

INTRODUCTION TO CO₂ SPECIATION CALCULATIONS

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MÉXICO • September 2016

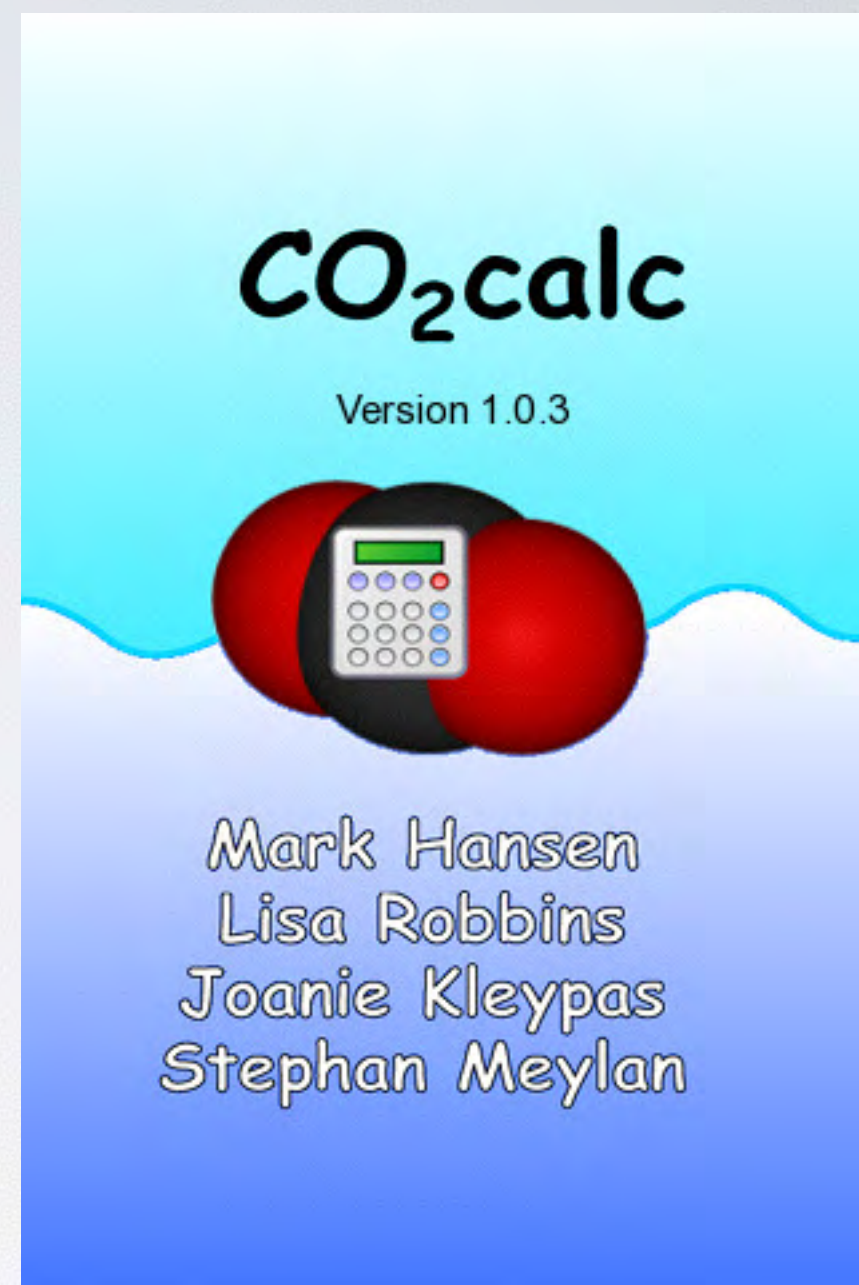
COMPUTER PROGRAMS EXIST FOR THESE CALCULATIONS

- Provide built in data for the various equilibrium constants which are functions of salinity, temperature, and pressure as well as for total concentrations such as boron that are proportional to salinity.
- Allow some additional acid-base information to be added (*e.g.* total phosphate and/or total silicate concentrations)
- Allow calculation of CO₂ speciation (typically from 2 analytical parameters, salinity & temperature)

Florida Shelf Ecosystems Response to Climate Change Project

**CO₂calc: A User-Friendly Seawater Carbon Calculator
for Windows, Mac OS X, and iOS (iPhone)**

<http://pubs.usgs.gov/of/2010/1280/>



Open-File Report 2010–1280





Input

Results

Sample Information

Name (6 chars)

Date

Get Date

<M/d/yy>

15

Latitude

N

Comment

Time

Get Time

Longitude

W

File Capture

File Name



Record

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)Total Si ($\mu\text{mol/kgSW}$)

Air-sea Flux

pCO2 Air (μatm)

Windspeed

m/s

Clear

Preferences

CO2 Constants

KHSO4

pH Scale

Total Boron

Air-sea Flux

Select

Process



Input

Results

Sample Information

Name (6 chars)

Date

Get Date

<M/d/yy>

Latitude

N

Comment

Time

Get Time

Longitude

W

File Capture

File Name

☐

Record

Sample identifier information
can be logged in a file along with results

Pressure (dbars)

pH (chosen scale)

fCO₂ water (µatm)pCO₂ water (µatm)

Air-sea Flux

pCO₂ Air (µatm)

Windspeed

m/s

Clear

Preferences

CO₂ ConstantsKHSO₄

pH Scale

Total Boron

Air-sea Flux

Select

Process



Input

Results

Sample Information

Name (6 chars)

Date

Get Date

<M/d/yy>

15

Latitude

N

Comment

Time

Get Time

Longitude

W

File Capture

File Name

☐ Record

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Adjusted Conditions

Temperature (C)

Pressure(dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)Total Si ($\mu\text{mol/kgSW}$)

Air-sea Flux

pCO2 Air (μatm)

Windspeed

m/s

Clear

Sample information

Process



Input

Results

Sample Information

Name (6 chars)

Date

Get Date

<M/d/yy>

15

Latitude

N

Comment

Time

Get Time

Longitude

W

File Capture

File Name



Record

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)Total Si ($\mu\text{mol/kgSW}$)

Air-sea Flux

pCO2 Air (μatm)

Adjusted Conditions

Preferences

CO2 Constants

KHSO4

pH Scale

Total Boron

Air-sea Flux

Select

Process

Choice of CO₂ constants, etc.

STEP 1

Choose the set of equilibrium constants, *etc.* that you wish to use.

Preferences	
CO2 Constants	<input type="text"/>
KHSO4	<input type="text"/>
pH Scale	<input type="text"/>
Total Boron	<input type="text"/>
Air-sea Flux	<input type="text"/>
<input type="button" value="Select"/>	

These are the choices I would usually recommend for systems with $S > 20$; I am sure they could be argued against.



THE KINDS OF CHEMICAL QUESTIONS WE NEED TO BE ABLE TO ANSWER

- How can I estimate the CO₂ composition of a sample of sea water?
- If the CO₂ level in the atmosphere increases by 300 ppm, how much will the pH in the surface ocean change?
- What will be the consequent change in the saturation state of aragonite?
- Will this be the same all over the oceans? Why? (or Why not?)
- How should I modify the CO₂ composition of a sample of sea water to reach a desired target composition?

A SIMPLE EXAMPLE

Surface sea water from the central North Atlantic

Input

Results

Sample Information

Name (6 chars)

Date

<M/d/yy>

15

Latitude

N

Comment

Time

Longitude

W

File Capture

File Name

☐ Record**Leave blank**

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Adjusted Conditions

Temperature (C)

Pressure(dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)Total Si ($\mu\text{mol/kgSW}$)

Air-sea Flux

pCO2 Air (μatm)

Windspeed

m/s

Preferences

CO2 Constants

Lueker et al., 2000

KHSO4

Dickson, 1990

pH Scale

Total scale (mol/kg-

Total Boron

Lee et al., 2010

Air-sea Flux

Ho et al., 2006

Already set

These are needed because the equilibrium constants are functions of salinity, temperature, and pressure; also total boron is estimated from salinity

The form contains the following sections and fields:

- Physical Data** (highlighted with a red border):
 - Salinity
 - temperature(C)
 - Pressure (dbars)
- Carbonate Data**:
 - TA ($\mu\text{mol/kgSW}$)
 - TCO2 ($\mu\text{mol/kgSW}$)
 - pH (chosen scale)
 - $f\text{CO}_2$ water (μatm)
 - $p\text{CO}_2$ water (μatm)
- Nutrient Data**:
 - Total P ($\mu\text{mol/kgSW}$)
 - Total Si ($\mu\text{mol/kgSW}$)
- Adjusted Conditions**:
 - Temperature (C)
 - Pressure(dbars)
- Air-sea Flux**:
 - $p\text{CO}_2$ Air (μatm)
 - Windspeed (with a unit dropdown menu currently set to m/s)

A "Clear" button is located at the bottom right of the form.

Pressure here is gauge pressure, *i.e.* zero at the sea surface (also 1 dbar \approx pressure exerted by 1 m of seawater)

Remember: only 2 carbonate system measurements are needed to define the chemical state of the system for a particular S , T , and p

The image shows a web-based calculator interface for carbonate system calculations. It features five main input sections: Physical Data, Carbonate Data, Nutrient Data, Adjusted Conditions, and Air-sea Flux. The Carbonate Data section is highlighted with a red rounded rectangle. Each section contains text labels and input fields. A 'Clear' button is located at the bottom right of the interface.

Section	Parameter	Unit
Physical Data	Salinity	
	temperature(C)	
	Pressure (dbars)	
Carbonate Data	TA	$\mu\text{mol/kgSW}$
	TCO2	$\mu\text{mol/kgSW}$
	pH	(chosen scale)
	fCO2 water	μatm
	pCO2 water	μatm
Nutrient Data	Total P	$\mu\text{mol/kgSW}$
	Total Si	$\mu\text{mol/kgSW}$
Adjusted Conditions	Temperature (C)	
	Pressure(dbars)	
Air-sea Flux	pCO2 Air	μatm
	Windspeed	m/s

Clear

If you have more than 2 of these with non-zero values, then the top two are the ones that are used for the calculation

Leaving “Nutrient Data” blank is the same as entering zero total concentrations

The form is titled "Physical Data" and contains the following fields:

- Salinity
- temperature(C)
- Pressure (dbars)

The form is titled "Carbonate Data" and contains the following fields:

- TA ($\mu\text{mol/kgSW}$)
- TCO2 ($\mu\text{mol/kgSW}$)
- pH (chosen scale)
- fCO2 water (μatm)
- pCO2 water (μatm)

The form is titled "Nutrient Data" and contains the following fields:

- Total P ($\mu\text{mol/kgSW}$)
- Total Si ($\mu\text{mol/kgSW}$)

The form is titled "Adjusted Conditions" and contains the following fields:

- Temperature (C)
- Pressure(dbars)

The form is titled "Air-sea Flux" and contains the following fields:

- pCO2 Air (μatm)
- Windspeed
- m/s

Clear

Leaving “Adjusted Conditions” blank repeats the values above

Leaving “Air-sea Flux” blank is OK, but yields a zero result

$S = 35$ Surface sea water from the central North Atlantic

$t = 18\text{ }^{\circ}\text{C}$

$p = 0\text{ dbar}$ (sea surface)

*Nutrient concentrations
assumed to be negligible*

The image shows a web-based data entry interface for oceanographic parameters. It is organized into five main sections, each with a title and a list of input fields:

- Physical Data:** Includes fields for Salinity (value: 35), temperature(C) (value: 18), and Pressure (dbars) (empty).
- Carbonate Data:** Includes fields for TA ($\mu\text{mol/kgSW}$) (value: 2300), TCO2 ($\mu\text{mol/kgSW}$) (value: 2025), pH (chosen scale) (empty), $f\text{CO}_2$ water (μatm) (empty), and $p\text{CO}_2$ water (μatm) (empty).
- Nutrient Data:** Includes fields for Total P ($\mu\text{mol/kgSW}$) (empty) and Total Si ($\mu\text{mol/kgSW}$) (empty).
- Adjusted Conditions:** Includes fields for Temperature (C) (empty) and Pressure(dbars) (empty).
- Air-sea Flux:** Includes fields for $p\text{CO}_2$ Air (μatm) (empty) and Windspeed (empty) with a unit selector set to m/s.

A "Clear" button is located at the bottom right of the form.

Total Alkalinity = $2300\text{ }\mu\text{mol kg}^{-1}$

Total Dissolved Inorganic Carbon = $2025\text{ }\mu\text{mol kg}^{-1}$

The parameters provided originally are repeated here together with a variety of calculated results

Physical Parameters	Carbonate Parameters	Auxillary Results	
Salinity 35.000	TA (μmol/kgSW) 2300.000	HCO3 (μmol/kgSW) 1821.128	Si Alk (μmol/kgSW) 0.000
temperature(C) 18.000	TCO2 (μmol/kgSW) 2025.000	CO3 (μmol/kgSW) 192.179	Revelle 10.115
Pressure 0.000	pH 8.103	CO2 (μmol/kgSW) 11.693	Ω Ca 4.589
	fCO2 (μatm) 341.034	B Alk (μmol/kgSW) 90.517	Ω Ar 2.967
	pCO2 (μatm) 342.223	OH (μmol/kgSW) 4.005	xCO2 (dry @ 1 atm) (ppm) 349.196
Nutrient Data	Air-sea CO2 Flux	P Alk (μmol/kgSW) 0.000	
Total P (umol/kgSW) 0.000	Flux (mmol/m ² /d) 0.000		
Total Si (umol/kgSW) 0.000			

$$R = \frac{\partial \ln[\text{CO}_2]}{\partial \ln C_T} = \frac{\frac{\partial [\text{CO}_2]}{[\text{CO}_2]}}{\frac{\partial C_T}{C_T}}$$

$$\Omega(\text{aragonite}) = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K_{sp}(\text{aragonite})}$$

WHAT HAPPENS IF WE WARM UP THAT WATER?

Increase temperature from 18 °C to 25 °C

Can do the calculation twice, changing the temperature from 18 to 25 °C or can take advantage of the “Adjusted Conditions”

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)

TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)

pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

Total Si ($\mu\text{mol/kgSW}$)

Adjusted Conditions

Temperature (C)

Pressure(dbars)

Air-sea Flux

pCO2 Air (μatm)

Windspeed

m/s



Clear

Can do the calculation twice, changing the temperature from 18 to 25 °C or can take advantage of the “Adjusted Conditions”

Physical Data

Salinity

temperature(C)

Pressure (dbars)

Carbonate Data

TA ($\mu\text{mol/kgSW}$)

TCO2 ($\mu\text{mol/kgSW}$)

pH (chosen scale)

fCO2 water (μatm)

pCO2 water (μatm)

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

Total Si ($\mu\text{mol/kgSW}$)

Adjusted Conditions

Temperature (C)

Pressure(dbars)

Air-sea Flux

pCO2 Air (μatm)

Windspeed

m/s



Clear

$t = 18\text{ }^{\circ}\text{C}$ The change of temperature is for a closed system.

Results at Input

Results at Adjusted Conditions

Physical Parameters

Salinity

35.000

temperature(C)

18.000

Pressure

0.000

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

0.000

Total Si ($\mu\text{mol/kgSW}$)

0.000

Carbonate Parameters

TA ($\mu\text{mol/kgSW}$)

2300.000

TCO2 ($\mu\text{mol/kgSW}$)

2025.000

pH

8.103

$f\text{CO}_2$ (μatm)

341.034

pCO2 (μatm)

342.223

Air-sea CO2 Flux

Flux ($\text{mmol/m}^2/\text{d}$)

0.000

Auxillary Results

HCO3 ($\mu\text{mol/kgSW}$)

1821.128

CO3 ($\mu\text{mol/kgSW}$)

192.179

CO2 ($\mu\text{mol/kgSW}$)

11.693

B Alk ($\mu\text{mol/kgSW}$)

90.517

OH ($\mu\text{mol/kgSW}$)

4.005

P Alk ($\mu\text{mol/kgSW}$)

0.000

Si Alk ($\mu\text{mol/kgSW}$)

0.000

Revelle

10.115

Ω Ca

4.589

Ω Ar

2.967

xCO2 (dry @ 1
atm) (ppm)

349.196

$t = 25\text{ }^{\circ}\text{C}$ The change of temperature is for a closed system.

Results at Input

Results at Adjusted Conditions

Physical Parameters

Salinity

35.000

temperature(C)

25.000

Pressure

0.000

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

0.000

Total Si ($\mu\text{mol/kgSW}$)

0.000

Carbonate Parameters

TA ($\mu\text{mol/kgSW}$)

2300.000

TCO2 ($\mu\text{mol/kgSW}$)

2025.000

pH

7.997

$f\text{CO}_2$ (μatm)

453.285

pCO2 (μatm)

454.736

Air-sea CO2 Flux

Flux ($\text{mmol/m}^2/\text{d}$)

0.000

Auxillary Results

HCO3 ($\mu\text{mol/kgSW}$)

1816.992

CO3 ($\mu\text{mol/kgSW}$)

195.138

CO2 ($\mu\text{mol/kgSW}$)

12.870

B Alk ($\mu\text{mol/kgSW}$)

86.764

OH ($\mu\text{mol/kgSW}$)

5.978

P Alk ($\mu\text{mol/kgSW}$)

0.000

Si Alk ($\mu\text{mol/kgSW}$)

0.000

Revelle

10.008

Ω Ca

4.697

Ω Ar

3.096

xCO2 (dry @ 1
atm) (ppm)

469.117

WHAT HAPPENS TO pH OR $p(\text{CO}_2)$?

$t = 18\text{ }^{\circ}\text{C}$ The change of temperature is for a closed system.

Results at Input

Results at Adjusted Conditions

Physical Parameters

Salinity

35.000

temperature(C)

18.000

Pressure

0.000

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

0.000

Total Si ($\mu\text{mol/kgSW}$)

0.000

Carbonate Parameters

TA ($\mu\text{mol/kgSW}$)

2300.000

TCO2 ($\mu\text{mol/kgSW}$)

2025.000

pH

8.103

fCO2 (μatm)

341.034

pCO2 (μatm)

342.223

Air-sea CO2 Flux

Flux ($\text{mmol/m}^2/\text{d}$)

0.000

Auxillary Results

HCO3 ($\mu\text{mol/kgSW}$)

1821.128

CO3 ($\mu\text{mol/kgSW}$)

192.179

CO2 ($\mu\text{mol/kgSW}$)

11.693

B Alk ($\mu\text{mol/kgSW}$)

90.517

OH ($\mu\text{mol/kgSW}$)

4.005

P Alk ($\mu\text{mol/kgSW}$)

0.000

Si Alk ($\mu\text{mol/kgSW}$)

0.000

Revelle

10.115

Ω Ca

4.589

Ω Ar

2.967

xCO2 (dry @ 1
atm) (ppm)

349.196

$t = 25\text{ }^{\circ}\text{C}$ The change of temperature is for a closed system.

Results at Input

Results at Adjusted Conditions

Physical Parameters

Salinity

35.000

temperature(C)

25.000

Pressure

0.000

Nutrient Data

Total P ($\mu\text{mol/kgSW}$)

0.000

Total Si ($\mu\text{mol/kgSW}$)

0.000

Carbonate Parameters

TA ($\mu\text{mol/kgSW}$)

2300.000

TCO2 ($\mu\text{mol/kgSW}$)

2025.000

pH

7.997

fCO2 (μatm)

453.285

pCO2 (μatm)

454.736

Air-sea CO2 Flux

Flux ($\text{mmol/m}^2/\text{d}$)

0.000

Auxillary Results

HCO3 ($\mu\text{mol/kgSW}$)

1816.992

CO3 ($\mu\text{mol/kgSW}$)

195.138

CO2 ($\mu\text{mol/kgSW}$)

12.870

B Alk ($\mu\text{mol/kgSW}$)

86.764

OH ($\mu\text{mol/kgSW}$)

5.978

P Alk ($\mu\text{mol/kgSW}$)

0.000

Si Alk ($\mu\text{mol/kgSW}$)

0.000

Revelle

10.008

Ω Ca

4.697

Ω Ar

3.096

xCO2 (dry @ 1
atm) (ppm)

469.117

IF WE MEASURE pH IN THE LABORATORY,
WE CAN USE THIS APPROACH TO CONVERT IT
TO AN ESTIMATED IN SITU VALUE

Laboratory measurement of pH at 25 °C (“zero” pressure)

Physical Data	Carbonate Data	Nutrient Data
Salinity <input type="text" value="35"/>	TA ($\mu\text{mol/kgSW}$) <input type="text" value="2300"/>	Total P ($\mu\text{mol/kgSW}$) <input type="text"/>
temperature(C) <input type="text" value="25"/>	TCO2 ($\mu\text{mol/kgSW}$) <input type="text"/>	Total Si ($\mu\text{mol/kgSW}$) <input type="text"/>
Pressure (dbars) <input type="text" value="0"/>	pH (chosen scale) <input type="text" value="8.00"/>	
	fCO2 water (μatm) <input type="text"/>	
	pCO2 water (μatm) <input type="text"/>	

Adjusted Conditions	Air-sea Flux
Temperature (C) <input type="text" value="8"/>	pCO2 Air (μatm) <input type="text"/>
Pressure(dbars) <input type="text" value="1000"/>	Windspeed <input type="text"/> m/s ▼

in situ conditions 8 °C @ 1,000 m depth

Calculation is for a closed system.

Results at Input

Results at Adjusted Conditions

Physical Parameters

Salinity

35.000

temperature(C)

25.000

Pressure

0.000

Nutrient Data

Total P (umol/kgSW)

0.000

Total Si (umol/kgSW)

0.000

Carbonate Parameters

TA (μmol/kgSW)

2300.000

TCO2 (μmol/kgSW)

2023.271

pH

8.000

fCO2 (μatm)

449.433

pCO2 (μatm)

450.871

Air-sea CO2 Flux

Flux (mmol/m²/d)

0.000

Auxillary Results

HCO3 (μmol/kgSW)

1814.286

CO3 (μmol/kgSW)

196.225

CO2 (μmol/kgSW)

12.760

B Alk (μmol/kgSW)

87.254

OH (μmol/kgSW)

6.020

P Alk (μmol/kgSW)

0.000

Si Alk (μmol/kgSW)

0.000

Revelle

9.975

Ω Ca

4.724

Ω Ar

3.113

xCO2 (dry @ 1 atm) (ppm)

465.129

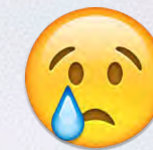
total dissolved inorganic carbon stays constant!

Calculation is for a closed system.

Results at Input	Results at Adjusted Conditions	
Physical Parameters Salinity <input type="text" value="35.000"/> temperature(C) <input type="text" value="8.000"/> Pressure <input type="text" value="1000.000"/>	Carbonate Parameters TA ($\mu\text{mol/kgSW}$) <input type="text" value="2300.000"/> TCO ₂ ($\mu\text{mol/kgSW}$) <input type="text" value="2023.271"/> pH <input type="text" value="8.225"/> $f\text{CO}_2$ (μatm) <input type="text" value="216.770"/> pCO ₂ (μatm) <input type="text" value="217.630"/> Air-sea CO₂ Flux Flux ($\text{mmol/m}^2/\text{d}$) <input type="text" value="0.000"/>	Auxillary Results HCO ₃ ($\mu\text{mol/kgSW}$) <input type="text" value="1827.364"/> CO ₃ ($\mu\text{mol/kgSW}$) <input type="text" value="185.735"/> CO ₂ ($\mu\text{mol/kgSW}$) <input type="text" value="10.173"/> B Alk ($\mu\text{mol/kgSW}$) <input type="text" value="99.040"/> OH ($\mu\text{mol/kgSW}$) <input type="text" value="2.132"/> P Alk ($\mu\text{mol/kgSW}$) <input type="text" value="0.000"/> Si Alk ($\mu\text{mol/kgSW}$) <input type="text" value="0.000"/> Revelle <input type="text" value="10.215"/> Ω Ca <input type="text" value="3.666"/> Ω Ar <input type="text" value="2.352"/> xCO ₂ (dry @ 1 atm) (ppm) <input type="text" value="219.912"/>
Nutrient Data Total P ($\mu\text{mol/kgSW}$) <input type="text" value="0.000"/> Total Si ($\mu\text{mol/kgSW}$) <input type="text" value="0.000"/>		

total dissolved inorganic carbon stays constant!

TIME TO TRY THIS FOR YOURSELVES



THE KINDS OF CHEMICAL QUESTIONS WE NEED TO BE ABLE TO ANSWER

- How can I estimate the CO_2 composition of a sample of sea water?
- If the CO_2 level in the atmosphere increases by 300 ppm, how much will the pH in the surface ocean change?
- What will be the consequent change in the saturation state of aragonite?
- Will this be the same all over the oceans? Why? (or Why not?)
- How should I modify the CO_2 composition of a sample of sea water to reach a desired target composition?

If the CO₂ level in the atmosphere increases by 300 ppm, how much will the pH in the surface ocean change?

What will be the consequent change in the saturation state of aragonite?

What information do we need to make this calculation?

1. Estimates of S , t , and P ($= 0$ at sea surface).
2. $\text{pH} = f(A_T, p(\text{CO}_2))$

The simplest assumption (which I recommend here) is to assume that the change in atmospheric $p(\text{CO}_2)$ does not affect S , t , & A_T .

A. Can do the calculation for average seawater values.

$$S = 35; t = 18 \text{ }^\circ\text{C}; A_T = 2300 \text{ } \mu\text{mol kg}^{-1}$$

Need to assume an initial $p(\text{CO}_2)$, *e.g.* 400 μatm

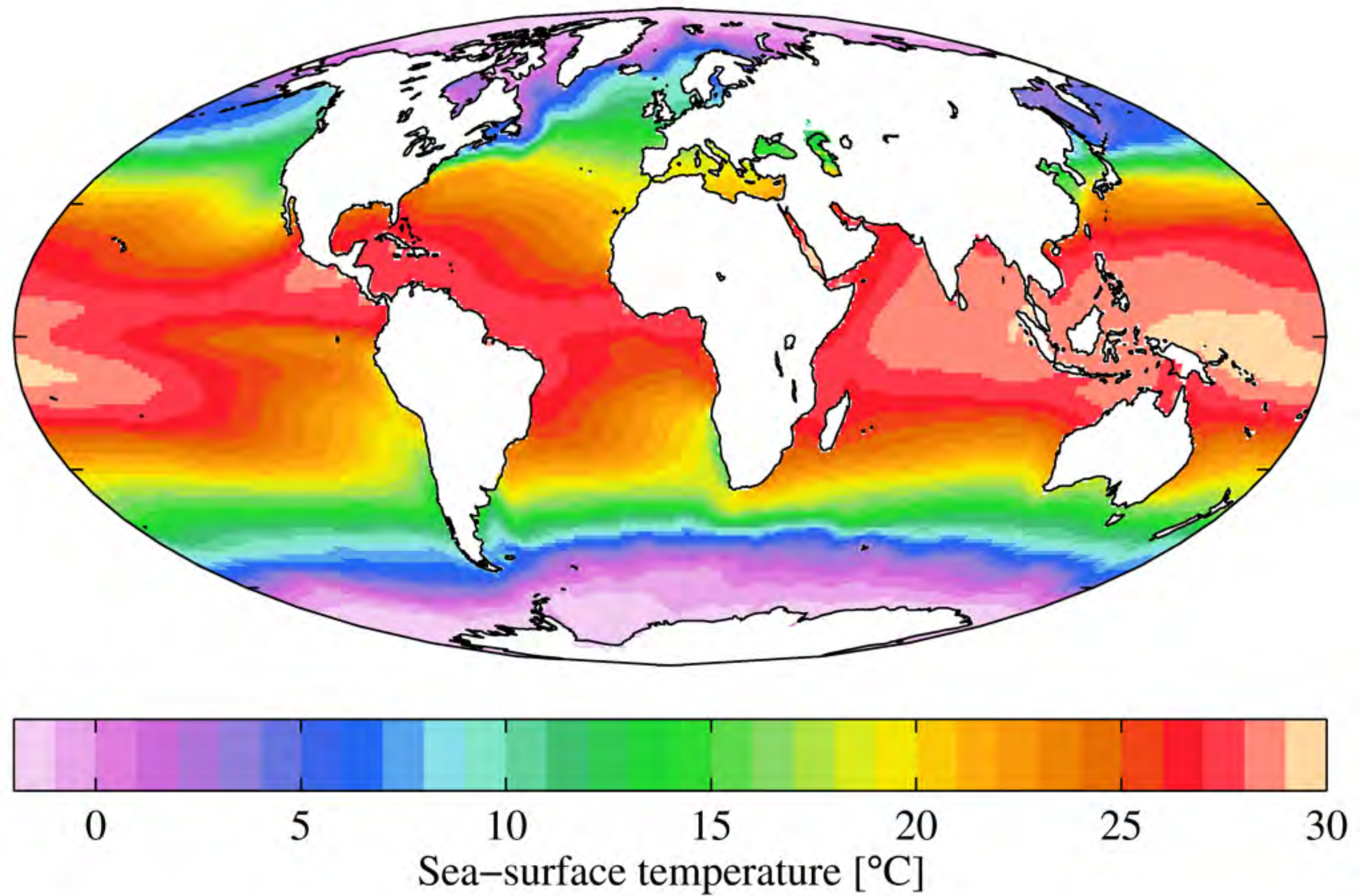
Repeat calculation for increased $p(\text{CO}_2)$, *i.e.* 700 μatm

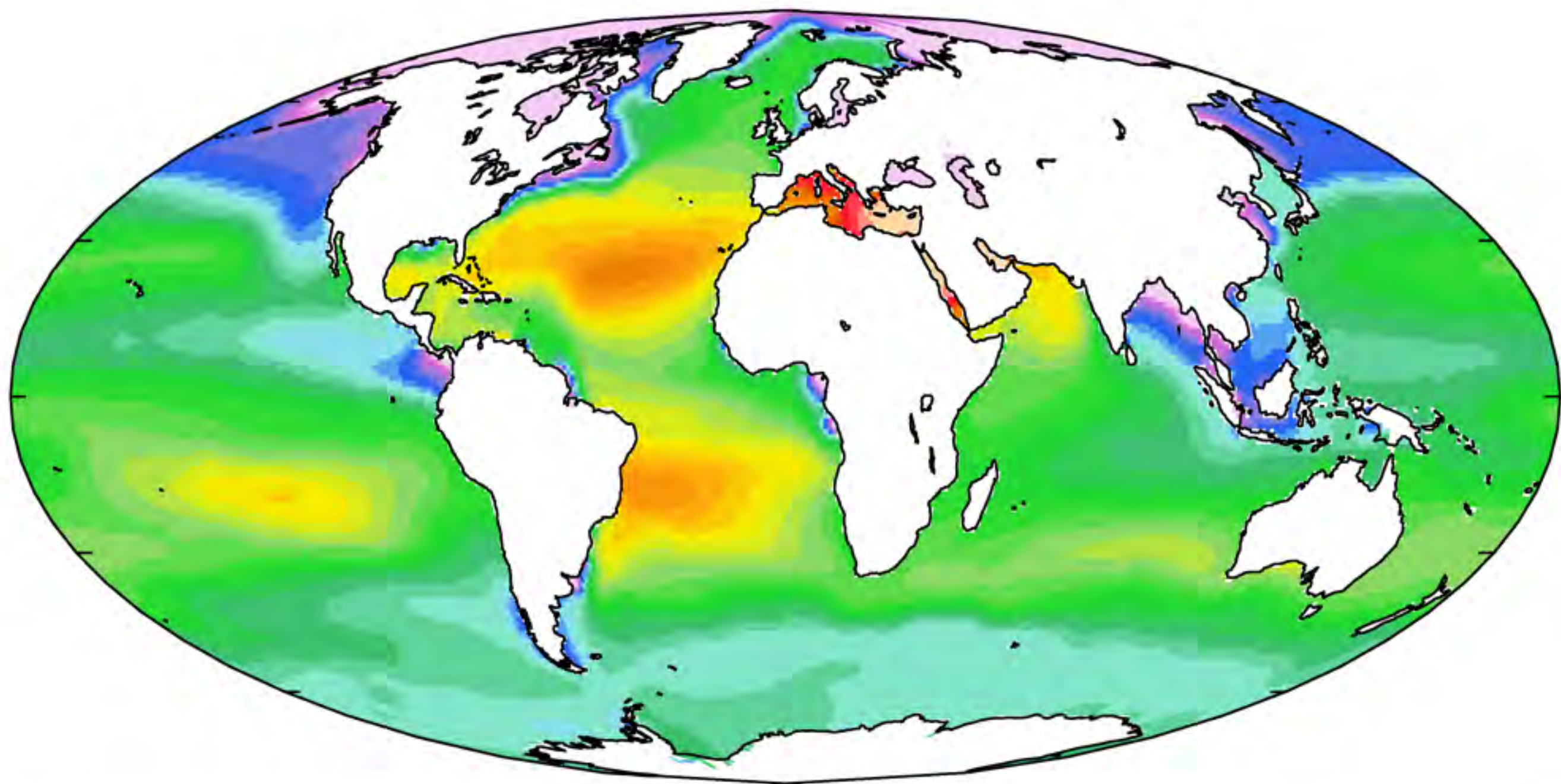
If the CO_2 level in the atmosphere increases by 300 ppm, how much will the pH in the surface ocean change?

What will be the consequent change in the saturation state of aragonite?

Will this be the same all over the oceans?

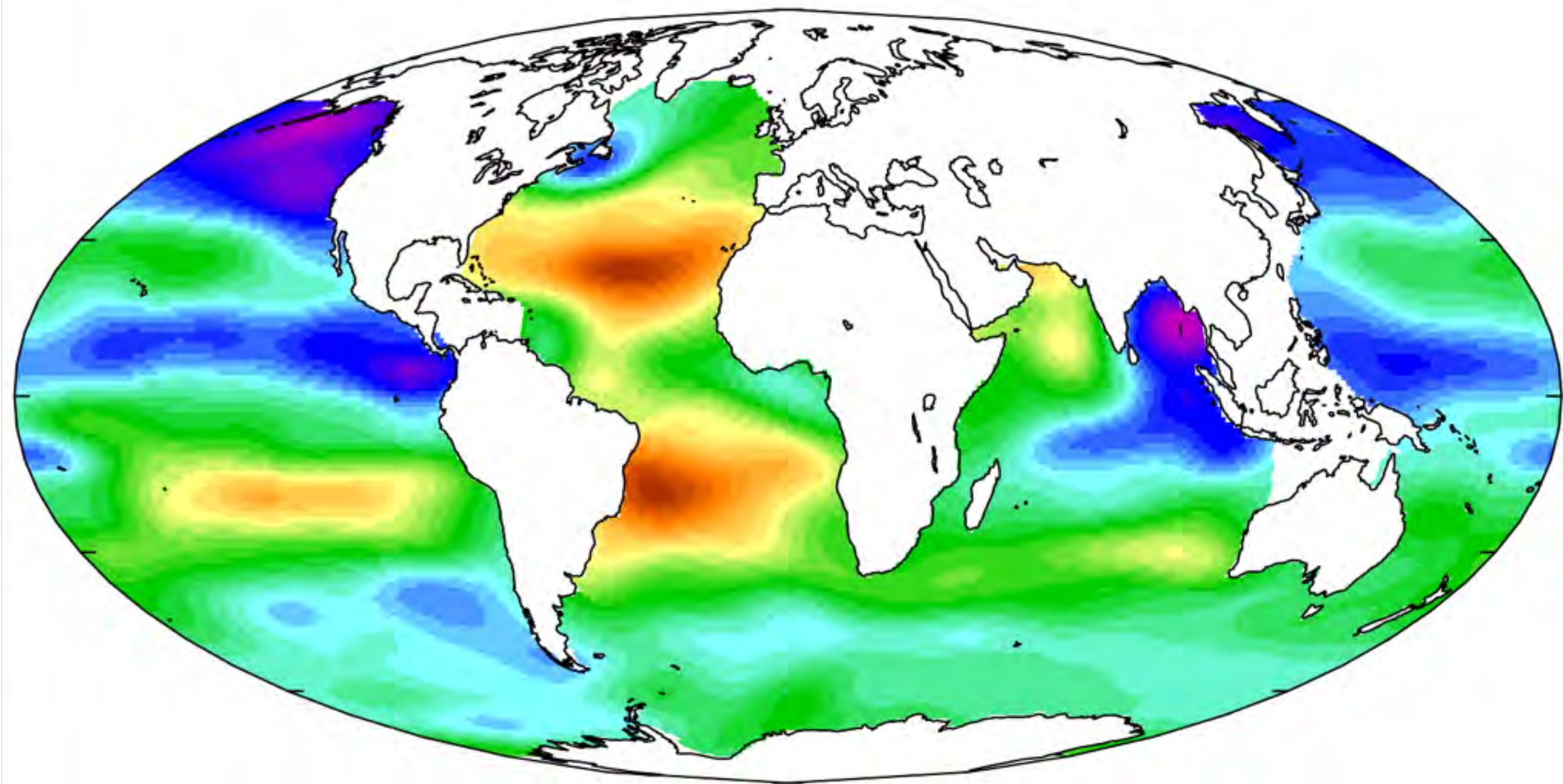
1. Need estimates of range of S , t , and A_T .
2. Repeat a few calculations to get an estimate of the likely variability in the pH change and in the the aragonite saturation state change





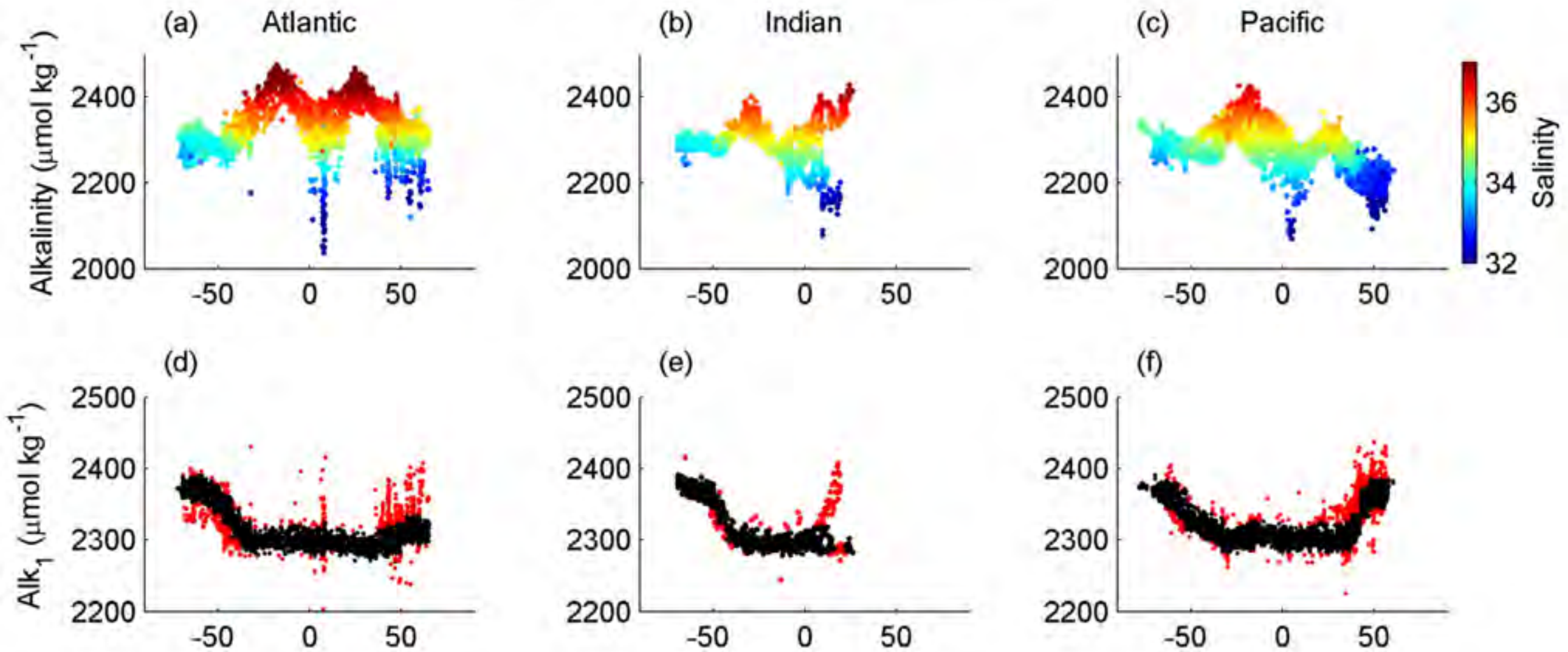
31 32 33 34 35 36 37 38 39

Sea-surface salinity



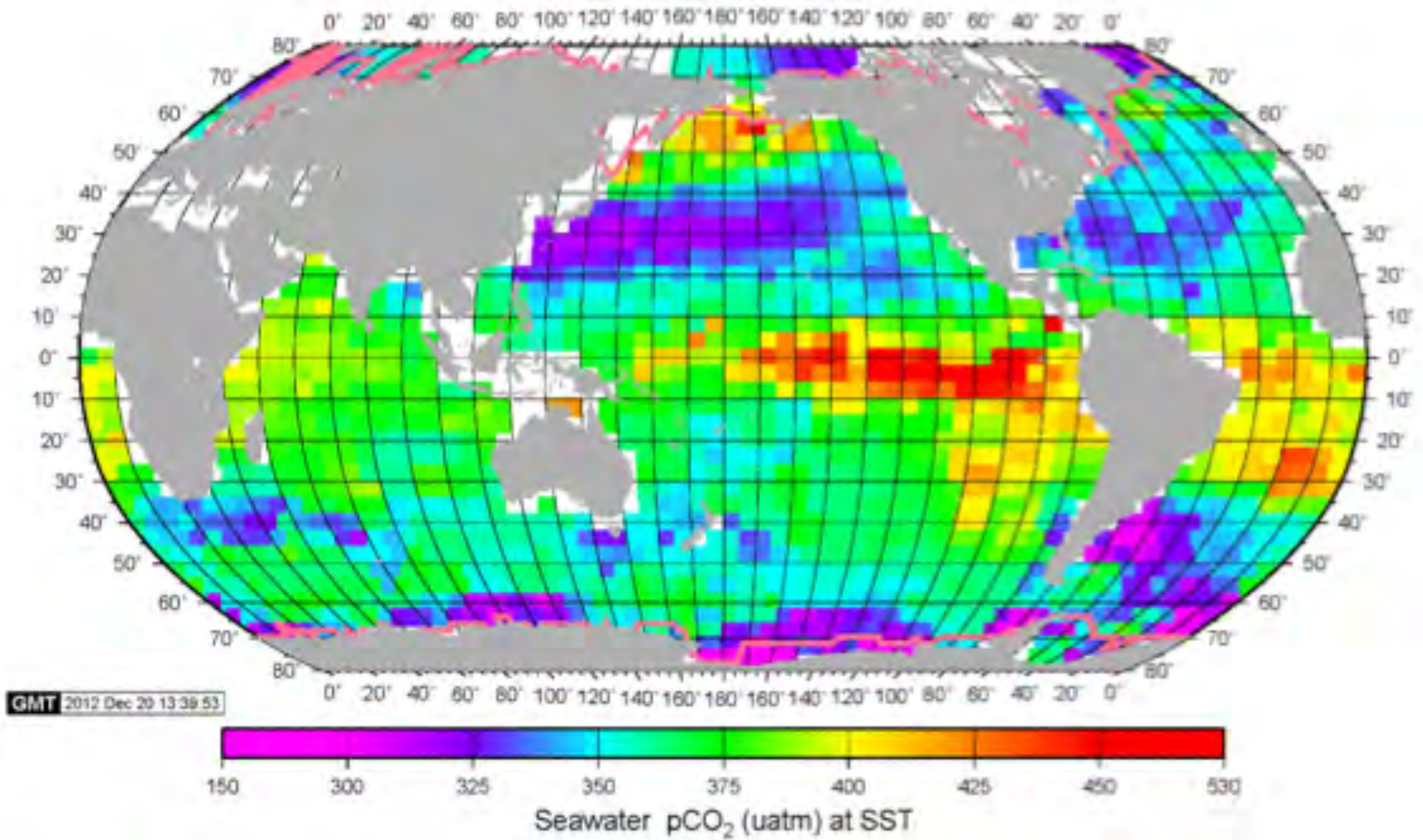
Sea-surface alkalinity [mmol kg⁻¹]





$$Alk_1 = \frac{Alk_m}{S} \times 35.$$

Reference year 2005



THE KINDS OF CHEMICAL QUESTIONS WE NEED TO BE ABLE TO ANSWER

- How can I estimate the CO_2 composition of a sample of sea water?
- If the CO_2 level in the atmosphere increases by 300 ppm, how much will the pH in the surface ocean change?
- What will be the consequent change in the saturation state of aragonite?
- Will this be the same all over the oceans? Why? (or Why not?)
- How should I modify the CO_2 composition of a sample of sea water to reach a desired target composition?

How should I modify the CO₂ composition of a sample of sea water to reach a desired target composition?

Need to know the initial composition of your water

Need to define the target (pH, $p(\text{CO}_2)$, $\Omega(\text{arag})$)

Need to decide what form of modification is simpler
(or more relevant)

Often it is most straightforward to keep A_T approximately constant, and to change the C_T by addition/removal of CO₂.

It is also simpler to monitor pH: rather than $p(\text{CO}_2)$ or $\Omega(\text{arag})$