, Z., Ma, J., Yuan, H., & Duan, L. (2022). Reconstruction of global surface ocean
- 788 pCO₂ using region-specific predictors based on a stepwise FFNN regression algorithm.
- 789 *Biogeosciences*, 19(3), 845–859. <https://doi.org/10.5194/bg-19-845-2022>
- 790



1
 2 **Fig. 1.** Distribution of the dissolved iron on the Ross Sea continental shelf with respect to a) location,
 3 b) water mass, c) longitude, d) latitude, e) sampling month, and f) sampling depth. The boxes
 4 in a) indicate coastal region of western Ross Sea (WRS), central Ross Ice Shelf Polynya (RISIP),
 5 and eastern Ross Sea (ERS). In panel (b), the dashed box indicates the characteristic potential
 6 temperature-salinity range of Circumpolar Deep Water (CDW). The two dashed curves in the lower
 7 part of the panel represent the seawater freezing temperatures at pressures corresponding to 0 (T_{frz0})
 8 and 350 m (T_{frz350}), respectively.



9

10 **Fig. 2.** Workflow for the model construction, transfer and statistical analysis. The black area in the
11 map indicates the reconstructed area.

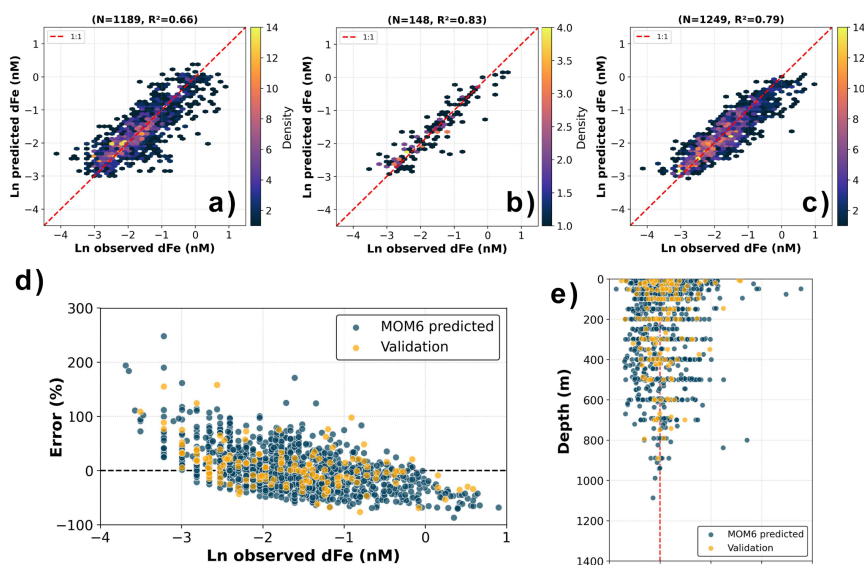


Fig. 3. Evaluation of the XGBoost model for dFe reconstruction in the Ross Sea. The density scatter plots compare the observational environmental parameters-driven reconstructed dFe with the in situ dFe during the a) block-based 4-fold validation during training phase, b) independent profiles validation and c) MOM6 output parameters-driven reconstructed dFe with in situ dFe; The model errors with d) dFe, and e) depth.

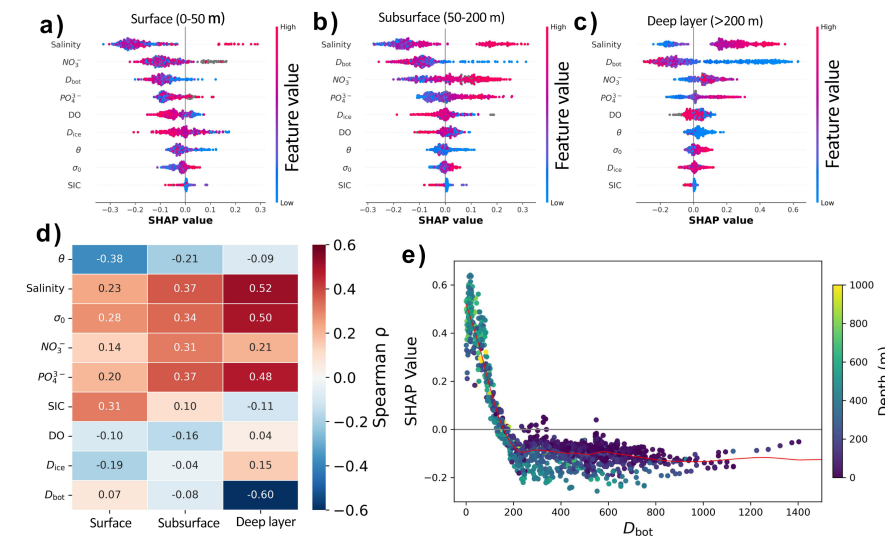


Fig. 4. Depth-dependent environmental associations with dissolved iron (dFe) and their contributions to the XGBoost reconstruction. a-c) SHAP summary plots for surface (0–50 m), mid-layer (50–200 m), and deep-water (>200 m) observations. Features are ranked within each depth layer according to their mean absolute SHAP values. Each point represents one observation; horizontal position indicates the SHAP contribution of a feature to the predicted $\ln(dFe)$, while color indicates the corresponding feature value from low (blue) to high (red). d) Depth-stratified Spearman rank correlations (ρ) between observed dFe and environmental variables. Positive and negative values indicate increasing and decreasing monotonic relationships with dFe, respectively. e) SHAP dependence plot between distance to bottom and dFe in cross-validation. The color bar represents sampling depth.

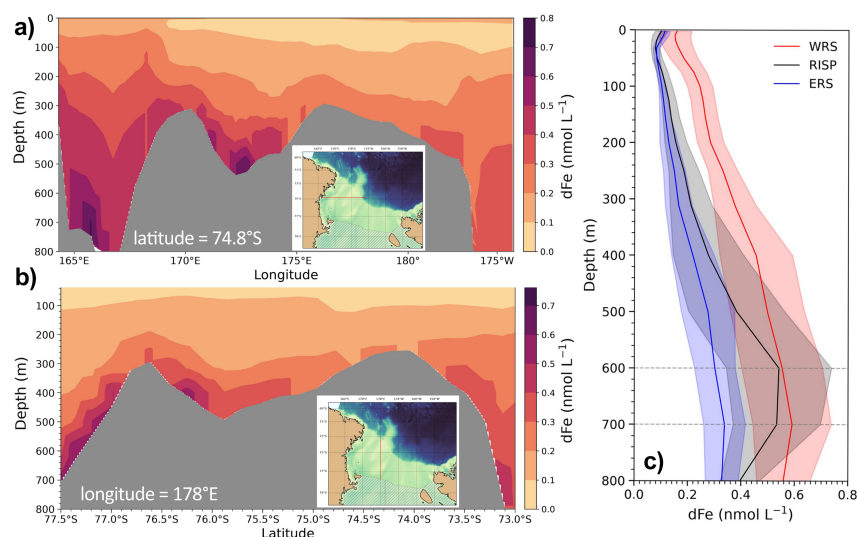


Fig. 5. Climatological (2005–2014) vertical distribution of dissolved iron (dFe) in the Ross Sea during the open water period (November–February). a) Zonal section along 74.8°S; b) meridional section along 178°E; and c) regional mean vertical dFe profiles for the western Ross Sea coastal region (WRS), central Ross Ice Shelf Polynya (RISP), and eastern Ross Sea (ERS). In panel c), solid lines and shading indicate the mean ± 1 standard deviation.

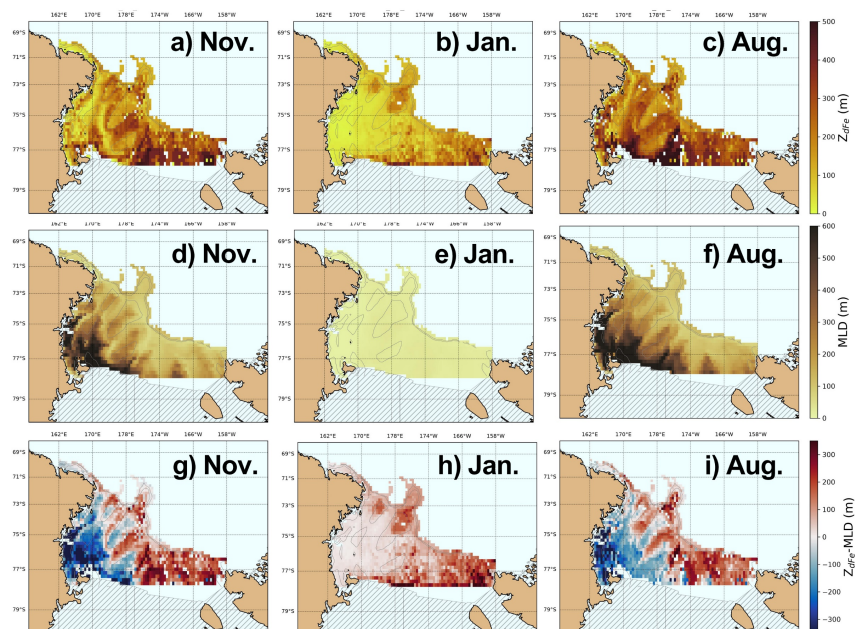


Fig. 6. The Climatological (2005–2014) distribution of a), b) and c) ferricline depth, d), e) and f) mixed layer depth, and g), h) and i) the difference between mixed layer depth (MLD) and ferricline depth in the Ross Sea in November (left), January (middle), and August (right).

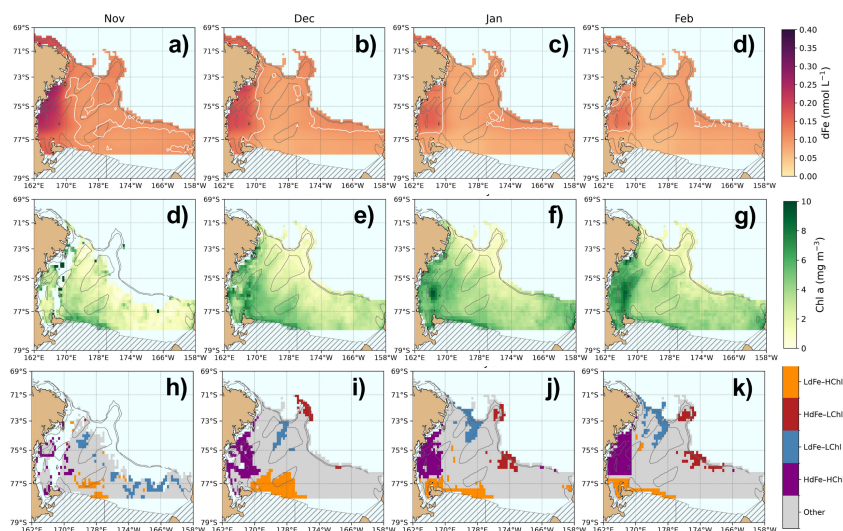


Fig. 7. Climatological (2005-2014) monthly spatial correspondence between a) though d) reconstructed dissolved iron (dFe) with gaussian smoothing; e) through g) chlorophyll a (Chl a) over the Ross Sea continental shelf during November February. For each month, panels show the 2005–2014 climatological mean values over the upper 50 m, with the 0.1 nM dFe isoline shown in white; h) through k) spatial combinations of extreme dFe and Chl a conditions from November to December (from left to right). High and low dFe and Chl a are defined independently as the upper and lower 25% of their respective area weighted spatial distributions. The four extreme combinations are high dFe-high Chl a (HdFe-HChl), low dFe-low Chl a (LdFe-LChl), high-dFe low Chl a (HdFe-LChl) and low dFe-high Chl a (LdFe-HChl). Gray cells in c) represent locations that do not fall within any of these four extreme combinations. Analyses are restricted to regions shallower than 1500 m.

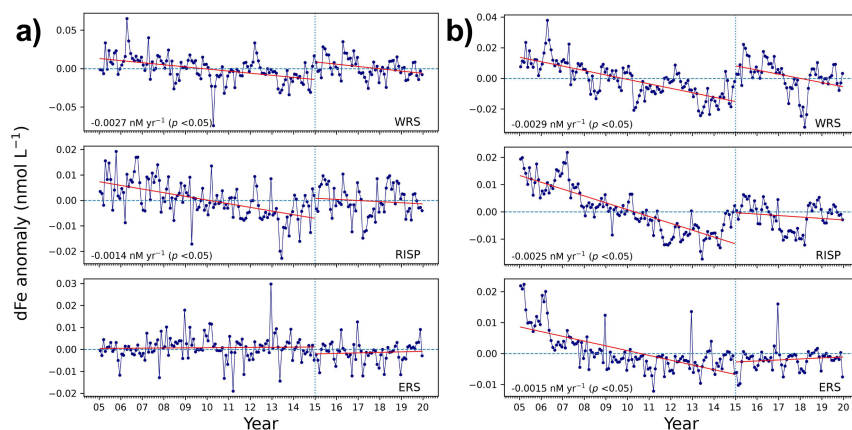


Fig. 8. Temporal changes of dFe anomalies at a) surface (0–50 m) and b) subsurface (50–200 m) in the western Ross Sea coastal region (WRS), central Ross Ice Shelf Polynya (RISP), and the eastern Ross Sea (ERS), with trends evaluated separately before and after 2014. Blue dots represent monthly area-averaged dFe anomalies, and red lines indicate linear trends. For statistically significant trends, the corresponding rates of change are shown in each region and panel.