



Getting started with the MARCHEMSPEC Marine Chemical Speciation Models

Supplement: Calculations for Natural Waters of Defined Alkalinity, Total Dissolved Inorganic Carbon, and Borate

Version 1.00

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The Marine Chemical Speciation Model (MARCHEMSPEC) was created by SCOR Working Group 145 (2015 – 2022), and it is being further developed under the auspices of the Joint Committee on the Properties of Seawater. The members of SCOR Working Group 145 were as follows:

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This document describes how to input natural water compositions into the models for defined values of alkalinity, total dissolved inorganic carbon, and borate.

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It is available from marchemspec.org.

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1. Introduction

This short Supplement describes how to carry out calculations for seawater solutions, or solutions containing the ions of seawater, for assigned alkalinities and total carbonate and borate concentrations. At the time of writing this document, the ability of the model to equilibrate solutions directly to pairs of specified values of pH, pCO₂, DIC (dissolved inorganic carbon) and/or alkalinity has not been implemented in the software. However, using the available forms of input for the standalone models, and the MARCHEMSPEC functions, it is possible to fix total borate, dissolved inorganic carbon, and alkalinity to user-defined values. This document summarises how to do this, and contains tables of input concentrations that can be used in calls of the MARCHEMSPEC functions for calculations of properties of seawater media.

2. The alkalinity of Reference Seawater

The compositions of Reference Seawater for practical salinity 35 are listed in Table 4 of Millero et al. (*Deep-Sea Research I*, **55**, 50-72, 2008), on both an amount content and molality basis. Acid-base speciation is assigned for the carbonate and borate systems, for this salinity, thus for example all of CO₂*, HCO₃⁻, CO₃²⁻, B(OH)₄⁻ and B(OH)₃ have assigned concentrations. Free H⁺ can be set to zero, for convenience, because it is so small.

These compositions can be re-arranged so that all borate is assigned to B(OH)₃, all carbonate is assigned to CO₂*, and all fluoride to F⁻ (as it already is in the table of Millero et al.). If this is done, then the concentration (*k*) of OH⁻ (amount content or molality) can be written:

$$k\text{OH}^- = k\text{OH}^-(\text{free}) + kB(\text{OH})_4^- + 2k\text{CO}_3^{2-} + k\text{HCO}_3^- - k\text{H}^+ - k\text{HF} \quad (1)$$

Taking amount contents from Table 4 of Millero et al. yields;

$$\begin{aligned} [\text{OH}^-] &= 0.0000080 + 0.0001008 + 2 \times 0.0002390 + 0.0017177 - 0.0 - 0.0 \\ &= 2.3045 \times 10^{-3} \text{ moles per kg of solution (amount content)} \end{aligned} \quad (2)$$

This is the alkalinity of the solution. The small difference between this value and that given by Millero et al. for this solution ($2.300 \times 10^{-3} \text{ mol kg}^{-1}$) is most likely due to rounding errors in the tabulated amount contents and is not significant.

The same calculation, on a molality basis (*m*), yields:

$$\begin{aligned} m\text{OH}^- &= 0.0000082 + 0.0001045 + 2 \times 0.0002477 + 0.0017803 - 0.0 - 0.0 \\ &= 2.33884 \times 10^{-3} \text{ moles per kg of pure water (molality)} \end{aligned} \quad (3)$$

(This conversion does not take into account the very small change in the moles of water solvent implied by the assignment of all carbonate to CO₂* and all borate to B(OH)₃.)

Compositions of seawater can be input into MARCHEMSPEC in this way, so that the OH⁻ input is equal to the alkalinity, and CO₂* and B(OH)₃ are total carbonate and borate, respectively. These two totals can be altered without affecting the alkalinity. For salinity 35 seawater on an amount content basis, the following two sets of seawater compositions in the table below are equivalent, and either can be used by the model.

Salinity 35 seawater, two equivalent compositions

	Seawater species composition			Equivalent composition, using alkalinity and total F, B, and DIC	
	No.	Species	Amount Content	Species	Amount Content
Cations	1	H	0.0	H	0.0
	2	Na	4.689674E-01	Na	4.689674E-01
	3	Mg	5.281710E-02	Mg	5.281710E-02
	4	Ca	1.028210E-02	Ca	1.028210E-02
	5	K	1.020770E-02	K	1.02077E-02
	6	MgOH	0.0	-	0.0
	7	Sr	9.070E-05	Sr	9.070E-05
	8	MgF	0.0	-	0.0
	9	CaF	0.0	-	0.0
Anions	1	Cl	5.458696E-01	Cl	5.458696E-01
	2	SO4	2.823520E-02	SO4	2.823520E-02
	3	HSO4	0.0	-	0.0
	4	OH	8.0E-06	ALK	2.3044118E-03
	5	Br	8.421E-04	Br	8.421E-04
	6	HCO3	1.7177E-03	-	0.0
	7	CO3	2.390E-04	-	0.0
	8	BOH4	1.008E-04	-	0.0
	9	F	6.83E-05	F	6.83E-05
Neutrals	1	BOH3	3.143E-04	B	4.151E-04
	2	CO2	9.6E-06	C (DIC)	1.9663E-03
	3	HF	0.0	-	0.0
	4	MgCO3	0.0	-	0.0
	5	CaCO3	0.0	-	0.0
	6	SrCO3	0.0	-	0.0

In the above table we have listed all the species in the MARCHEMSPEC seawater model. The model that includes trace metals contains these same species, plus the trace metals and their complexes, and also phosphate and silicate species.

In the next part of this document we list compositions of reference seawater expressed in terms of the totals in the rightmost column above for a wide range of salinities.

Whichever way the composition of the seawater or other natural water solution is expressed, the input into MARCHEMSPEC must be charge balanced. The simplest way to achieve this is, for any change Δ to the alkalinity, is to add an equivalent Δ to one or more of the major cations. One or both of Na^+ or Ca^{2+} are reasonable choices. So, for example:

If $\Delta\text{ALK} = -1.0\text{E-}4$, then:

$$[\text{Na}^+] \text{ becomes } 0.4689674 + \Delta\text{ALK} = 0.4689674 - 1.0\text{E-}4 = 0.4688674$$

or:

$$[\text{Ca}^{2+}] \text{ becomes } 0.01028210 + \Delta\text{ALK} = 0.01028210 - 1.0\text{E-}4/2 = 0.0102321$$

Note that we only change $[\text{Ca}^{2+}]$ by half as much because it is doubly charged. The identical calculation can be done on a molality basis.

3. Tables of Reference Seawater compositions (various salinities)

On this and the following pages we list amount content compositions of reference seawater over a wide range of salinities. In the tables the column for OH is equivalent to the total alkalinity (ALK), that for $B(OH)_3$ to total borate (B), and that for CO_2^* to total dissolved inorganic carbon (C).

These tables contain the values required for input into the MARCHEMSPEC functions for the iCalc values 5 and 7. In the input arrays the minor product species such as HSO_4^- and ion pairs are omitted and the concentrations of the reactant species are therefore all total values. However, the executable standalone programs read input data from files, and these data must include values for all species (even if zero). The supplied data files for the standalone programs include equivalents of the tables below in which all the necessary values are present.

Table 1a. Cation amount contents of reference seawater of various practical salinities.

Salinity	H	NA	MG	CA	K	SR
0.1	0.0	1.3399064E-03	1.5090594E-04	2.9377298E-05	2.9164759E-05	2.5912706E-07
0.2	0.0	2.6798134E-03	3.0181194E-04	5.8754591E-05	5.8329507E-05	5.1825424E-07
0.5	0.0	6.6995337E-03	7.5452987E-04	1.4688647E-04	1.4582381E-04	1.2956358E-06
1	0.0	1.3399064E-02	1.5090593E-03	2.9377294E-04	2.9164758E-04	2.5912709E-06
2	0.0	2.6798133E-02	3.0181191E-03	5.8754589E-04	5.8329515E-04	5.1825421E-06
3	0.0	4.0197203E-02	4.5271792E-03	8.8131884E-04	8.7494262E-04	7.7738127E-06
4	0.0	5.3596275E-02	6.0362393E-03	1.1750914E-03	1.1665907E-03	1.0365086E-05
5	0.0	6.6995344E-02	7.5452992E-03	1.4688648E-03	1.4582374E-03	1.2956354E-05
6	0.0	8.0394410E-02	9.0543586E-03	1.7626379E-03	1.7498852E-03	1.5547626E-05
7	0.0	9.3793477E-02	1.0563421E-02	2.0564108E-03	2.0415332E-03	1.8138895E-05
8	0.0	1.0719253E-01	1.2072478E-02	2.3501838E-03	2.3331806E-03	2.0730166E-05
9	0.0	1.2059161E-01	1.3581539E-02	2.6439570E-03	2.6248276E-03	2.3321443E-05
10	0.0	1.3399071E-01	1.5090594E-02	2.9377296E-03	2.9164753E-03	2.5912709E-05
11	0.0	1.4738976E-01	1.6599653E-02	3.2315027E-03	3.2081230E-03	2.8503977E-05
12	0.0	1.6078878E-01	1.8108716E-02	3.5252755E-03	3.4997708E-03	3.1095252E-05
13	0.0	1.7418787E-01	1.9617775E-02	3.8190481E-03	3.7914178E-03	3.3686527E-05
14	0.0	1.8758695E-01	2.1126840E-02	4.1128216E-03	4.0830661E-03	3.6277796E-05
15	0.0	2.0098604E-01	2.2635900E-02	4.4065942E-03	4.3747130E-03	3.8869061E-05
16	0.0	2.1438506E-01	2.4144957E-02	4.7003670E-03	4.6663606E-03	4.1460337E-05
17	0.0	2.2778420E-01	2.5654011E-02	4.9941400E-03	4.9580088E-03	4.4051607E-05
18	0.0	2.4118320E-01	2.7163071E-02	5.2879134E-03	5.2496560E-03	4.6642883E-05
19	0.0	2.5458225E-01	2.8672139E-02	5.5816862E-03	5.5413031E-03	4.9234149E-05
20	0.0	2.6798137E-01	3.0181193E-02	5.8754586E-03	5.8329513E-03	5.1825419E-05
21	0.0	2.8138039E-01	3.1690255E-02	6.1692317E-03	6.1245987E-03	5.4416694E-05
22	0.0	2.9477949E-01	3.3199314E-02	6.4630044E-03	6.4162463E-03	5.7007959E-05
23	0.0	3.0817861E-01	3.4708370E-02	6.7567778E-03	6.7078941E-03	5.9599235E-05
24	0.0	3.2157764E-01	3.6217434E-02	7.0505510E-03	6.9995414E-03	6.2190506E-05
25	0.0	3.3497671E-01	3.7726495E-02	7.3443241E-03	7.2911891E-03	6.4781774E-05
26	0.0	3.4837581E-01	3.9235553E-02	7.6380970E-03	7.5828363E-03	6.7373043E-05
27	0.0	3.6177487E-01	4.0744618E-02	7.9318699E-03	7.8744840E-03	6.9964314E-05
28	0.0	3.7517388E-01	4.2253670E-02	8.2256426E-03	8.1661312E-03	7.2555590E-05
29	0.0	3.8857297E-01	4.3762729E-02	8.5194153E-03	8.4577791E-03	7.5146864E-05
30	0.0	4.0197203E-01	4.5271794E-02	8.8131889E-03	8.7494265E-03	7.7738128E-05
31	0.0	4.1537108E-01	4.6780855E-02	9.1069614E-03	9.0410745E-03	8.0329404E-05
32	0.0	4.2877022E-01	4.8289911E-02	9.4007347E-03	9.3327220E-03	8.2920675E-05
33	0.0	4.4216926E-01	4.9798973E-02	9.6945100E-03	9.6243693E-03	8.5511942E-05
34	0.0	4.5556832E-01	5.1308030E-02	9.9882792E-03	9.9160151E-03	8.8103218E-05
35	0.0	4.6896739E-01	5.2817091E-02	1.0282053E-02	1.0207664E-02	9.0694486E-05
36	0.0	4.8236648E-01	5.4326147E-02	1.0575830E-02	1.0499311E-02	9.3285755E-05
37	0.0	4.9576551E-01	5.5835215E-02	1.0869597E-02	1.0790963E-02	9.5877029E-05
38	0.0	5.0916456E-01	5.7344266E-02	1.1163373E-02	1.1082609E-02	9.8468329E-05
39	0.0	5.2256366E-01	5.8853329E-02	1.1457146E-02	1.1374256E-02	1.0105960E-04
40	0.0	5.3596270E-01	6.0362393E-02	1.1750913E-02	1.1665903E-02	1.0365080E-04
41	0.0	5.4936179E-01	6.1871448E-02	1.2044692E-02	1.1957546E-02	1.0624211E-04
42	0.0	5.6276084E-01	6.3380513E-02	1.2338462E-02	1.2249195E-02	1.0883341E-04
43	0.0	5.7615994E-01	6.4889567E-02	1.2632240E-02	1.2540847E-02	1.1142468E-04
44	0.0	5.8955901E-01	6.6398629E-02	1.2926014E-02	1.2832489E-02	1.1401592E-04
45	0.0	6.0295804E-01	6.7907687E-02	1.3219782E-02	1.3124141E-02	1.1660718E-04

Table 1b. Anion amount contents of reference seawater of various practical salinities (Sal.).

Sal.	CL	SO4	ALK (OH)	BR	HCO3	CO3	BOH4	F
0.1	1.5596273E-03	8.0672054E-05	6.5840337E-06	2.4060222E-06	0.0	0.0	0.0	1.9517229E-07
0.2	3.1192551E-03	1.6134407E-04	1.3168067E-05	4.8120459E-06	0.0	0.0	0.0	3.9034465E-07
0.5	7.7981366E-03	4.0336027E-04	3.2920165E-05	1.2030114E-05	0.0	0.0	0.0	9.7586162E-07
1	1.5596274E-02	8.0672056E-04	6.5840340E-05	2.4060232E-05	0.0	0.0	0.0	1.9517231E-06
2	3.1192545E-02	1.6134414E-03	1.3168068E-04	4.8120451E-05	0.0	0.0	0.0	3.9034465E-06
3	4.6788815E-02	2.4201612E-03	1.9752105E-04	7.2180679E-05	0.0	0.0	0.0	5.8551703E-06
4	6.2385091E-02	3.2268823E-03	2.6336135E-04	9.6240910E-05	0.0	0.0	0.0	7.8068936E-06
5	7.7981367E-02	4.0336026E-03	3.2920165E-04	1.2030111E-04	0.0	0.0	0.0	9.7586163E-06
6	9.3577635E-02	4.8403231E-03	3.9504204E-04	1.4436137E-04	0.0	0.0	0.0	1.1710339E-05
7	1.0917394E-01	5.6470440E-03	4.6088241E-04	1.6842160E-04	0.0	0.0	0.0	1.3662064E-05
8	1.2477021E-01	6.4537641E-03	5.2672274E-04	1.9248185E-04	0.0	0.0	0.0	1.5613784E-05
9	1.4036646E-01	7.2604854E-03	5.9256303E-04	2.1654206E-04	0.0	0.0	0.0	1.7565506E-05
10	1.5596271E-01	8.0672059E-03	6.5840339E-04	2.4060230E-04	0.0	0.0	0.0	1.9517237E-05
11	1.7155896E-01	8.8739265E-03	7.2424371E-04	2.6466250E-04	0.0	0.0	0.0	2.1468956E-05
12	1.8715531E-01	9.6806471E-03	7.9008404E-04	2.8872271E-04	0.0	0.0	0.0	2.3420680E-05
13	2.0275155E-01	1.0487369E-02	8.5592443E-04	3.1278298E-04	0.0	0.0	0.0	2.5372408E-05
14	2.1834780E-01	1.1294091E-02	9.2176471E-04	3.3684316E-04	0.0	0.0	0.0	2.7324125E-05
15	2.3394414E-01	1.2100811E-02	9.8760492E-04	3.6090339E-04	0.0	0.0	0.0	2.9275850E-05
16	2.4954039E-01	1.2907526E-02	1.0534454E-03	3.8496363E-04	0.0	0.0	0.0	3.1227571E-05
17	2.6513663E-01	1.3714248E-02	1.1192857E-03	4.0902390E-04	0.0	0.0	0.0	3.3179294E-05
18	2.8073287E-01	1.4520973E-02	1.1851261E-03	4.3308407E-04	0.0	0.0	0.0	3.5131018E-05
19	2.9632921E-01	1.5327686E-02	1.2509665E-03	4.5714427E-04	0.0	0.0	0.0	3.7082739E-05
20	3.1192544E-01	1.6134412E-02	1.3168066E-03	4.8120454E-04	0.0	0.0	0.0	3.9034465E-05
21	3.2752176E-01	1.6941134E-02	1.3826471E-03	5.0526473E-04	0.0	0.0	0.0	4.0986192E-05
22	3.4311798E-01	1.7747849E-02	1.4484873E-03	5.2932498E-04	0.0	0.0	0.0	4.2937909E-05
23	3.5871428E-01	1.8554570E-02	1.5143282E-03	5.5338522E-04	0.0	0.0	0.0	4.4889632E-05
24	3.7431056E-01	1.9361292E-02	1.5801683E-03	5.7744541E-04	0.0	0.0	0.0	4.6841357E-05
25	3.8990683E-01	2.0168010E-02	1.6460081E-03	6.0150567E-04	0.0	0.0	0.0	4.8793084E-05
26	4.0550307E-01	2.0974738E-02	1.7118486E-03	6.2556586E-04	0.0	0.0	0.0	5.0744807E-05
27	4.2109938E-01	2.1781452E-02	1.7776895E-03	6.4962610E-04	0.0	0.0	0.0	5.2696524E-05
28	4.3669565E-01	2.2588175E-02	1.8435291E-03	6.7368633E-04	0.0	0.0	0.0	5.4648252E-05
29	4.5229189E-01	2.3394892E-02	1.9093694E-03	6.9774660E-04	0.0	0.0	0.0	5.6599978E-05
30	4.6788817E-01	2.4201617E-02	1.9752099E-03	7.2180683E-04	0.0	0.0	0.0	5.8551698E-05
31	4.8348450E-01	2.5008336E-02	2.0410502E-03	7.4586707E-04	0.0	0.0	0.0	6.0503419E-05
32	4.9908078E-01	2.5815062E-02	2.1068911E-03	7.6992725E-04	0.0	0.0	0.0	6.2455147E-05
33	5.1467698E-01	2.6621780E-02	2.1727311E-03	7.9398750E-04	0.0	0.0	0.0	6.4406870E-05
34	5.3027331E-01	2.7428494E-02	2.2385712E-03	8.1804775E-04	0.0	0.0	0.0	6.6358594E-05
35	5.4586956E-01	2.8235220E-02	2.3044118E-03	8.4210795E-04	0.0	0.0	0.0	6.8310315E-05
36	5.6146581E-01	2.9041940E-02	2.3702526E-03	8.6616821E-04	0.0	0.0	0.0	7.0262039E-05
37	5.7706206E-01	2.9848660E-02	2.4360923E-03	8.9022838E-04	0.0	0.0	0.0	7.2213763E-05
38	5.9265840E-01	3.0655384E-02	2.5019324E-03	9.1428858E-04	0.0	0.0	0.0	7.4165483E-05
39	6.0825462E-01	3.1462105E-02	2.5677726E-03	9.3834885E-04	0.0	0.0	0.0	7.6117205E-05
40	6.2385090E-01	3.2268820E-02	2.6336139E-03	9.6240863E-04	0.0	0.0	0.0	7.8068927E-05
41	6.3944724E-01	3.3075541E-02	2.6994534E-03	9.8646919E-04	0.0	0.0	0.0	8.0020652E-05
42	6.5504343E-01	3.3882263E-02	2.7652942E-03	1.0105299E-03	0.0	0.0	0.0	8.1972378E-05
43	6.7063975E-01	3.4688980E-02	2.8311346E-03	1.0345896E-03	0.0	0.0	0.0	8.3924101E-05
44	6.8623599E-01	3.5495706E-02	2.8969746E-03	1.0586501E-03	0.0	0.0	0.0	8.5875826E-05
45	7.0183233E-01	3.6302426E-02	2.9628156E-03	1.0827103E-03	0.0	0.0	0.0	8.7827549E-05

Note that the entries for HCO_3^- , CO_3^{2-} , and B(OH)_4^- have been set to zero and assigned to CO_2^* (total dissolved inorganic carbon) and B(OH)_3 (total borate) in Table 1c. The column for OH^- is also the total alkalinity (ALK).

Table 1c. Anion amount contents of reference seawater of various practical salinities (Sal.).

Salinity	B (BOH3)	C (CO2)	HF
0.1	1.1861957E-06	5.6180961E-06	0.0
0.2	2.3723913E-06	1.1236192E-05	0.0
0.5	5.9309790E-06	2.8090477E-05	0.0
1	1.1861957E-05	5.6180964E-05	0.0
2	2.3723916E-05	1.1236193E-04	0.0
3	3.5585867E-05	1.6854291E-04	0.0
4	4.7447824E-05	2.2472385E-04	0.0
5	5.9309778E-05	2.8090477E-04	0.0
6	7.1171744E-05	3.3708578E-04	0.0
7	8.3033697E-05	3.9326677E-04	0.0
8	9.4895654E-05	4.4944773E-04	0.0
9	1.0675761E-04	5.0562865E-04	0.0
10	1.1861957E-04	5.6180963E-04	0.0
11	1.3048152E-04	6.1799057E-04	0.0
12	1.4234350E-04	6.7417153E-04	0.0
13	1.5420541E-04	7.3035254E-04	0.0
14	1.6606735E-04	7.8653345E-04	0.0
15	1.7792935E-04	8.4271432E-04	0.0
16	1.8979126E-04	8.9889540E-04	0.0
17	2.0165324E-04	9.5507635E-04	0.0
18	2.1351519E-04	1.0112573E-03	0.0
19	2.2537720E-04	1.0674383E-03	0.0
20	2.3723917E-04	1.1236190E-03	0.0
21	2.4910108E-04	1.1798001E-03	0.0
22	2.6096304E-04	1.2359810E-03	0.0
23	2.7282500E-04	1.2921625E-03	0.0
24	2.8468700E-04	1.3483432E-03	0.0
25	2.9654889E-04	1.4045237E-03	0.0
26	3.0841089E-04	1.4607049E-03	0.0
27	3.2027286E-04	1.5168863E-03	0.0
28	3.3213483E-04	1.5730666E-03	0.0
29	3.4399674E-04	1.6292474E-03	0.0
30	3.5585873E-04	1.6854285E-03	0.0
31	3.6772063E-04	1.7416095E-03	0.0
32	3.7958259E-04	1.7977910E-03	0.0
33	3.9144455E-04	1.8539717E-03	0.0
34	4.0330654E-04	1.9101524E-03	0.0
35	4.1516848E-04	1.9663336E-03	0.0
36	4.2703048E-04	2.0225150E-03	0.0
37	4.3889236E-04	2.0786953E-03	0.0
38	4.5075434E-04	2.1348761E-03	0.0
39	4.6261633E-04	2.1910570E-03	0.0
40	4.7447834E-04	2.2472388E-03	0.0
41	4.8634020E-04	2.3034190E-03	0.0
42	4.9820221E-04	2.3596004E-03	0.0
43	5.1006410E-04	2.4157815E-03	0.0
44	5.2192608E-04	2.4719620E-03	0.0
45	5.3378806E-04	2.5281436E-03	0.0

Note that the entry for B(OH)₃ above is equivalent to the total borate in solution (B), and that for CO₂* is equivalent to the total dissolved inorganic carbon (C).