Model data for simulations of ocean biogeochemistry after the Chicxulub impact (http://doi.org/10.5880/PIK.2020.008)

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Citation

When using the data please cite:

Brugger, J.; Feulner, G.; Hofmann, M.; Petri, S. (2021): Model data for simulations of ocean biogeochemistry after the Chicxulub impact. GFZ Data Services. https://doi.org/10.5880/PIK.2020.008.

The data are supplementary material to:

Brugger, J.; Feulner, G.; Hofmann, M.; Petri, S. (2021): A pronounced spike in ocean productivity triggered by the Chicxulub impact. Geophysical Research Letters, Vol 48, e2020GL092260. https://doi.org/10.1029/2020GL092260.

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Abstract

In "A pronounced spike in ocean productivity triggered by the Chicxulub impact" we study the combined effect of sulfate aerosols, carbon dioxide and dust on the oceans and the marine biosphere after the Chicxulub impact using simulations with a climate model including ocean biogeochemistry. The data presented here is the model output the results of this manuscript are based on. Additionally, the figures of the publication and scripts (Python) to analyse the model output and generate the figures are contained. The model output is provided in different netcdf files. The structure of the model output is explained in this readme file. The data are generated using the coupled ocean-atmosphere model CLIMBER-3α+C which model climate globally on a 3.75° x 3.75° (ocean) and 22.5° (longitude) x 7.5° (latitude) (atmosphere) grid. More information about the model can be found in the manuscript. This Readme contains the description of model output data (Part 1), the description of the generation of model input data, the files for figures and for the calculation of values discussed in the article (Part 2) and the description of the files for figures of the Supplementary Information (Part 3). In addition, the files for the corrected figures in the Correction were added to this Readme.

Part 1: Description of model output data

Each run's name gives all relevant information about the parameter setting:

c3beta_cret_065Ma_carboncycle_eq_globaldust…

c3beta	model version
cret	period in Earth history (Cretaceous)
065Ma	continental configuration
carboncycle	carbon cylce in the ocean model included
eq	run has reached equilibrium state
globaldust	dust is distributed globally (in contrast to CLIMBER2 model version)

Original equilibrium run is 11455 years long. Alkalinity was adjusted to equilibrate at an atmospheric CO_2 concentration of 500 ppm

…_1000years

Original equilibrium run is shortened: last 1000 years of the equilibrium run. Then 100 years with the parameter C13SAM (value linked to $\delta^{13}C$) fixed to the value of the equilibrated run: 1.001860. All impact runs are started on this run.

…_1000years_control

Continuation of the …_1000years run with unchanged parameters as a control run

Impact runs

- for all impact runs the atmospheric effect of 100 Gt S (which equals 3.1Pmol) is considered using transmission curves for a stratospheric residence time of Pierazzo et al. 2003
- for the runs with dust distribution (all but not …dust0) a mass of $2.9*10^{18}$ g dust is assumed to be distributed, as described in more detail in the SI to the article and in the readme to the Python script (folder regridding _dust_bioavail, readme_regridding_dust.txt)
- dust and C are equally distributed over 10 days
- the C amount is given in Gt, i.e. *C115* means 115 Gt C, minx means a ^{13}C signature of minus x

- the bioavailability is increased by a factor of 10 after the impact outside the (*BioavailFe10P10*), but is scaled in the 3000km radius around the impact site (*scaledbioavail*), as described in the SI to the article and the readme of the Python script (folder regridding _dust_bioavail, readme_regridding_dust.txt)
- in the standard case 3.1 Pmol sulfur are given to the ocean over 6 years, as described in the SI and in the readme to the Python script to create the input amounts (folder Scalculation_ocean, readme_Scalculation_ocean). This is done in all impact runs presented here
- additional S is added equally distributed over 10 days in some impact runs *(Sfast* in Pmol)
- Impact year, i.e., the first year of solar constant reduction and with additional S, C dust flux, is 11555. This is saved in year 1101 in the shortened history files and in the "snapshots" files named 11556 (snapshot named with year x contains data for year x-1)

Impact run without dust:
…_Impact_dust0_C115_Sfast0_Sslow3p1
Standard run:
…_Impact_C115min3_Sfast0_BioavailFe10P10_scaledbioavail
3 additional runs to investigate SST and $\delta^{13}C$ for different C amounts:
…_Impact_C1615min25_Sfast0_BioavailFe10P10_scaledbioavail
…_Impact_C2615min26_Sfast0_BioavailFe10P10_scaledbioavail
…_Impact_C4115min26_Sfast0_BioavailFe10P10_scaledbioavail
run to investigate ocean acidification:
…_Impact_C1615min25_S325Gt6yrsscaled_Sfast0_BioavailFe10P10_scaledbioavail
2 runs only used for material in the SI to deepen the investigation of ocean acidification:
…_Impact_C115min3_Sfast60_BioavailFe10P10_scaledbioavail
…_Impact_C4115min26_Sfast60_BioavailFe10P10_scaledbioavail

In addition, we tested the sensitivity to higher CO_2 concentrations for the Late Cretaceous: in the pre-impact run, we reached 1165 ppm. For this higher CO_2 concentration, we added the standard impact run and the impact run with additional 1500 Gt C: The new pre-impact run with higher CO_2 concentration was added to the 500ppm pre-impact run (c3beta_cret_065Ma_carboncycle_eq_globaldust) at year 11455. We cut the history files, i.e., they consist of 1000 years of the 500ppm run and then we changed alkalinity to reach higher CO_2 concentrations. A state close to equilibrium (but still with a small drift of ~ 5ppm/100 years) is reached after ~ 3400 years. C13SAM is fixed to 1.002989 and the run continued for 100 years until the impact runs were started. The impact year for this high CO_2 pre-impact run is 14960. This is saved in year 4507 in the shortened history files and in the snapshots files named 14961.

Control run:
…_highCO2-2_ControlC13SAMconst
standard run for high CO2:
…_highCO2-2_Impact_C115min3_Sfast0_BioavailFe10P10_scaledbioavail
with additional 1500 Gt C:
_highCO2-2_Impact_C1615min25_Sfast0_BioavailFe10P10_scaledbioavail

Model output

Most relevant files:

snapshots contain monthly values of the variables for the model year given in the name
Ocean model data: snapshots.00….01.01.dta.nc
Atmosphere model data: snapshots_potsdam2.00….01.01.dta.nc
for some model runs, nc files containing selected snapshot variables for 10, 100 and 1000 years were generated using cdo. They are saved in separate folders, called for example snapshots10yrsafterimpact
history files contain yearly values of the variables for each model year the simulation was run
Ocean model data: history.nc
Atmosphere model data: history_potsdam2.nc
Ice model data: history_isis.nc
topog.dta.nc contains information about topography and cells

Part 2: Description of files for creating model input, figures and for calculation of values used in the article (PythonScriptsKPg2_20210426.tar.xz)

The Python scripts in this .tar directory are an updated and extended version of the scripts in PythonScriptsKPg2_20200904.tar.xz.

Scalculation_ocean/S_in_ocean.py
Calculation of S amounts given to the ocean on the slow timescale, as described in the SI to the article. This is based on Pierazzo et al. 2003, Fig. 4b
regridding_dust_bioavail/dustdistribution_withbioavail.py
Calculation and regridding of dustdistribution and bioavailability, as described in the SI to the article and the readme and comments in this directory. Calculation of dust distribution is based on Artemieva et al. 2009 and personal communication with Natalia Artemieva.

Figure 1: Global annual mean sea surface temperatures (SSTs) for simulations with different C amounts with dust and without dust emission for 500 years after the impact on two different time scales *(SST_global.pdf)*
globalSST.py
script to generate Fig. 1 (SST_global.pdf)

Figure 2: Global annual mean net primary productivity (NPP) for simulations with and without dust emission and 115 Gt C emission for 500 years after the impact on two different time scales (NPP_global.*pdf*)
NPPmean.py
script to generate Fig. 2 (NPP_global.pdf)

Figure 3: δ^{13}C from proxy data and modeled for different C amounts from 60.000 years before the impact to 1.000.000 years after the impact on three different timescales for location around Shatsky Rise (*delta13C_proxies_Climber_ShatskyRise_surface.pdf*)
delta13C.py
script to generate Fig.3 (delta13C_proxies_Climber_ShatskyRise_surface.pdf)
proxydata_delta13C.xlsx
extract from Table S11 from SI to Hull et al. 2020, containing δ13C proxy data before and after the impact

Figure 4: Aragonite saturation Ω_a for preimpact state and for 10-year mean after the impact
(omega_a_C1615_S325.pdf)
omega_a.py
script to generate Fig. 4 (omega_a_C1615_S325.pdf)

Calculation of all SST, NPP and pH values or differences discussed in the article can be found in

SSTcalculation/SSTcalculation.py, SSTcalulation_1165ppm.py (same for higher pre-impact CO_2)
NPPcalculation/NPPcalculation.py
PHcalculation/pHcalculation.py

Ocean characteristics for pre-impact climate state in
LateCretaceousClimate/oceancharacteristics_preimpact.py

Part 3: Description of files for figures in Supplementary Information

Figure S1: Surface air temperature for pre-impact late-Cretaceous climate state, 500 ppm: zonal means and maps of surface air temperature *(ts_ann_preimpact_500ppm.pdf)*
Ts_ann_preimpact_500ppm.py
script to generate Fig. S1 (ts_ann_preimpact_500ppm.pdf)

Figure S2: Surface air temperature for pre-impact late-Cretaceous climate state, 1165 ppm: zonal means and maps of surface air temperature *(ts_ann_preimpact_1165ppm.pdf)*
Ts_ann_preimpact_1165ppm.py
script to generate Fig. S2 (ts_ann_preimpact_1165ppm.pdf)

Figure S3: Maps of annual mean NPP for the preimpact state and 2, 3, 5, 10, 100 years for the standard run *(NPP_maps_Impact_C115min3_Sfast0_BioavailFe10P10_map.pdf)*
NPPmaps.py
script to generate Fig. S3 (NPP_maps_Impact_C115min3_Sfast0_BioavailFe10P10_map.pdf)

Figure S4: Global annual mean pH after the impact for different C and S amounts (phmean_Sens.pdf)
phmean.py
script to generate Fig. S4 (pHmean_Sens.pdf)

Figure S5: Calcite saturation Ω_c for preimpact state and for 10-year mean after the impact, as in Fig.4 in the main article *(omega_c_C1615_S325.pdf)*
omega_c.py
script to generate Fig. S5 (omega_c_C1615_S325.pdf)

Figure S6 and S7: Aragonite and calcite saturation ($\Omega_{a\ \mathrm{and}}\ \Omega_c$) for runs with different C amounts (115, 4115 Gt) and different S amounts (0, 60 Pmol) to investigate the sensitivity of ocean acidification *(SaturationState_115GtCSSens.pdf, SaturationState_4115GtCSSens.pdf)*
SaturationState_CSSensitivity.py
script to generate Fig. S6 and S7
(SaturationState_115GtCSSens.pdf, SaturationState_4115GtCSSens.pdf)

Figure S8: Maps of mixed-layer depth (left) and global overturning stream function (right) for the preimpact state, impact year, year 3, 10, 100 years after the impact for the standard run
(hmxl_glb_over_C115min3_Sfast0_BioavailFe10P10_scaledbioavail_map.pdf)
Hmxl_maps.py
script to generate Fig. S8 (hmxl_glb_over_C115min3_Sfast0_BioavailFe10P10_scaledbioavail_map.pdf)

Figure S9: Global annual mean sea surface temperatures (SSTs) for pre-impact simulations with 500 ppm (as in Figure 1 main manuscript) and 1165 ppm, with emission of 115 Gt C and additional 1500 Gt C for 500 years after the impact on two different time scales
(SST_global_1000ppm.pdf)
globalSST_1000ppm.py
script to generate Fig. S9 (SST_global_1000ppm.pdf)

Figure S10: $\delta^{13}C$ from proxy data and modeled for pre-impact CO_2 concentrations of 500 (as in Figure 3 main manuscript) and 1165 ppm and 115 as well as additional 1500 Gt C emitted during the impact; from 60.000 years before the impact to 1.000.000 years after the impact on three different timescales for location around Shatsky Rise
(*delta13C_proxies_Climber_ShatskyRise_surface_1165ppm.pdf*)

Delta13C_1165ppm.py
script to generate Fig.S10 (delta13C_proxies_Climber_ShatskyRise_surface_1165ppm.pdf)
proxydata_delta13C.xlsx
extract from Table S11 from SI to Hull et al. 2020, containing δ13C proxy data before and after the impact

Figure S11: Global annual mean pH after the impact for pre-impact CO_2 concentrations of 500 (as in Figure S4) and 1165 ppm and 115 as well as additional 1500 Gt C emitted during the impact *(phmean_Sens_with1000ppm.pdf)*

phmean_1000ppm.py
script to generate Fig. S11 (pHmean_Sens_with1000ppm.pdf)

SST differences in **Table S1** can be calculated with SSTcalculation/SSTcalculation.py
Calculations of temperature gradients and other temperature variables for late-Cretaceous climate can be found in Python scripts to S1 and S2.

Part 4: Description of files for corrected figures in Correction

These files are written in Python 3 (instead of Python 2.7 for the rest)
Figure C1: Correction to Figure 2 of the manuscript: Global annual mean net primary productivity (NPP) for simulations with and without dust emission and 115 Gt C emission for 500 years after the impact on two different time scales (NPP_global_corr.*pdf*)

NPPmean_corr.py
script to generate Fig. C1 (NPP_global_corr.pdf)
The file *gridarea.nc*, which contains the gridarea of each grid cell in m^2, is needed for the correction as the unit of the model output g C/(m^2 year) needs to be transformed in Gt C/year by multiplication with the gridarea for each grid cell.

Figure C2: Correction to Figure S3 of the manuscript: Maps of annual mean NPP for the preimpact state and 2, 3, 5, 10, 100 years for the standard run
(NPP_maps_Impact_C115min3_Sfast0_BioavailFe10P10_map_correctedunits.pdf)

NPPmaps_correctedunits.py
script to generate Fig. C2
(NPP_maps_Impact_C115min3_Sfast0_BioavailFe10P10_map_correctedunits.pdf)

this figure is identical with Figure S3 and differs only in the correction of the unit from Gt C/year to g C/(m^2 year)

Calculation of NPP:

NPP_calculation_corr.py
Using *gridarea.nc*, which contains the gridarea of each grid cell in m^2, the output is calculated in Gt C/year from the unit g C/(m^2 year).

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The initial conditions and boundary conditions for the model runs of this study are derived from the here listed references. See the article and its SI for further details.

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