

# Geophysical Research Letters

### Supporting Information for

# **Global analysis of surface ocean CO**<sub>2</sub> **fugacity and air-sea fluxes with low latency**

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### 1. Evaluation and analysis for surface ocean CO<sub>2</sub> fugacity and air-sea fluxes

# 1.1. Quality assessment for regional reconstruction and prediction of $CO_2$ fugacity ( $fCO_2$ )

In reconstruction mode (1985-2020), FFNNv2021 and FFNNv2 models perform with good skill over many ocean provinces (Figures 2, S3, and S5). Subtropical and tropical provinces (i.e., 3.NA-PS, 5.SA, 7.NP-PS, 8.PEQU-W, 10.SP, and 12.SIO) have the highest model skill among the ocean basins (RMSD < 14  $\mu$ atm and  $r^2$  > 0.74). Interestingly, these sub-basins are not dominant in data density compared to subpolar regions (2.NA-SS and 6.NP-SS) for the northern hemisphere and to the southern ocean (13.SO-SS) for the southern hemisphere (Figure 2). Data-rich provinces involve many observations distributed in coastal bands or in ocean upwelling systems with substantial fCO<sub>2</sub> inter-annual variations. These data put high weight on the calculated model-data mismatch (Figures S5 and S6). The model tends to get high biases from SOCAT data outliers (Figure S3), i.e., data beyond the 95% confidence interval ([279, 443] µatm) of the full data range. Overestimates of  $fCO_2$  with a model-data bias greater than 100 µatm are distributed along the Arctic (1.ARC) and the subpolar-polar regions (2.NA-SS, 6.NP-SS, and 14.SO-ICE) (Figure S3 and Figure S5). Most of the poor estimates of fCO<sub>2</sub> belong to the coastal sector of these regions (Figure S5) where  $fCO_2$  is characterized with high variability driven by multiple and complex physical and biological conditions (Feely et al., 2008; Bakker et al., 2016; Chavez et al., 2018; Chau et al., 2022). RMSD ranges from 21.1  $\mu$ atm to 40  $\mu$ atm and  $r^2$  is between 0.57 and 0.76 over these regimes. In contrast, the FFNN models underestimate SOCAT  $fCO_2$  at the right tail of its global distribution. Most of these data belong to the coastal sectors of NA-SS and NP-SS or are found in PEQU-E and NIO (see further analysis in Chau et al. (2022). Among these provinces, the eastern equatorial Pacific (9.PEQU-E) yields the largest RMSD (~27 µatm). Nevertheless, the reconstruction of the interannual variability of  $fCO_2$  over PEQU-E has an *r*<sup>2</sup> of 0.71.

Despite general good performance as analyzed in the main manuscript, FFNNv2021 shows the poorest one-year prediction in 2021 relative to the 1985-2020 reconstruction skill in ARC (RMSD: 49.1 µatm vs 40 µatm;  $r^2$ : 0.25 vs 0.57), in AEQU (RMSD: 34.2 µatm vs 19.96 µatm;  $r^2$ : 0.36 vs 0.57), and in PEQU-E (RMSD: 37.2 µatm vs 27 µatm;  $r^2$ : 0.55 vs 0.71). The FFNNv2022 model reconstruction in 2021 benefits from more than 919 additional data (411 data points in the year 2021), resulting in an improvement in the fCO2 estimates in 2021 over the Arctic: the RMSD reduces to 41.8 µatm and  $r^2$  rises up

to 0.35 (Figure S7). In 2022, the FFNNv2022 model scores slightly better in one-year prediction (RMSD = 37.0  $\mu$ atm and  $r^2$  = 0.60) relative to the FFNNv2021 two-year prediction (RMSD = 37.7  $\mu$ atm and  $r^2$  = 0.56). To a smaller extent, this improvement holds for the equatorial Atlantic (4.AEQU) and the eastern equatorial Pacific (9.PEQU-E). For instance, the FFNNv2021 prediction (RMSD = 34.2  $\mu$ atm and  $r^2$  = 0.36) in AEQU in 2021 shows similar skill scores compared to the FFNNv2022 reconstruction (RMSD = 32.9  $\mu$ atm and  $r^2$  = 0.43). By contrast, the two model predictions perform well in 2022 (RMSD < 17.5 µatm and  $r^2$  < 0.6), knowing that the evaluation data in SOCATv2023 in the years 2021 and 2022 do not have the same quantity and distribution over AEQU as well as other ocean provinces (Table S4 and Figure S5). For both reconstruction and prediction modes, the two time series of the mean  $fCO_2$  derived from the two models deviate in interannual variability of  $fCO_2$  in the equatorial Atlantic (Figure S6). Over the equatorial Pacific (9.PEQU-E), FFNNv2022 predicts fCO<sub>2</sub> in 2022 with a high deviation from SOCAT data (RMSD = 47.1  $\mu$ atm) but reproduces its temporal variations well ( $r^2$  = 0.76). FFNNv2021 makes the two-year prediction (RMSD = 45.1  $\mu$ atm and  $r^2$  = 0.77) marginally more precise than the latest model. The contradictory effects observed in the two FFNN performances over the tropical regions (4.AEQU and 9.PEQU-E) may derive from the discrepancy in SOCAT data used for model fits from one to another version; e.g., SOCATv2022 removed 234 [164] data from the previous version over AEQU [PEQU-E] for the period 1985-2020 (7% [2%] of the total data in this region) and added 116 [180] data for the year 2021 (Figures S2 and S7 and Table S4).

# 1.2. Computation of air-sea fluxes (fgCO<sub>2</sub>)

An air-sea flux density of  $CO_2$  is calculated in molC.m<sup>-2</sup>.yr<sup>-1</sup> by using the formulation as follows,

$$fgCO_2 = K \times dpCO_2 = k \times L \times (1 - f_{ice}) \times (pCO_2^{air} - pCO_2^{sea}),$$
(1)

where *K* is the gas transfer coefficient and  $dpCO_2$  is the air-sea difference in partial pressure of  $CO_2$  ( $pCO_2$ ). *K* is the product of gas transfer velocity (*k*), temperature-dependent solubility of  $CO_2$  (*L*), and sea ice coverage ratio ( $f_{ice}$ ). *L* is estimated with sea surface temperature (Weiss, 1974) while the computation of *k* replies on a quadratic dependence of 10-m wind speed (Ho et al., 2006; Wanninkhof., 2014) and a scaling to match the global mean *k* of 16.5 cm.h<sup>-1</sup> (Naegler, 2009). The derivation of atmospheric partial pressure of  $CO_2$  ( $pCO_2^{air}$ ) comes from  $CO_2$  mole fraction multiplied with total pressure in dry air conditions.  $pCO_2^{sea}$  is converted from FFNN *f*CO<sub>2</sub> following Körtzinger., (1999). Data products used in the air-sea flux

calculation are presented in Table S1. Given flux density per grid cell ( $fgCO_2^{(i)}$ ), an integration of CO<sub>2</sub> fluxes (PgC.yr<sup>-1</sup>) over a region or the global ocean derives from

$$fgCO_2 = \sum_{i=1:N} fgCO_2^{(i)} \times A^{(i)},$$
 (2)

where  $A^{(i)}$  is the area in  $m^2$  of grid cell (i).

### 1.3. Multi-year time series of fCO<sub>2</sub> and fgCO<sub>2</sub>

Figures S6 and S8 (right sector of the red vertical line) respectively show the time series of mean fCO<sub>2</sub> predicted with FFNNv2022 models and of fgCO<sub>2</sub> integrated over different provinces. fCO<sub>2</sub> predicted for 2022 continues to increase resulting in an increment of the global average of sea surface partial pressure of CO<sub>2</sub> (pCO<sub>2</sub><sup>sea</sup>) of 2.9 µatm relative to the year 2021 (Table S5) and much higher than its global growth rate of 1.7 µatm.yr<sup>-1</sup> (2.0 µatm.yr<sup>-1</sup>) estimated over the period 1985-2022 (2010s). The one-year increment in atmospheric  $pCO_2$  ( $pCO_2^{air}$ ) between the two years (2.5 µatm) is less than in  $pCO_2^{sea}$  implying a reduction in the global ocean uptake of  $CO_2$  predicted for 2022 (2.25±0.5 PgC.yr<sup>-1</sup>) compared to the previous year (2.36±0.43 PgC.yr<sup>-1</sup>). When adjusting the estimated global net fluxes with the riverine outgassing of CO<sub>2</sub> of 0.65 PgC.yr<sup>-1</sup> (Regnier et al., 2022) and the total ocean surface area (FFNNv2022 data covers 95% of the global ocean), one obtains the estimates of anthropogenic ocean carbon uptake about 3.13±0.46 PgC.yr<sup>-1</sup> and 3.02±0.52 PgC.yr<sup>-1</sup> in 2021 and 2022, respectively. The non-increasing imprint in the ocean sink of anthropogenic CO<sub>2</sub> found in this study is consistent with the 2022 projection proposed by Friedlingstein et al, (2022): the anthropogenic ocean sink in 2021 was 2.9±0.4 PgC.yr<sup>-1</sup> remains unchanged for the year 2022. This evidence supports the hypothesis that the persistence of cooling climate patterns (La Niña conditions) weakened CO<sub>2</sub> ocean uptake in 2021-2022 (high peaks appeared in mid-2022, Figure S9). For January to August in 2023, FFNNv2022 predicts a global net flux of 2.45±0.56 PgC.yr<sup>-1</sup> (w.r.s.t., 3.23±0.59 PgC.yr<sup>-1</sup> for anthropogenic uptake) higher than the 8-month net flux in 2022 of 2.17±0.50 PgC.yr<sup>-1</sup> (w.r.s.t., 2.94±0.53 PgC.yr<sup>-1</sup> for anthropogenic uptake).

# 1.4. Substantial intra- to inter-annual changes of $fCO_2$ and air-sea fluxes ( $fgCO_2$ ) at the eastern equatorial Pacific (EEP) driven by the El Niño Southern Oscillation (ENSO)

The ENSO phenomenon does not only constrain ocean  $CO_2$  outgassing at the tropical Pacific air-sea interface but also strongly affects the global net  $CO_2$  uptake (Rödenbeck et al., 2015; Chau et al., 2022; Friedlingstein et al., 2022). In El Niño conditions, warmer

surface temperature weakens vertical upwelling of subsurface water rich in dissolved inorganic carbon (DIC) and nutrients, therefore, El Niño leads to lower surface partial pressure of CO<sub>2</sub> (Feely et al., 2006; Wang et al., 2015). A decrease of fCO<sub>2</sub> reached 410  $\mu$ atm and the intra-annual variation of  $fCO_2$  was as large as 40  $\mu$ atm in the year 2015 (Figure S6) as the strongest El Niño events of the last decade happened (Figure S9a). The dampening  $fCO_2$  resulted in a reduction of the EEP source of  $CO_2$  and thus an enhancement in the global ocean CO<sub>2</sub> uptake (Figure S8). The net flux excessed -0.15±0.03 PgC.yr<sup>-1</sup> in 2015/2016 while the EEP normally released an average source of CO<sub>2</sub> of -0.31±0.02 PgC.yr<sup>-1</sup> in the last decade. The spatial pattern in Figure S9bc confirms that the El Niño events spreading until the 2016 summer probably reduced fCO<sub>2</sub> below 400  $\mu$ atm (fgCO<sub>2</sub> < -0.5 molC.m<sup>-2</sup>.yr<sup>-1</sup>) around 90°W and 150°W westward. Later in this period, the opposite conditions - La Niña - triggered in the 2017 summer became dominant and  $fCO_2$  was, for the first time, rising over 460 µatm in the 2018 spring. La Niña has turned back and governed since the year 2020 (Figure S9a). The cooling phase persisted in 2021 and reached its maximum in the 2022 spring-summer. Anomalies in  $fCO_2$  enhancement have been found throughout the year 2021 (Figure S9(b,c)). Likewise, FNNNv2022 correspondingly projects extremely high fCO<sub>2</sub> exceeding 484  $\mu$ atm (fgCO<sub>2</sub> < -2.5 molC.m<sup>-2</sup>.yr<sup>-1</sup>) in the eastern Niño3 and Niño4 sectors in the first half of 2022. By then, a reduction of  $fCO_2$  is predicted according to the lessening cooling conditions.

### 2. Tables

Variables	Notati	Product name	References
	on		
Measureme	fCO <sub>2</sub>	Surface ocean CO2 ATlas (SOCAT):	Bakker et al. (2021,
fugacity fugacity		SOCATV2021, SOCATV2022 (last access 17/06/2022), and SOCATV2023 (last access 20/06/2023)	2022, 2023)
Sea surface	SST	Copernicus Marine Service (CMEMS):	Good et al. (2020)
temperatur e		<u>SST GLO SST L4 REP OBSERVATIONS 010 011</u> (1985-2021)	
Sea ice	$f_{\sf ice}$	SST_GLO_SST_L4_NRT_OBSERVATIONS_010_001	
Sea surface salinity	SSS	CMEMS: MULTIOBS GLO PHY S SURFACE MYNRT 015 013 (1993-2023)	Buongiorno et al. (2016); Droghei et al. (2018)
Sea surface height	SSH	CMEMS: <u>SEALEVEL_GLO_PHY_L4_MY_008_047</u> (1993-2021) <u>SEALEVEL_GLO_PHY_L4_NRT_OBSERVATIONS_008_046</u> (2022-2023)	Pujol et al. (2016, 2018)

Table S1. Input datasets used for reconstructions and prediction of surface ocean  $CO_2$  fugacity ( $fCO_2$ ) and air-sea fluxes ( $fgCO_2$ ) in 1985-2023.

Mixed layer	MLD	Estimating the Circulation and Climate of the Ocean project Phase II (ECCO2):	Menemenlis et al.			
depth		<u>cube92_latlon_quart_90S90N</u> (1992-2022)	(2008)			
Chlorophyll-	Chl-a	CMEMS:	Garnesson et al .			
a		<u>OCEANCOLOUR GLO BGC L4 MY 009 104</u> (1998-2023)	(2019)			
Atmospheri c CO <sub>2</sub> mole fraction	xCO <sub>2</sub>	CO <sub>2</sub> atmospheric inversion from the Copernicus Atmosphere Monitoring Service (CAMS): Surface: <u>v20r2</u> (1985-2020) Satellite: FT21r2 (2021)	Chevallier et al. (2005, 2010); Chevallier. (2013)			
<i>p</i> CO <sub>2</sub>	pCO2 <sup>cli</sup>	Lamont Doherty Earth Observatory (LDEO) climatology of sea surface partial pressure of $CO_2$	Takahashi et al.			
climatology	m		(2009)			
Wind speed	U	FRA5 hourly data on single levels from 1959 to present	Hersbach et al			
Total pressure	Ps	(1985-2023)	(2020)			

Notes:

- Preprocessing for missing data in the reconstruction mode (before the 2000s):
  - SSS and CHL-*a* (MLD) are set to climatologies computed on the available data (in 1992-1997).
  - SSH is set to climatologies plus linear trends computed on the available data
- Preprocessing for missing data in the prediction mode (2022-2023):

Input datasets for prediction are set to the same data resources as for reconstruction, these data are available within a few weeks behind real time. This condition is not met for the  $xCO_2$  and MLD datasets that we use in 2023. For  $xCO_2$ , we extrapolated the original dataset (the atmospheric inversion of the Copernicus Atmosphere Monitoring Service for years 1985- 2022, Table S1), knowing the recent measurements of the atmospheric  $CO_2$  mole fraction at the Mauna Loa Observatory, Hawaii (https://gml.noaa.gov/ccgg/trends/mlo.html, last access: 11/9/2023). For MLD, given the dominance of seasonality in its variability (Menemenlis et al. 2008, Zhang et al. 2018), we use the last 5-year climatology of the Estimating the Circulation and Climate of the Ocean project Phase II (ECCO2) data in the prediction mode.

### Table S2. Indicators of ocean provinces (Figure S1) used in this study.

No	Ocean provinces	Remarks
0	Global ocean (GLO)	

1	Arctic (ARC)	Aggregated from Arctic, North Atlantic, and North Pacific ice biomes and the Barents Sea (biomes 1, 2, 3, and 4)
2	North Atlantic seasonally stratified (NA-SS)	Aggregated from North Atlantic subpolar and subtropical seasonally stratified biomes (biomes 5 and 6)
3	North Atlantic permanently stratified (NA-PS)	North Atlantic subtropical permanently stratified biome (biome 7)
4	Atlantic equatorial (AEQU)	Biome 8
5	South Atlantic (SA)	South Atlantic subtropical permanently stratified biome (biome 9)
6	North Pacific seasonally stratified (NP-SS)	Aggregated from North Pacific subpolar and subtropical seasonally stratified biomes (biomes 11 and 12)
7	North Pacific permanently stratified (NP-PS)	North Pacific subtropical permanently stratified biome (biome 13)
8	Pacific western equatorial (PEQU-W)	Biome 14
9	Pacific eastern equatorial (PEQU-E)	Biome 15
10	South Pacific (SP)	South Pacific subtropical permanently stratified biome (Biome 16)
11	Northern Indian Ocean (NIO)	Aggregated from the Arabian Sea, Bay of Bengal, and Equatorial Indian Ocean above the Equator (biomes 17, 18, and 19)
12	Southern Indian Ocean (SIO)	Aggregated from the Equatorial Indian Ocean blow the Equator and the South Indian Ocean (biomes 19 and 20)
13	Southern Ocean seasonally stratified (SO-SS)	Aggregated from Southern Ocean subpolar and subtropical seasonally stratified biomes (biomes 21 and 22)
14	Southern Ocean icea (SO-ICE)	Biome 23

# Table S3. Comparison of CMEMS-LSCE-FFNN models (FFNNv2021 and FFNNv2022)

u) 5u			used for	inouci i uns un	amouc	evaluati	VII			
	Mod	el fitting		Model evaluation						
FFNN	Target Data	Time	Number	Target Data	Recons	struction	Prediction			
		span	ordata		Time span	Number of data	Time span	Number of data		

### a) Summary of SOCAT data used for model runs and model evaluation

v2021	SOCATv2021	1985- 2020	306357	COCAT-2022	1985- 2020	302255	2021- 2022	10908 8602
v2022	SOCATv2022	1985- 2021	311694	SUCATV2023	1985- 2021	313163	2022	8602

b) Model evaluation between global reconstructions of fCO<sub>2</sub> [µatm] in 1985-2020 and between FFNNv2021 prediction and FFNNv2022 reconstruction (prediction) in 2021 (2022). Statistics include the number of SOCAT monthly gridded data (N), mean fCO<sub>2</sub> (µ), mean uncertainty (*c*), and model-data misfit (RMSD) and coefficient of determination (*r*<sup>2</sup>).

		Years													
FFNN		1985	-2020			20	21		2022						
	μ	σ	RMSD	r <sup>2</sup>	μ	σ	RMSD	r <sup>2</sup>	μ	σ	RMSD	r²			
v2021	361.6	8.7	19.1	0.78	395.2	11.4	24.3	0.74	397.8	12.2	23.1	0.75			
v2022	361.5	8.5	19.1	0.78	395.7	10.9	23.3	0.76	398.5	11.3	22.6	0.76			

Table S4. Regional comparison (a) between FFNN model reconstructions of  $fCO_2$  [µatm] in 1985-2020, (b) between FFNNv2021 prediction and FFNNv2022 reconstruction in 2021, and (c) between FFNN model predictions in 2022. Statistics include 1) the number (N) of monthly gridded data used in FFNN fits (SOCATv2021 and SOCATv2022) and in data evaluation (SOCATv2023, see values in brackets), 2) mean  $fCO_2$  (µ), 3) mean uncertainty ( $\sigma$ ), and 4) model-data misfit (RMSD), and 5) determination coefficient ( $r^2$ ).

Ν	Biome			Years													
0			1985-2020					2021				2022					
		FFNN	N	μ	σ	RM SD	r <sup>2</sup>	N	μ	σ	RM SD	r²	Ν	μ	σ	RM SD	r²
1	ARC	v2021	5043 (5646)	320.5	30.0	40.0	0.57	0 (411)	356.3	31.3	49.1	0.25	0 (225)	351. 4	29.6	37.7	0.56
		v2022	5551 (5646)	318.0	29.3	40.0	0.57	411 (411)	348.5	29.5	41.8	0.35	0 (225)	345. 6	27.5	37.0	0.60
2	NA-SS	v2021	57808 (55738)	339.8	8.0	23.1	0.76	0 (2350)	368.8	9.0	26.0	0.76	0 (2265)	373. 6	10.1	24.6	0.74

	-			-							-		-				
		v2022	55714 (55738)	339.9	7.7	23.1	0.76	2167 (2350)	369.1	8.3	26.2	0.75	0 (2265)	374. 8	9.1	24.0	0.75
3	NA-PS	v2021	37951 (37011)	364.5	5.3	13.9	0.74	0 (1161)	398.4	6.3	20.4	0.50	0 (1007)	401. 0	7.0	18.2	0.61
		v2022	36991 (37011)	364.5	5.1	13.8	0.75	945 (1161)	399.3	5.9	20.1	0.51	0 (1007)	402. 7	6.5	17.0	0.65
4	AEQU	v2021	3313 (3179)	376.9	10.0	20.0	0.57	0 (182)	400.2	12.8	34.2	0.36	0 (144)	403. 1	14.2	17.3	0.64
		v2022	3179 (3179)	376.0	10.0	19.9	0.57	116 (182)	400.5	13.2	32.9	0.43	0 (144)	404. 2	13.6	16.7	0.65
5	SA	v2021	6575 (6497)	369.6	7.9	13.2	0.79	0 (273)	398.5	9.5	14.3	0.55	0 (161)	401. 1	10.2	12.8	0.51
		v2022	6497 (6497)	369.7	7.6	12.9	0.80	212 (273)	401.9	9.2	12.4	0.59	0 (161)	404. 3	9.6	12.0	0.55
6	NP-SS	v2021	57531 (58165)	349.1	8.2	21.1	0.73	0 (2334)	378.9	10.1	28.3	0.76	0 (1495)	383. 1	11.1	31.0	0.62
		v2022	58161 (58165)	349.5	8.0	21.0	0.74	2147 (2334)	380.8	9.4	27.4	0.77	0 (1495)	385. 9	10.2	30.2	0.64
7	NP-PS	v2021	40176 (40300)	360.7	5.3	11.9	0.85	0 (1705)	397.0	7.1	16.4	0.76	0 (1608)	401. 3	8.4	13.2	0.78
		v2022	40287 (40300)	360.6	5.1	11.8	0.85	1443 (1705)	397.1	6.5	16.1	0.77	0 (1608)	401. 5	7.3	12.4	0.81
8	PEQU-W	v2021	14845 (14821)	366.6	6.1	11.2	0.72	0 (484)	407.2	9.2	11.2	0.76	0 (326)	411. 6	10.7	12.0	0.73
		v2022	14821 (14821)	366.6	6.0	11.2	0.72	430 (484)	407.8	8.2	11.1	0.74	0 (326)	411. 8	9.1	10.9	0.78
9	PEQU-E	v2021	9470 (9306)	415.7	9.9	27.0	0.71	0 (199)	460.0	14.4	37.2	0.55	0 (146)	462. 4	15.7	45.0	0.77
		v2022	9306 (9306)	415.5	9.7	26.9	0.71	180 (199)	459.8 9	13.1	35.2	0.59	0 (146)	461. 9	13.8	47.1	0.76
10	SP	v2021	21551 (20968)	363.1	9.0	11.9	0.86	0 (689)	398.4	11.9	10.2	0.85	0 (592)	399. 8	12.6	10.1	0.80
		v2022	20968 (20968)	363.5	8.8	11.8	0.87	605 (689)	399.3	11.3	9.8	0.86	0 (592)	400. 5	11.5	10.0	0.80
11	NIO	v2021	1335 (1335)	382.8	15.0	24.0	0.53	0 (0)	418.3	23.6	nan	nan	0 (0)	419. 8	24.4	nan	nan
		v2022	1335 (1335)	382.1	14.7	23.9	0.54	0 (0)	416.8	23.7	nan	nan	0 (0)	419. 7	23.4	nan	nan
12	SIO	v2021	4583 (4562)	357.2	9.3	10.8	0.88	0 (133)	392.6	14.1	11.2	0.80	0 (73)	394. 1	14.8	8.8	0.43
		v2022	4562 (4562)	356.7	9.0	10.8	0.88	133 (133)	392.8	13.8	12.0	0.81	0 (73)	394. 2	13.6	9.3	0.45

Table S5. Area-integrated air-sea  $CO_2$  fluxes ( $fgCO_2$ ) derived from FFNNv2022  $fCO_2$  reconstruction in 1985-2021 and from FFNNv2022 predictions in 2022-2023. The units of  $fgCO_2$  are in PgC.yr<sup>-1</sup>. Area-averaged surface temperature (SST), 10-m wind speed (U), sea surface partial pressure of  $CO_2$  ( $pCO_2^{sea}$ ), air-sea  $pCO_2$  difference ( $dpCO_2$ ), and gas transfer coefficient (K) are provided for the global ocean and each ocean province (see province indicator in Figure S1).

No	Biome					١	/ariables		
		<b>Area</b> [10 <sup>6</sup> km <sup>2</sup> ]	Years	<b>SST</b> [°C]	<b>U</b> [ms <sup>-1</sup> ]	<b>pCO<sub>2</sub>sea</b> [µatm]	<b>dpCO₂</b> [µatm]	<b>K</b> [molC.m <sup>-2</sup> .y r <sup>-1</sup> .µatm <sup>-1</sup> ]	<b>fgCO</b> <sub>2</sub> [PgC.yr <sup>-1</sup> ]
0	GLO	343.3	1985-2020	18.8	7.8	362.8±10.5	2.8	0.0526	1.583±0.341
			2021	19.0	7.9	397.1±13.0	6.0	0.0524	2.355±0.434
			2022	19.2	7.9	400.0±13.0	5.7	0.0528	2.249±0.495
			2023/01-08	19.1	7.8	401.5±14.1	7.0	0.0519	2.449±0.557
1	ARC	6.9	1985-2020	-0.5	7.3	324.9±33.3	50.3	0.0228	0.082±0.017
			2021	-0.1	7.5	355.5±34.2	55.9	0.026	0.107±0.020
			2022	-0.1	7.5	356.4±32.6	60.0	0.0281	0.106±0.017
			2023/01-08	-0.5	6.5	366.0±39.9	53.8	0.0137	0.077±0.015
2	NA-SS	15.9	1985-2020	11.8	9.2	341.2±9.5	30.4	0.0733	0.384±0.041
			2021	12.3	9.4	370.4±9.8	38.6	0.0750	0.503±0.045
			2022	12.5	9.3	376.1±10.4	37.0	0.0731	0.475±0.048
			2023/01-08	12.0	9.0	376.2±11.2	39.4	0.0697	0.467±0.052

3	NA-PS	22.2	1985-2020	25.1	7.0	365.7±5.9	0.8	0.0397	0.042±0.025
			2021	25.4	7.0	400.6±6.6	3.1	0.0389	0.064±0.027
			2022	25.4	6.9	403.6±7.0	3.5	0.0383	0.073±0.031
			2023/01-08	25.4	6.8	404.2±7.7	5.8	0.037	0.092±0.034
4	AEQU	8.5	1985-2020	26.9	5.5	377.2±12.5	-14.2	0.0254	-0.040±0.010
			2021	27.4	5.5	401.8±15.5	-1.9	0.0251	-0.009±0.017
			2022	27.2	5.5	405.9±15.5	-3.5	0.0245	-0.012±0.016
			2023/01-08	27.6	5.4	404.0±17.1	0.6	0.0241	-0.002±0.018
5	SA	19.5	1985-2020	22.6	7.2	371.0±8.5	-5.2	0.0419	-0.012±0.033
			2021	22.8	7.3	403.2±10.1	0.5	0.0423	0.049±0.048
			2022	22.8	7.2	405.6±10.6	-0.4	0.0406	0.036±0.047
			2023/01-08	23.5	7.1	411.0±11.8	-2.9	0.0405	0.024±0.059
6	NP-SS	24.7	1985-2020	12.7	8.7	350.8±10.2	21.4	0.0651	0.393±0.056
			2021	13.3	8.5	382.2±11.8	27.6	0.0618	0.476±0.060
			2022	13.6	8.6	387.6±12.0	26.4	0.0632	0.477±0.073
			2023/01-08	12.6	8.3	389.1±13.0	27.8	0.0589	0.436±0.078
7	NP-PS	40.2	1985-2020	26.3	7.0	361.7±6.1	2.9	0.0404	0.130±0.040
			2021	26.4	6.9	398.4±7.6	3.7	0.0388	0.152±0.053
			2022	26.5	6.8	402.8±8.2	2.5	0.0373	0.126±0.052
			2023/01-08	26.1	7.1	403.4±8.6	5.1	0.0412	0.176±0.069
8	PEQU-W	13.1	1985-2020	29.3	5.1	367.7±7.6	-7.9	0.0220	-0.023±0.010
			2021	29.4	5.2	409.0±9.4	-12.4	0.0222	-0.040±0.013
			2022	29.3	5.4	413.3±10.0	-14.0	0.0236	-0.052±0.016
			2023/01-08	29.5	5.2	412.1±10.7	-10.2	0.0227	-0.036±0.016
9	PEQU-E	15.1	1985-2020	26.3	5.9	416.8±10.8	-54.0	0.0292	-0.294±0.023
			2021	25.9	6.3	461.3±14.2	-60.8	0.0314	-0.350±0.030
			2022	25.6	6.4	463.5±15.0	-60.4	0.0328	-0.370±0.037

			2023/01-08	27.5	5.8	460.2±15.0	-55.7	0.0277	-0.297±0.036
10	SP	54.8	1985-2020	22.0	7.5	364.7±9.9	0.1	0.0470	0.103±0.117
			2021	22.1	7.6	400.6±12.4	2.6	0.0468	0.161±0.146
			2022	22.0	7.6	401.9±12.5	3.3	0.0464	0.166±0.146
			2023/01-08	22.8	7.5	405.0±13.3	2.2	0.0463	0.201±0.168
11	ΝΙΟ	11.4	1985-2020	28.2	6.0	383.3±17.0	-21.7	0.0317	-0.113±0.042
			2021	28.5	6.0	418.1±25.8	-19.8	0.0305	-0.099±0.077
			2022	28.4	6.0	421.1±25.2	-20.1	0.0311	-0.104±0.075
			2023/01-08	28.6	6.0	421.3±23.8	-17.4	0.0324	-0.096±0.076
12	SIO	32.9	1985-2020	24.8	7.1	357.8±9.6	5.8	0.0421	0.187±0.064
			2021	25.0	7.2	394.0±14.8	7.1	0.0422	0.216±0.114
			2022	24.9	7.2	395.4±14.5	7.6	0.0423	0.223±0.119
			2023/01-08	25.3	7.1	397.9±13.8	8.1	0.0414	0.222±0.109
13	SO-SS	59.6	1985-2020	8.0	10.5	353.0±9.4	13.3	0.0951	0.721±0.185
			2021	8.2	10.7	386.2±11.6	18.0	0.0956	1.006±0.232
			2022	8.2	10.7	388.4±12.1	17.8	0.0955	0.980±0.269
			2023/01-08	8.7	10.6	391.7±13.4	17.8	0.0950	1.006±0.314
14	SO-ICE	17.3	1985-2020	-1.1	9.1	366.1±11.9	-5.0	0.0421	0.022±0.040
			2021	-1.0	9.1	392.3±14.0	5.2	0.0423	0.119±0.042
			2022	-1.0	9.5	394.4±14.6	4.7	0.0525	0.122±0.054
			2023/01-08	-0.7	9.4	392.3±14.7	11.1	0.0575	0.175±0.073

# 3. Figures



Figure S1. Ocean provinces aggregated from the biomes used in the RECCAP2 project (source: https://github.com/RECCAP2-ocean/RECCAP2-shared-resources/tree/master/data

/regions, last access: 20/3/2023). See Table S2 for the province indicator.



Figure S2. Number of  $fCO_2$  data ( $\Delta N$ ) added in (red) or removed from (blue) SOCATv2022 compared to SOCATv2021 for different time frames.



**Figure S3.** Scatter plots of FFNNv2022 versus SOCATv2023  $fCO_2$  [µatm] for 36-year reconstruction (1985-2020: points), 1-year reconstruction (2021: stars) and 1-year prediction (2022: pluses). Values of FFNNv2022 and SOCATv2023 data are shown in y- and x-axis, respectively. Light-grey rectangles mark the 95% SOCAT data range (i.e., [279, 443] µatm) over the global ocean in 1985-2021. Red lines represent the bisector corresponding to ideal model-data fits: objects above this line indicate FFNN overestimates of SOCAT  $fCO_2$  and vice versa. Metrics for reconstruction and prediction in the legend are model-data standard deviation (D: RMSD) and correlation (C:  $r^2$ ).



**Figure S4.** Spatial distribution of temporal means of  $fCO_2$  [µatm] derived from FFNNv2021 (left) and FFNNv2022 (middle) and their discrepancy (right).



Figure S5. Spatial distribution of model-data deviation (RMSD) in  $\mu$ atm:  $fCO_2$  derived from FFNNv2021 (left) and FFNNv2022 (middle) and their RMSD difference (right). SOCATv2023 is used for this evaluation.



Figure S6. Time series of  $fCO_2$  [µatm] averaged over ocean provinces. Vertical dashed lines mark the starting date for model prediction (blue: FFNNv2021, red: FFNNv2022).



Figure S7. Time series of differences in  $fCO_2$  [µatm] (left y-axis) and number of SOCAT data (right y-axis). Vertical dashed line marks the starting date for prediction (FFNNv2021: blue, FFNNv2022: red).



**Figure S8.** Time series of monthly air-sea fluxes integrated over ocean provinces [PgC.yr<sup>-1</sup>]. Plain curve and shaded area represent model's best estimate and 1σ-uncertainty. Vertical dashed lines mark the starting date for FFNNv2022 prediction.



Figure S9. Illustration of the relationship between ENSO events (a) and FFNNv2022  $fCO_2$  (air-sea fluxes) variations (Hovmöller plots in b and c) over the eastern Equatorial Pacific (9.PEQU-E). ENSO events are plotted with the NOAA bi-monthly Multivariate El Niño/Southern Oscillation (ENSO) index (https://psl.noa35.5, 50.5a.gov/enso/mei/, last access: 11/09/2023). The black horizontal dotted line marks the starting date for the FFNNv2022 prediction (January 2022).



Figure S10. Anomalies of surface temperature (SST), salinity (SSS), Chlorophyll-*a* (CHL-*a*), air-sea  $pCO_2$  difference  $(dpCO_2)$ , gas transfer coefficient (K) over the Atlantic in June 2023 (top) and June 2022 (bottom) are computed by subtracting long-term trends and seasonal climatologies relative to the years 1985-2022. Blue box limits the region of interest where the extreme marine heat wave appeared in the northeastern Atlantic in June 2023.

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