Supplement of Biogeosciences, 18, 5447–5463, 2021
https://doi.org/10.5194/bg-18-5447-2021-supplement

Biogeosciences
Open Access

Supplement of

Modeling the marine chromium cycle: new constraints on global-scale processes

Frerk Pöppelmeier et al.

Correspondence to: Frerk Pöppelmeier (frerk.poeppelmeier@climate.unibe.ch)

Table S1: Parameter space varied for the tuning with the Latin hyper cube approach.

Tuning parameter	Minimum	Maximum
Benthic flux (F_{bs}) (nmol cm^{-2} yr^{-1})	0	1.2
Oxidation rate (r_{oxi}) (yr^{-1})	0.002	0.015
OMZ reduction rate (r_{OMZ}) (nmol m^{-3} yr^{-1})	0.2	10
$K_{d,ref}$(Cr(III))	5.0×10^{4}	1.0×10^{6}
$K_{d,ref}$(Cr(VI))	5.0×10^{2}	1.0×10^{4}

Table S2: Scavenging parameters for the control run, which are multiplied by the reference scavenging parameters of 2.31×10^{5} and 8.4×10^{2}, for Cr(III) and Cr(VI), respectively.

Particle type	K_d (Cr(III))	K_d (Cr(VI))
POM	1	5
$CaCO_3$	1	5
Biogenic opal	1	5
Lithogenics	0.5	10

Table S3: Model-data agreement determined by two the different cost functions of the Mean Absolute Error (MAE) and the Root Mean Squared Error (RMSE) (n = 701).

Run	MAE (nmol kg^{-1})	RMSE (nmol kg^{-1})
CTRL	0.48	0.66
NoArcticBFlux	0.44	0.59
OMZrem	0.45	0.60
OMZrem20	0.45	0.59
OMZrem30	0.45	0.59

Text S1: Data compilation

Model outputs were assessed by comparison to a compilation of all known oceanic Cr data in peer review publications and theses. However, not all literature data for Cr (and other contamination-prone trace metals) are likely to be free of analytical artefacts, including contamination during sampling and handling. Indeed, this has been a significant limitation throughout the history of trace metal oceanographic studies. With the development of clean sampling techniques and the publication of the first coherent metal data (e.g. Boyle, et al., 1977; Bruland et al., 1978), the initial criteria developed for quality control were based on "oceanographic consistency":

> "A priori arguments on the extent of precautions in sampling and analysis are not in themselves sufficient nor is the fact that the numbers are lower than previously reported. The primary criteria must be interlaboratory agreement [6,7] and the oceanographic consistency of the data themselves; detailed profiles should show smooth variations related to the hydrographic and chemical features displayed by conventionally measured properties. Regional variations should be compatible with what is known of the large-scale physical and chemical circulation of the oceans." (Boyle et al. 1977)

These criteria assess data validity based on other oceanographic parameters (salinity, temperature, distributions of better-studied parameters such as nutrients) and processes controlling elemental distribution (e.g. biological cycling, circulation, atmospheric deposition). It should be stressed that these criteria do not indicate that the processes governing trace metal distributions are fully understood nor preclude the discovery of new processes controlling metal distributions (cf. Bruland, 1980), nor do they invalidate data outright; however, the criteria maintain that erratic profiles with no correlation to any other oceanographic parameters should be treated as suspect until confirmed through replicate analysis and interlaboratory agreement. This latter point has been a topic of substantial subsequent developments for trace metal research. Reference materials established through collaborative efforts (e.g. SAFe standards, Johnson et al., 2007; the GEOTRACES program, Schlitzer et al., 2018) have greatly improved quality control standards. Unfortunately, adoption of these materials is not uniform across analytes, and intercalibration and standardization for Cr has lagged behind that of other transition metals, though recent developments suggest this is changing.

Any compilation of literature data should apply modern quality control measures, including re-assessments of oceanographic consistency based on new data and understandings of the oceanic Cr cycle, especially for studies where reference materials were not available or were not analyzed. Following the principles outlined above, in order to ensure a meaningful comparison between the body of literature data and our model results, quality controls were applied to the data compilation. The basis of these controls were the oceanographic consistency of data as well as discussions in subsequent studies highlighting which datasets are unlikely to reflect natural processes for known and unknown reasons (e.g. see discussions in Isshiki et al., 1989; Goring-Harford et al., 2018; Rickli et al., 2019; Moos et al., 2020; Nasemann et al., 2020; Huang et al., 2021; Janssen et al., 2021). In addition, data that pass the above criteria but with high analytical uncertainty were omitted. Finally, due to the intermediate resolution of the model, coastal data that might be controlled by processed not resolved by the model were excluded from the compilation.

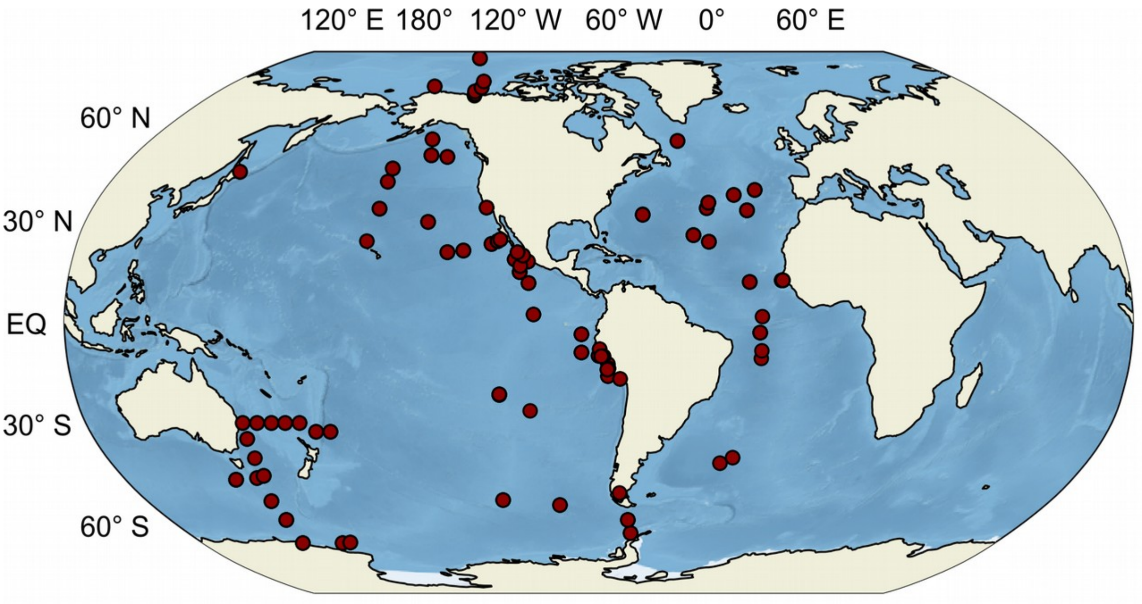

Figure S1: World map with locations of all seawater stations of the data compilation indicated as red circles. For details please Supplementary Data 2.

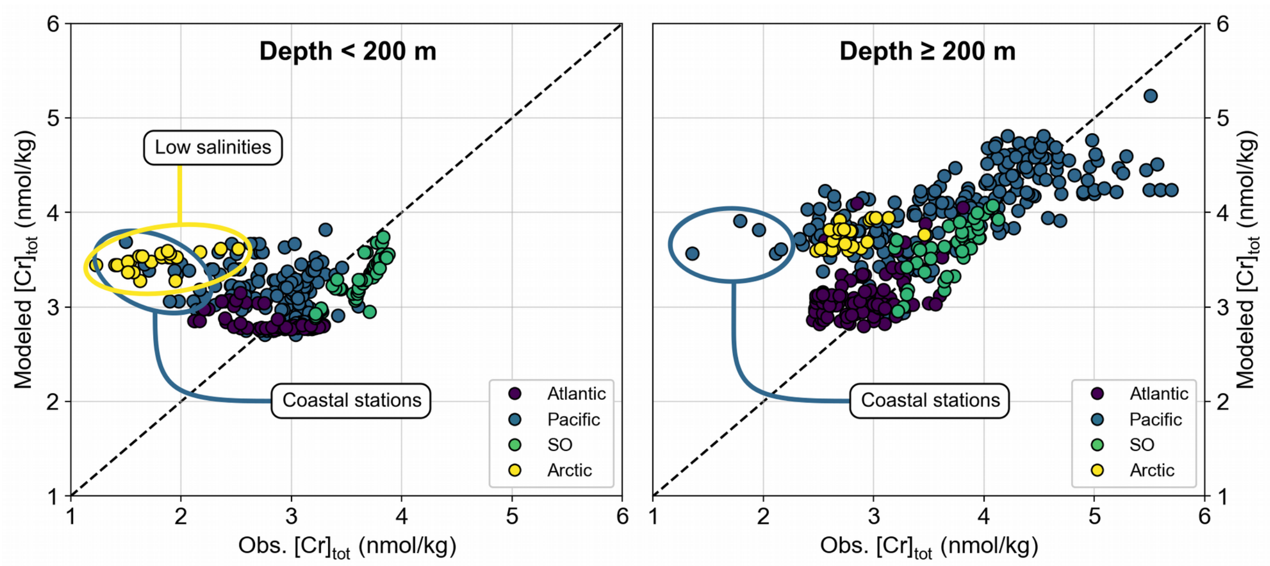

Figure S2: Observational versus modeled total Cr concentrations subdivided into the four main ocean basins (SO: Southern Ocean) (n = 701) and into shallow **(left)** and deeper depths than 200 m **(right)**. To date no data for the Indian Ocean exists. Dashed line marks the 1-to-1 relationship. Arctic data with very low observed Cr concentrations all have low salinities indicating influence of meltwater.

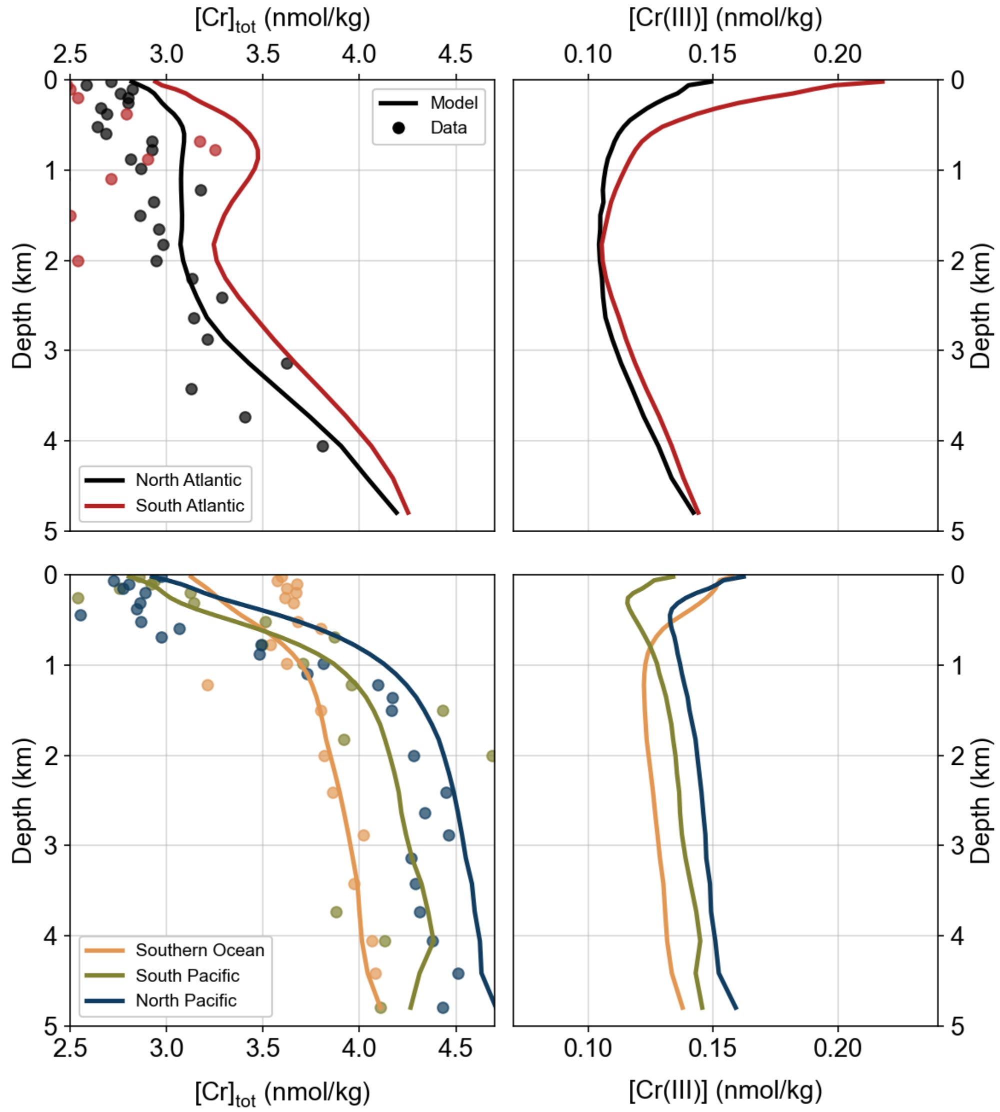

Figure S3: Averaged basin Cr_{tot} **(left)** and Cr(III) **(right)** concentrations as functions of water depth. Observational data was binned into the 32 depth layers of the Bern3D model, where at least one data point per depth layer was available. The North Atlantic and North Pacific are defined as the latitudinal band between 0°-70°N, the South Atlantic and South Pacific as 30°S-0°, and the Southern Ocean as south of 30°S.

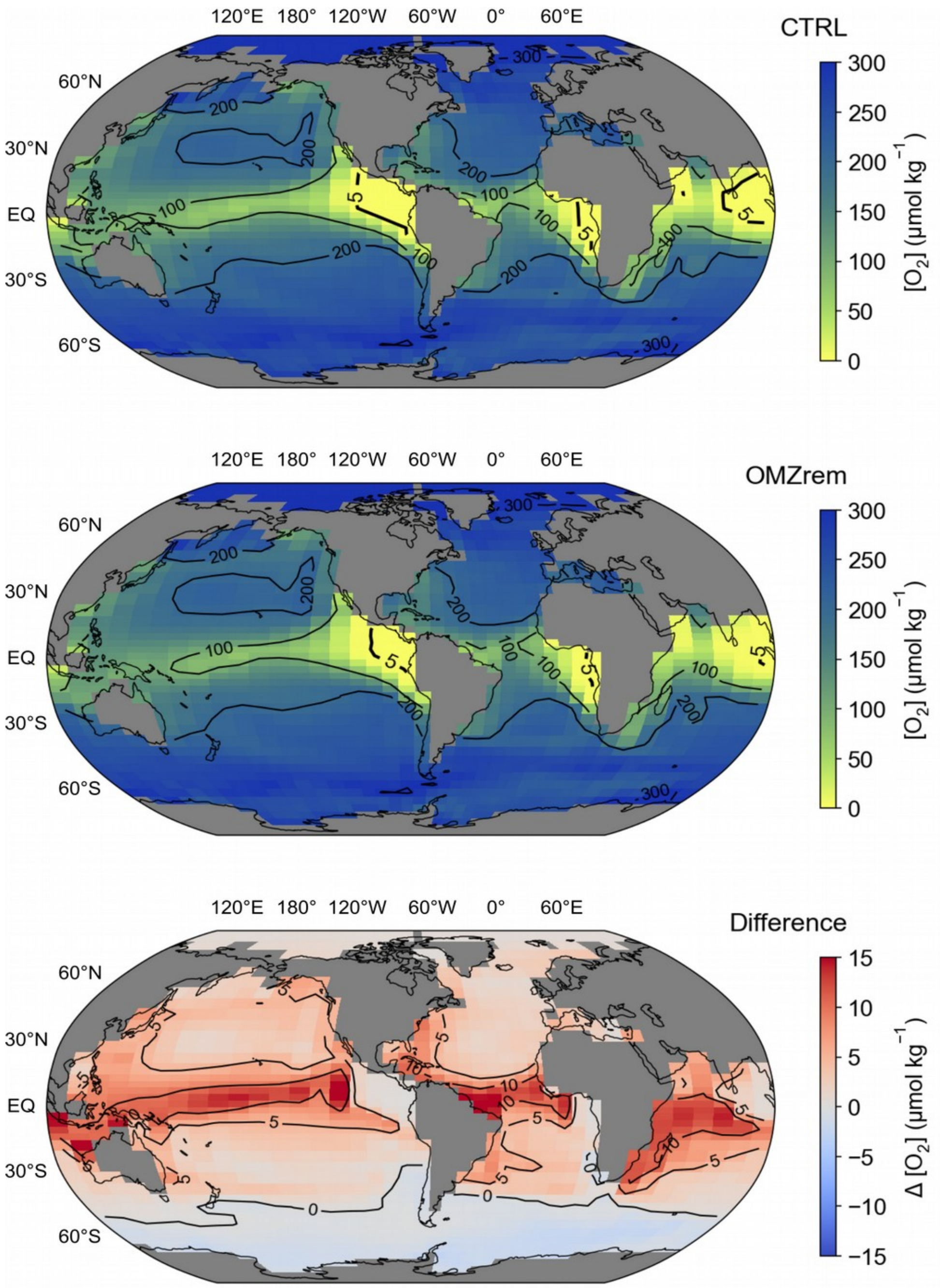

Figure S4: Dissolved oxygen concentrations at 200 m water depth. **(top)** For the control run, i.e., POM remineralization after Martin et al. (1987), and **(mid)** simulations with the O_2-dependent remineralization after Battaglia et al. (2018). **(bottom)** Difference between middle and top panel.

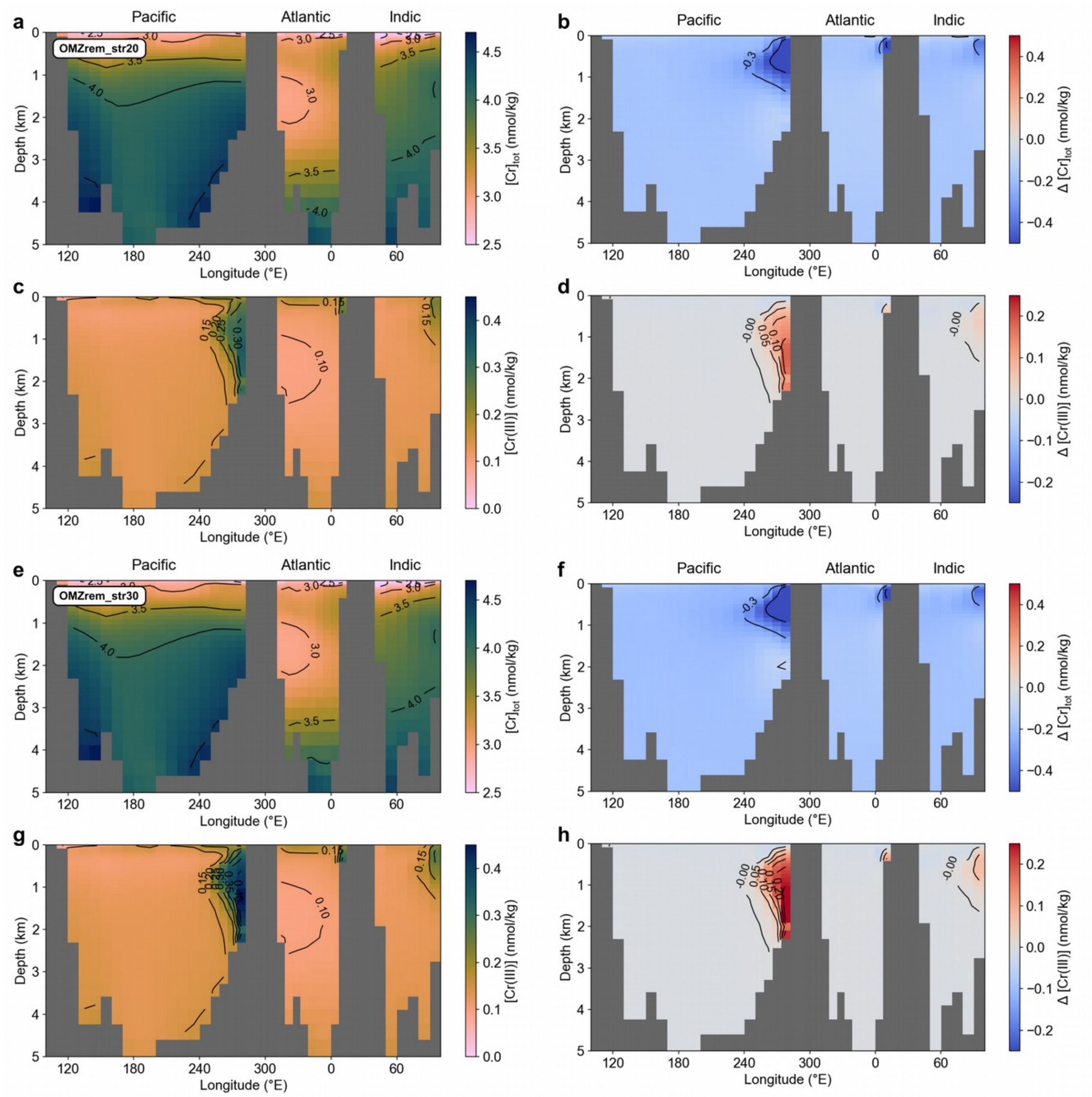

Figure S5: Total Cr and Cr(III) concentrations **(left)** as well as their anomalies **(right)** with respect to the control run along the equator for simulations OMZrem20 (a-d) and OMZrem30 (e-h).

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