

The general 'Sea-Water_Calc' program displays in text format all the relevant parameters for seawater, including :

Temp = temperature in degree Celsius (°C)
CO2 = ppmv, parts per million in volume of CO2 in dry air
pptF = fraction of CaCO3(calcite) which precipitates, ratio to complete precipitation(when omega=1)
Pres = pressure in atm x 100
Saln = salinity in grams of dissolved salts per kg of solution
pHfr. pHtot pHsws = different pH scales, free, total and seawater
pOH = -log10[OH-]
H2CO3 HCO3 CO3 = concentrations in millimol/kg-solution
DIC = Dissolved Inorganic Carbon in mmol/kg-soln
Alk = alkalinity in mmol/kg-soln Alk = 2*CO3+HCO3+OH+BOH4-H
Ca++ CaCO3 = concentrations in mmol/kg-soln
sovr1 sovr2 = Calcite and aragonite over saturation (omega)
pH2O = water vapour pressure above sea level
Cout = mmol/kg-soln of carbon absorbed(-) or outgassed (+) from the first iteration

One over the following six parameters can be varied inside a proper , user selectabel, for..endfor cycle.
If not varied , the parameter assumes as default the following values

Tc = 4; % temperature in Celsius (°C) *

ppmCO2 = 410; % parts per million (in volume) of CO2 in the atmosphere *

P = 0; % pressure in atm. P=0 means ambient pressure, 1 atm. *

S = 35; % salinity, in grams of salts in 1 kg of solution *

pptF = 0; % fraction of CaCO3 which actually precipitates *

pH2O = 100; % H2O vapour pressure in %saturation at sea level *

Standar seawater composition (S=35 g/ Kg(solution)) is as follows

Cl_i = 0.54586; % Cl⁻ Mol/kg(solution)

Na_i = 0.46906; % Na⁺ Mol/kg(solution)

Mg_i = 0.05282; % Mg⁺⁺ Mol/kg(solution)

Ca_i = 0.01028; % Ca⁺⁺ Mol/kg(solution)

SO_{4i} = 0.02824; % SO₄₋₋ Mol/kg(solution)

K_i = 0.01021; % K⁺ Mol/kg(solution)

Br_i = 0.00084; % Br⁻ Mol/kg(solution)

Sr_i = 0.00009; % Sr⁺⁺ Mol/kg(solution)

Fi = 0.00007; % F⁻ Mol/kg(solution)

Bi = 0.00042; % B(OH)₃ + B(OH)₄⁻ Mol/kg(solution)

Some text output are listed as examples in the following (script follows at the end):

1) Temperature ranging from 0 to 30 °C while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHtot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
0.00	410	0.00	0.00	35.0	8.099	8.068	8.061	6.239	0.0255	2.149	0.0989	2.274	10.280	2.400	0.000	2.369	1.489	0.0059	0.00
1.00	410	0.00	0.00	35.0	8.102	8.070	8.062	6.189	0.0245	2.139	0.1028	2.267	10.280	2.400	0.000	2.461	1.548	0.0064	0.01
2.00	410	0.00	0.00	35.0	8.106	8.072	8.064	6.139	0.0236	2.130	0.1069	2.260	10.280	2.400	0.000	2.556	1.609	0.0068	0.01
3.00	410	0.00	0.00	35.0	8.109	8.073	8.066	6.090	0.0227	2.119	0.1111	2.253	10.280	2.400	0.000	2.653	1.672	0.0073	0.02
4.00	410	0.00	0.00	35.0	8.112	8.075	8.067	6.041	0.0219	2.109	0.1153	2.246	10.280	2.400	0.000	2.753	1.736	0.0079	0.03
5.00	410	0.00	0.00	35.0	8.115	8.076	8.068	5.993	0.0211	2.098	0.1197	2.239	10.280	2.400	0.000	2.855	1.803	0.0084	0.03
6.00	410	0.00	0.00	35.0	8.118	8.078	8.070	5.946	0.0204	2.088	0.1241	2.232	10.280	2.400	0.000	2.959	1.871	0.0090	0.04
7.00	410	0.00	0.00	35.0	8.121	8.079	8.071	5.898	0.0196	2.077	0.1287	2.225	10.280	2.400	0.000	3.066	1.941	0.0097	0.05
8.00	410	0.00	0.00	35.0	8.125	8.080	8.072	5.852	0.0190	2.065	0.1333	2.218	10.280	2.400	0.000	3.176	2.013	0.0104	0.06
9.00	410	0.00	0.00	35.0	8.128	8.081	8.073	5.806	0.0183	2.054	0.1381	2.210	10.280	2.400	0.000	3.288	2.088	0.0111	0.06
10.0	410	0.00	0.00	35.0	8.131	8.082	8.074	5.760	0.0177	2.042	0.1429	2.203	10.280	2.400	0.000	3.402	2.164	0.0119	0.07
11.0	410	0.00	0.00	35.0	8.133	8.083	8.075	5.715	0.0171	2.030	0.1478	2.195	10.280	2.400	0.000	3.519	2.242	0.0127	0.08
12.0	410	0.00	0.00	35.0	8.136	8.084	8.075	5.671	0.0166	2.018	0.1528	2.188	10.280	2.400	0.000	3.639	2.323	0.0136	0.09
13.0	410	0.00	0.00	35.0	8.139	8.085	8.076	5.626	0.0160	2.006	0.1580	2.180	10.280	2.400	0.000	3.761	2.405	0.0145	0.09
14.0	410	0.00	0.00	35.0	8.142	8.086	8.077	5.583	0.0155	1.993	0.1632	2.172	10.280	2.400	0.000	3.886	2.490	0.0155	0.10
15.0	410	0.00	0.00	35.0	8.145	8.086	8.077	5.540	0.0151	1.981	0.1684	2.164	10.280	2.400	0.000	4.013	2.577	0.0165	0.11
16.0	410	0.00	0.00	35.0	8.148	8.087	8.077	5.497	0.0146	1.968	0.1738	2.156	10.280	2.400	0.000	4.143	2.666	0.0176	0.12
17.0	410	0.00	0.00	35.0	8.150	8.087	8.078	5.455	0.0141	1.954	0.1793	2.148	10.280	2.400	0.000	4.275	2.758	0.0187	0.13
18.0	410	0.00	0.00	35.0	8.153	8.088	8.078	5.413	0.0137	1.941	0.1848	2.140	10.280	2.400	0.000	4.410	2.852	0.0200	0.13
19.0	410	0.00	0.00	35.0	8.156	8.088	8.078	5.372	0.0133	1.928	0.1904	2.131	10.280	2.400	0.000	4.548	2.948	0.0213	0.14
20.0	410	0.00	0.00	35.0	8.158	8.088	8.078	5.331	0.0129	1.914	0.1961	2.123	10.280	2.400	0.000	4.688	3.047	0.0226	0.15
21.0	410	0.00	0.00	35.0	8.161	8.088	8.078	5.291	0.0126	1.900	0.2018	2.114	10.280	2.400	0.000	4.830	3.148	0.0241	0.16
22.0	410	0.00	0.00	35.0	8.163	8.088	8.078	5.251	0.0122	1.886	0.2077	2.106	10.280	2.400	0.000	4.975	3.251	0.0256	0.17
23.0	410	0.00	0.00	35.0	8.166	8.088	8.078	5.211	0.0119	1.872	0.2135	2.097	10.280	2.400	0.000	5.123	3.357	0.0272	0.18
24.0	410	0.00	0.00	35.0	8.168	8.088	8.078	5.172	0.0116	1.857	0.2195	2.088	10.280	2.400	0.000	5.273	3.465	0.0289	0.19
25.0	410	0.00	0.00	35.0	8.171	8.088	8.077	5.134	0.0112	1.842	0.2255	2.079	10.280	2.400	0.000	5.426	3.577	0.0307	0.19
26.0	410	0.00	0.00	35.0	8.173	8.087	8.077	5.095	0.0109	1.828	0.2316	2.070	10.280	2.400	0.000	5.582	3.690	0.0325	0.20
27.0	410	0.00	0.00	35.0	8.176	8.087	8.076	5.057	0.0107	1.813	0.2377	2.061	10.280	2.400	0.000	5.739	3.807	0.0345	0.21
28.0	410	0.00	0.00	35.0	8.178	8.087	8.076	5.020	0.0104	1.798	0.2439	2.052	10.280	2.400	0.000	5.900	3.926	0.0366	0.22
29.0	410	0.00	0.00	35.0	8.180	8.086	8.075	4.983	0.0101	1.782	0.2501	2.042	10.280	2.400	0.000	6.063	4.047	0.0388	0.23
30.0	410	0.00	0.00	35.0	8.183	8.086	8.074	4.946	0.0099	1.767	0.2564	2.033	10.280	2.400	0.000	6.228	4.172	0.0411	0.24

2) ppmCO2 ranging from 300 to 500 (step : 10) while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHtot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
4.00	300	0.00	0.00	35.0	8.231	8.194	8.186	5.922	0.0160	2.032	0.1462	2.194	10.280	2.400	0.000	3.491	2.201	0.0079	0.00
4.00	310	0.00	0.00	35.0	8.219	8.182	8.174	5.934	0.0166	2.040	0.1427	2.200	10.280	2.400	0.000	3.407	2.149	0.0079	-0.01
4.00	320	0.00	0.00	35.0	8.207	8.170	8.162	5.946	0.0171	2.049	0.1394	2.205	10.280	2.400	0.000	3.328	2.099	0.0079	-0.01
4.00	330	0.00	0.00	35.0	8.195	8.158	8.150	5.958	0.0176	2.057	0.1362	2.210	10.280	2.400	0.000	3.252	2.051	0.0079	-0.02
4.00	340	0.00	0.00	35.0	8.184	8.147	8.139	5.969	0.0182	2.064	0.1332	2.216	10.280	2.400	0.000	3.180	2.005	0.0079	-0.02
4.00	350	0.00	0.00	35.0	8.173	8.136	8.128	5.980	0.0187	2.071	0.1303	2.220	10.280	2.400	0.000	3.111	1.962	0.0079	-0.03
4.00	360	0.00	0.00	35.0	8.162	8.125	8.117	5.991	0.0192	2.078	0.1275	2.225	10.280	2.400	0.000	3.044	1.920	0.0079	-0.03
4.00	370	0.00	0.00	35.0	8.152	8.114	8.107	6.002	0.0198	2.085	0.1249	2.230	10.280	2.400	0.000	2.981	1.880	0.0079	-0.04
4.00	380	0.00	0.00	35.0	8.141	8.104	8.096	6.012	0.0203	2.091	0.1223	2.234	10.280	2.400	0.000	2.921	1.842	0.0079	-0.04
4.00	390	0.00	0.00	35.0	8.131	8.094	8.086	6.022	0.0208	2.098	0.1199	2.238	10.280	2.400	0.000	2.862	1.805	0.0079	-0.04
4.00	400	0.00	0.00	35.0	8.122	8.084	8.077	6.032	0.0214	2.103	0.1176	2.242	10.280	2.400	0.000	2.806	1.770	0.0079	-0.05
4.00	410	0.00	0.00	35.0	8.112	8.075	8.067	6.041	0.0219	2.109	0.1153	2.246	10.280	2.400	0.000	2.753	1.736	0.0079	-0.05
4.00	420	0.00	0.00	35.0	8.103	8.065	8.058	6.051	0.0224	2.114	0.1131	2.250	10.280	2.400	0.000	2.701	1.704	0.0079	-0.06
4.00	430	0.00	0.00	35.0	8.094	8.056	8.049	6.060	0.0230	2.120	0.1111	2.254	10.280	2.400	0.000	2.651	1.672	0.0079	-0.06
4.00	440	0.00	0.00	35.0	8.085	8.047	8.040	6.069	0.0235	2.125	0.1091	2.257	10.280	2.400	0.000	2.603	1.642	0.0079	-0.06
4.00	450	0.00	0.00	35.0	8.076	8.039	8.031	6.077	0.0240	2.130	0.1071	2.261	10.280	2.400	0.000	2.557	1.613	0.0079	-0.07
4.00	460	0.00	0.00	35.0	8.067	8.030	8.022	6.086	0.0246	2.134	0.1053	2.264	10.280	2.400	0.000	2.513	1.585	0.0079	-0.07
4.00	470	0.00	0.00	35.0	8.059	8.022	8.014	6.094	0.0251	2.139	0.1035	2.267	10.280	2.400	0.000	2.470	1.558	0.0079	-0.07
4.00	480	0.00	0.00	35.0	8.051	8.013	8.006	6.103	0.0256	2.143	0.1017	2.271	10.280	2.400	0.000	2.428	1.531	0.0079	-0.08
4.00	490	0.00	0.00	35.0	8.043	8.005	7.997	6.111	0.0262	2.147	0.1000	2.274	10.280	2.400	0.000	2.388	1.506	0.0079	-0.08
4.00	500	0.00	0.00	35.0	8.035	7.997	7.989	6.119	0.0267	2.152	0.0984	2.277	10.280	2.400	0.000	2.349	1.482	0.0079	-0.08

3) Pressure ranging from 0 to 600 bar(step : 20) while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHTot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
4.00	410	0.00	0.00	35.0	8.112	8.075	8.067	6.041	0.0219	2.109	0.1153	2.246	10.280	2.400	0.000	2.753	1.736	0.0079	0.00
4.00	410	0.00	0.20	35.0	8.103	8.066	8.058	6.041	0.0219	2.110	0.1145	2.247	10.280	2.400	0.000	2.626	1.660	0.0079	-0.00
4.00	410	0.00	0.40	35.0	8.094	8.058	8.050	6.040	0.0219	2.112	0.1138	2.247	10.280	2.400	0.000	2.506	1.588	0.0079	-0.00
4.00	410	0.00	0.60	35.0	8.085	8.049	8.042	6.039	0.0219	2.113	0.1130	2.248	10.280	2.400	0.000	2.392	1.519	0.0079	-0.00
4.00	410	0.00	0.80	35.0	8.076	8.040	8.033	6.038	0.0219	2.114	0.1123	2.248	10.280	2.400	0.000	2.283	1.454	0.0079	-0.00
4.00	410	0.00	1.00	35.0	8.066	8.032	8.025	6.037	0.0219	2.115	0.1116	2.249	10.280	2.400	0.000	2.180	1.392	0.0079	-0.00
4.00	410	0.00	1.20	35.0	8.057	8.023	8.016	6.037	0.0219	2.116	0.1109	2.249	10.280	2.400	0.000	2.082	1.332	0.0079	-0.00
4.00	410	0.00	1.40	35.0	8.048	8.015	8.008	6.036	0.0219	2.118	0.1101	2.250	10.280	2.400	0.000	1.989	1.276	0.0079	-0.00
4.00	410	0.00	1.60	35.0	8.039	8.006	8.000	6.035	0.0219	2.119	0.1094	2.250	10.280	2.400	0.000	1.901	1.222	0.0079	-0.00
4.00	410	0.00	1.80	35.0	8.030	7.998	7.991	6.035	0.0219	2.120	0.1088	2.250	10.280	2.400	0.000	1.817	1.171	0.0079	-0.00
4.00	410	0.00	2.00	35.0	8.021	7.989	7.983	6.034	0.0219	2.121	0.1081	2.251	10.280	2.400	0.000	1.736	1.122	0.0079	-0.00
4.00	410	0.00	2.20	35.0	8.012	7.981	7.975	6.033	0.0219	2.122	0.1074	2.251	10.280	2.400	0.000	1.660	1.075	0.0079	-0.01
4.00	410	0.00	2.40	35.0	8.003	7.972	7.967	6.032	0.0219	2.123	0.1067	2.252	10.280	2.400	0.000	1.588	1.031	0.0079	-0.01
4.00	410	0.00	2.60	35.0	7.994	7.964	7.958	6.032	0.0219	2.124	0.1061	2.252	10.280	2.400	0.000	1.519	0.988	0.0079	-0.01
4.00	410	0.00	2.80	35.0	7.986	7.955	7.950	6.031	0.0219	2.125	0.1054	2.253	10.280	2.400	0.000	1.453	0.948	0.0079	-0.01
4.00	410	0.00	3.00	35.0	7.977	7.947	7.942	6.031	0.0219	2.126	0.1048	2.253	10.280	2.400	0.000	1.391	0.909	0.0079	-0.01
4.00	410	0.00	3.20	35.0	7.968	7.938	7.934	6.030	0.0219	2.127	0.1042	2.253	10.280	2.400	0.000	1.331	0.872	0.0079	-0.01
4.00	410	0.00	3.40	35.0	7.959	7.930	7.926	6.030	0.0219	2.128	0.1035	2.254	10.280	2.400	0.000	1.274	0.837	0.0079	-0.01
4.00	410	0.00	3.60	35.0	7.950	7.921	7.917	6.029	0.0219	2.129	0.1029	2.254	10.280	2.400	0.000	1.220	0.804	0.0079	-0.01
4.00	410	0.00	3.80	35.0	7.941	7.913	7.909	6.029	0.0219	2.130	0.1023	2.254	10.280	2.400	0.000	1.169	0.771	0.0079	-0.01
4.00	410	0.00	4.00	35.0	7.932	7.904	7.901	6.028	0.0219	2.131	0.1017	2.255	10.280	2.400	0.000	1.120	0.741	0.0079	-0.01
4.00	410	0.00	4.20	35.0	7.923	7.896	7.893	6.028	0.0219	2.132	0.1011	2.255	10.280	2.400	0.000	1.073	0.712	0.0079	-0.01
4.00	410	0.00	4.40	35.0	7.915	7.887	7.885	6.027	0.0219	2.133	0.1005	2.255	10.280	2.400	0.000	1.028	0.684	0.0079	-0.01
4.00	410	0.00	4.60	35.0	7.906	7.879	7.876	6.027	0.0219	2.134	0.0999	2.256	10.280	2.400	0.000	0.986	0.657	0.0079	-0.01
4.00	410	0.00	4.80	35.0	7.897	7.871	7.868	6.027	0.0219	2.135	0.0994	2.256	10.280	2.400	0.000	0.945	0.631	0.0079	-0.01
4.00	410	0.00	5.00	35.0	7.888	7.862	7.860	6.026	0.0219	2.136	0.0988	2.256	10.280	2.400	0.000	0.907	0.607	0.0079	-0.01
4.00	410	0.00	5.20	35.0	7.880	7.854	7.852	6.026	0.0219	2.137	0.0983	2.257	10.280	2.400	0.000	0.870	0.584	0.0079	-0.01
4.00	410	0.00	5.40	35.0	7.871	7.845	7.844	6.026	0.0219	2.137	0.0977	2.257	10.280	2.400	0.000	0.834	0.561	0.0079	-0.01
4.00	410	0.00	5.60	35.0	7.862	7.837	7.836	6.026	0.0219	2.138	0.0972	2.257	10.280	2.400	0.000	0.801	0.540	0.0079	-0.01
4.00	410	0.00	5.80	35.0	7.854	7.829	7.827	6.026	0.0219	2.139	0.0966	2.258	10.280	2.400	0.000	0.769	0.520	0.0079	-0.01
4.00	410	0.00	6.00	35.0	7.845	7.820	7.819	6.026	0.0219	2.140	0.0961	2.258	10.280	2.400	0.000	0.738	0.500	0.0079	-0.01

4) Salinity ranging from 30 to 40 g/kg-soln(step:0.5) while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHtot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
4.00	410	0.00	0.00	30.0	8.060	8.024	8.016	6.124	0.0226	1.853	0.0799	1.956	8.8114	2.057	0.000	1.957	1.220	0.0079	0.00
4.00	410	0.00	0.00	30.5	8.065	8.029	8.022	6.115	0.0225	1.880	0.0831	1.985	8.9583	2.091	0.000	2.029	1.267	0.0079	-0.03
4.00	410	0.00	0.00	31.0	8.071	8.035	8.027	6.107	0.0224	1.906	0.0863	2.015	9.1051	2.126	0.000	2.103	1.315	0.0079	-0.06
4.00	410	0.00	0.00	31.5	8.077	8.040	8.032	6.098	0.0224	1.932	0.0896	2.044	9.2520	2.160	0.000	2.178	1.364	0.0079	-0.09
4.00	410	0.00	0.00	32.0	8.082	8.045	8.038	6.089	0.0223	1.958	0.0930	2.073	9.3989	2.194	0.000	2.255	1.414	0.0079	-0.12
4.00	410	0.00	0.00	32.5	8.087	8.050	8.043	6.081	0.0222	1.984	0.0965	2.102	9.5457	2.229	0.000	2.334	1.465	0.0079	-0.15
4.00	410	0.00	0.00	33.0	8.092	8.055	8.048	6.073	0.0222	2.009	0.1001	2.131	9.6926	2.263	0.000	2.414	1.517	0.0079	-0.18
4.00	410	0.00	0.00	33.5	8.097	8.060	8.053	6.065	0.0221	2.034	0.1037	2.160	9.8394	2.297	0.000	2.496	1.570	0.0079	-0.20
4.00	410	0.00	0.00	34.0	8.102	8.065	8.058	6.057	0.0220	2.059	0.1075	2.189	9.9863	2.331	0.000	2.580	1.624	0.0079	-0.23
4.00	410	0.00	0.00	34.5	8.107	8.070	8.062	6.049	0.0220	2.084	0.1114	2.218	10.133	2.366	0.000	2.666	1.680	0.0079	-0.26
4.00	410	0.00	0.00	35.0	8.112	8.075	8.067	6.041	0.0219	2.109	0.1153	2.246	10.280	2.400	0.000	2.753	1.736	0.0079	-0.29
4.00	410	0.00	0.00	35.5	8.117	8.079	8.072	6.034	0.0218	2.134	0.1194	2.275	10.427	2.434	0.000	2.842	1.794	0.0079	-0.32
4.00	410	0.00	0.00	36.0	8.121	8.084	8.076	6.026	0.0218	2.158	0.1235	2.303	10.574	2.469	0.000	2.932	1.852	0.0079	-0.35
4.00	410	0.00	0.00	36.5	8.126	8.088	8.081	6.019	0.0217	2.182	0.1278	2.331	10.721	2.503	0.000	3.025	1.912	0.0079	-0.38
4.00	410	0.00	0.00	37.0	8.130	8.093	8.085	6.012	0.0216	2.205	0.1322	2.359	10.867	2.537	0.000	3.119	1.972	0.0079	-0.40
4.00	410	0.00	0.00	37.5	8.134	8.097	8.089	6.005	0.0216	2.229	0.1366	2.387	11.014	2.571	0.000	3.215	2.034	0.0079	-0.43
4.00	410	0.00	0.00	38.0	8.139	8.101	8.093	5.998	0.0215	2.252	0.1412	2.415	11.161	2.606	0.000	3.314	2.097	0.0079	-0.46
4.00	410	0.00	0.00	38.5	8.143	8.106	8.098	5.991	0.0214	2.275	0.1459	2.443	11.308	2.640	0.000	3.414	2.160	0.0079	-0.49
4.00	410	0.00	0.00	39.0	8.147	8.110	8.102	5.984	0.0214	2.298	0.1508	2.470	11.455	2.674	0.000	3.515	2.225	0.0079	-0.51
4.00	410	0.00	0.00	39.5	8.151	8.114	8.106	5.978	0.0213	2.321	0.1557	2.498	11.602	2.709	0.000	3.619	2.291	0.0078	-0.54
4.00	410	0.00	0.00	40.0	8.155	8.118	8.110	5.971	0.0213	2.343	0.1608	2.525	11.749	2.743	0.000	3.725	2.358	0.0078	-0.57

5) pptF (fraction of CaCO3 which precipitates) from 0 to 1(step : 0.05) while all other 5 parameters remain as default

Temp	CO2	pptF	Pres	Saln	pHfr.	pHtot	pHsws	pOH	H2CO3	HCO3-	CO3--	DIC	Ca++	Alk	CaCO3	over1	over2	pH2O	Cout
4.00	410	0.00	0.00	35.0	8.112	8.075	8.067	6.041	0.0219	2.109	0.1153	2.246	10.280	2.400	0.000	2.753	1.736	0.0079	0.00
4.00	410	0.05	0.00	35.0	8.025	7.988	7.980	6.129	0.0219	1.725	0.0772	1.824	10.045	1.930	0.235	1.800	1.135	0.0079	0.19
4.00	410	0.10	0.00	35.0	7.979	7.942	7.934	6.174	0.0219	1.552	0.0624	1.636	9.9415	1.723	0.338	1.442	0.909	0.0079	0.27
4.00	410	0.15	0.00	35.0	7.955	7.918	7.910	6.198	0.0219	1.469	0.0560	1.547	9.8925	1.625	0.388	1.285	0.811	0.0079	0.31
4.00	410	0.20	0.00	35.0	7.941	7.904	7.896	6.212	0.0219	1.423	0.0525	1.497	9.8652	1.570	0.415	1.202	0.758	0.0079	0.33
4.00	410	0.25	0.00	35.0	7.932	7.895	7.887	6.221	0.0219	1.394	0.0503	1.466	9.8481	1.536	0.432	1.152	0.726	0.0079	0.35
4.00	410	0.30	0.00	35.0	7.926	7.889	7.881	6.227	0.0219	1.374	0.0489	1.445	9.8365	1.513	0.444	1.118	0.705	0.0079	0.36
4.00	410	0.35	0.00	35.0	7.921	7.884	7.876	6.232	0.0219	1.359	0.0479	1.429	9.8281	1.496	0.452	1.093	0.690	0.0079	0.37
4.00	410	0.40	0.00	35.0	7.918	7.881	7.873	6.235	0.0219	1.349	0.0471	1.418	9.8217	1.483	0.458	1.075	0.678	0.0079	0.37
4.00	410	0.45	0.00	35.0	7.915	7.878	7.870	6.238	0.0219	1.340	0.0465	1.408	9.8168	1.474	0.463	1.061	0.669	0.0079	0.37
4.00	410	0.50	0.00	35.0	7.913	7.876	7.868	6.240	0.0219	1.333	0.0461	1.401	9.8128	1.466	0.467	1.050	0.662	0.0079	0.38
4.00	410	0.55	0.00	35.0	7.911	7.874	7.866	6.242	0.0219	1.328	0.0457	1.395	9.8095	1.459	0.470	1.041	0.656	0.0079	0.38
4.00	410	0.60	0.00	35.0	7.910	7.872	7.864	6.244	0.0219	1.323	0.0454	1.390	9.8068	1.454	0.473	1.033	0.652	0.0079	0.38
4.00	410	0.65	0.00	35.0	7.908	7.871	7.863	6.245	0.0219	1.319	0.0451	1.386	9.8045	1.449	0.476	1.027	0.648	0.0079	0.38
4.00	410	0.70	0.00	35.0	7.907	7.870	7.862	6.246	0.0219	1.316	0.0449	1.382	9.8025	1.445	0.477	1.021	0.644	0.0079	0.39
4.00	410	0.75	0.00	35.0	7.906	7.869	7.861	6.247	0.0219	1.313	0.0447	1.379	9.8008	1.442	0.479	1.017	0.641	0.0079	0.39
4.00	410	0.80	0.00	35.0	7.905	7.868	7.860	6.248	0.0219	1.310	0.0445	1.376	9.7993	1.439	0.481	1.012	0.639	0.0079	0.39
4.00	410	0.85	0.00	35.0	7.905	7.867	7.859	6.249	0.0219	1.308	0.0443	1.374	9.7980	1.436	0.482	1.009	0.636	0.0079	0.39
4.00	410	0.90	0.00	35.0	7.904	7.867	7.859	6.250	0.0219	1.306	0.0442	1.372	9.7968	1.434	0.483	1.006	0.634	0.0079	0.39
4.00	410	0.95	0.00	35.0	7.903	7.866	7.858	6.250	0.0219	1.304	0.0441	1.370	9.7957	1.431	0.484	1.003	0.632	0.0079	0.39
4.00	410	1.00	0.00	35.0	7.903	7.865	7.858	6.251	0.0219	1.302	0.0440	1.368	9.7948	1.430	0.485	1.000	0.631	0.0079	0.39

For those curious to try, here is the complete Octave script:

```
clear;clc;format short;format compact;
global SO4 KS K1 K2 Kw K7 K8 H2CO3 HCO3 CO3 OH F KF KB B BOH4 Ksp1 pptF Mg Sr Na K Cl Br H HT
global Hsws Ca Cal
% No [Mg(OH)+] or [Ca(OH)+] formation because they seem to be negligible effects

function y = neut(pH) % ==> pH free scale, i.e. chemical true scale, always used if not otherwise stated !!
    global SO4 KS K1 K2 Kw K7 K8 H2CO3 HCO3 CO3 OH F KF KB B BOH4 Ksp1 pptF Mg Sr Na K Cl Br H HT
    global Hsws Ca Cal
    H = 10^(-pH);Ca = Cal;
    HCO3 = K1*H2CO3/H;
    CO3 = K2*HCO3/H;
    HF = H*F/(KF + H);
    HSO4 = H*SO4/(KS + H);
    Hsws = H + HF + HSO4; % ==> pH SWS scale only here
    OH = Kw/Hsws; % ==> pH SWS scale only here
    HT = H + HSO4; % ==> pH total scale only here
    BOH4 = KB*B/(HT + KB); % ==> pH total scale only here
    % solubility check for CaCO3
    if (Ca*CO3)>Ksp1
        x1 = (Ca*CO3 - Ksp1)/CO3; % primo grado
        Ca = Ca - x1*pptF;
    end
    % end of solubility check
    y = H - OH + 2*Ca + 2*Mg + 2*Sr + Na + K - 2*(SO4-HSO4) - BOH4 - HCO3 - 2*CO3 - Cl - (F-HF) - Br - HSO4;
endfunction

Cini = 0;
% Display of data in condensed form is prepared.
disp('Temp = temperature in degree Celsius (°C)');
disp('CO2 = ppmv, parts per million in volume of CO2 in dry air');
disp('pptF = fraction of CaCO3(calcite) which precipitates, ratio to complete precipitation(when omega=1)');
disp('Pres = pressure in atm x 100');
disp('Saln = salinity in grams of dissolved salts per kg of solution');
disp('pHfr. pHtot pHsws = different pH scales, free, total and seawater');
disp('pOH = -log10[OH-]');
disp('H2CO3 HCO3 CO3 = concentrations in millimol/kg-solution');
disp('DIC = Dissolved Inorganic Carbon in mmol/kg-soln');
disp('Alk = alkalinity in mmol/kg-soln Alk = 2*CO3+HCO3+OH+BOH4-H');
disp('Ca++ CaCO3 = concentrations in mmol/kg-soln');
```



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% --> Waters, Millero, Woosley (Mar. Chem., 165, 66-67, 2014) [H+]=free scale
LnK1 = -log(10)*(6320.813/T + 19.568224*log(T) -126.34048 + 5.592953*S^0.5 + 0.028845*S - (6.388e-5)*S^2 + (-
225.7489*S^0.5 - 4.761*S)/T -0.8715109*S^0.5*log(T));
% HCO3- <==> H+ + CO3--
% --> Waters, Millero, Woosley (Mar. Chem., 165, 66-67, 2014) [H+]=free scale
LnK2 = -log(10)*(5143.692/T + 14.613358*log(T) - 90.18333 + 13.396949*S^0.5 + 0.12193009*S - (3.8362e-4)*S^2 + (-
472.8633*S^0.5 - 19.03634*S)/T - 2.1563270*S^0.5*log(T));

% H2O <==> H+ + OH- (DOE 1994) % pH = pH(SWS) !!
LnKw = 148.9802 - 13847.26/T - 23.6521*log(T) + (118.67/T - 5.977 + 1.0495*log(T))*S^0.5 - 0.01615*S;

% HSO4- <==> H+ + SO4--
I = 19.924*S/(1000 - 1.005*S); % ionic strenght, useful for KS and KF calculations
LnKS = -4276.1/T + 141.328 - 23.039*log(T) + (-13856/T + 324.57 - 47.986*log(T))*I^0.5 + (35474/T - 771.54 +
114.723*log(T))*I -2698/T*I^1.5 + 1766/T*I^2 + log(1-0.001005*S);

% HF <==> H+ + F-
LnKF = 1590.2/T - 12.641 + 1.525*I^0.5 + log(1-0.001005*S); % pH = pH free NO conversion to total

% CaCO3calcite <==> Ca++ + CO3--
LogKspCal = -171.9065 - 0.077993*T + 2839.319/T + 71.595*log10(T) + (-0.77712 + 0.0028426*T + 178.34/T)*S^0.5 -
0.07711*S + 0.0041249*S^1.5;
LnKspCal = LogKspCal*log(10);

% CaCO3aragonite <==> Ca++ + CO3--
LogKspAra = -171.945 - 0.077993*T + 2903.293/T + 71.595*log10(T) + (-0.068393 + 0.0017276*T + 88.135/T)*S^0.5 -
0.10018*S + 0.0059415*S^1.5;
LnKspAra = LogKspAra*log(10);

% B(OH)3 + H2O <==> H+ + B(OH)4-
LnKB = (-8966.9 - 2890.53*S^0.5 - 77.942*S + 1.728*S^1.5 - 0.0996*S^2)/T + 148.0248 + 137.1942*S^0.5 + 1.62142*S -
(24.4344 + 25.085*S^0.5 + 0.2474*S)*log(T) + 0.053105*S^0.5*T;

% The log(K) are modified according to hydrostatic pressure (on the sea surface P=0)
LnK1P = LnK1 + (25.5 - 0.1271*Tc)/R1/T*P + 0.5*(-3.08e-3 + 0.0877e-3*Tc)/R1/T*P^2;
LnK2P = LnK2 + (15.82 + 0.0219*Tc)/R1/T*P + 0.5*(1.13e-3 - 0.1475e-3*Tc)/R1/T*P^2;
LnKwP = LnKw + (25.6 - 0.2324*Tc + 3.6246e-3*Tc^2)/R1/T*P + 0.5*(-5.13e-3 + 0.0794e-3*Tc)/R1/T*P^2;
LnKBP = LnKB + (29.48 - 0.1622*Tc - 2.608e-3*Tc^2)/R1/T*P + 0.5*(-2.84e-3)/R1/T*P^2;
LnKspCalP = LnKspCal + (48.76 - 0.5304*Tc)/R1/T*P + 0.5*(-11.76e-3 + 0.3692e-3*Tc)/R1/T*P^2;
LnKspAraP = LnKspAra + (46 - 0.5304*Tc)/R1/T*P + 0.5*(-11.76e-3 + 0.3692e-3*Tc)/R1/T*P^2;
LnKSP = LnKS + (18.03 - 0.0466*Tc - 0.3160e-3*Tc^2)/R1/T*P + 0.5*(-4.53e-3 + 0.09e-3*Tc)/R1/T*P^2;
LnKFP = LnKF + (9.78 + 0.009*Tc + 0.942e-3*Tc^2)/R1/T*P + 0.5*(-3.91e-3 + 0.054*Tc)/R1/T*P^2;

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% The K(eq) values are calculated from their logarithms.
K1 = exp(LnK1P);K2 = exp(LnK2P);K0 = exp(LnK0);Kw = exp(LnKwP);Ksp1 = exp(LnKspCalP);
Ksp2 = exp(LnKspAraP);KS = exp(LnKSP);KF = exp(LnKFP);KB = exp(LnKBP);

% CO2 fugacity is introduced, according to Koertzing (pag 65 Zeebe and Gladrow 2001)
fCO2 = ppmCO2*exp(101325*((-1636.75 + 12.0408*T - 3.27957e-2*T^2 + 3.16528e-5*T^3)*1e-6 + 2*(57.7 -
0.118*T)*1e-6)/R/T);

% H2O vapour pressure is calculated for seawater, Weiss and Price 1980
LnpH2O = 24.4543 -6745.09/T - 4.8489*log(T/100) -0.000544*S;

% CO2 fugacity is corrected according to water vapour partial pressure
fCO2 = fCO2*(1 - exp(LnpH2O)*pH2O/100);
H2CO3 = K0*fCO2*1e-6;

[pH,fval,info] = fzero(@neut,[0,14]); % call to fzero

CaCO3 = (Ca1 - Ca)*1000;
DIC = (H2CO3+HCO3+CO3)*1000;          % Dissolved Inorganic Carbon in mmol/kg-soln
Alk = 1000*(2*CO3+HCO3+OH+BOH4-H);    % Total Alkalinity mmol/kg-soln
OverSatCal = Ca*CO3/Ksp1;             % Oversaturation of CaCO3 (calcite form)
OverSatAra = Ca*CO3/Ksp2;            % Oversaturation of CaCO3 (aragonite form)
if Cini == 0;Cini = 1000*(H2CO3 + HCO3 + CO3) + CaCO3;end %DIC iniziale
Cout = Cini - 1000*(H2CO3 + HCO3 + CO3) - CaCO3;          %CO2 outgassed during the for/endfor cycles

% The results are displayed.
if Tc<10;T1 = ['|',num2str(Tc,'%2f')];else T1 = ['|',num2str(Tc,'%1f')];endif
T1 = [T1,'|',num2str(ppmCO2,3),'|',num2str(pptF,'%2f'),'|',num2str(P/100,'%2f'),'|',num2str(S,'%1f')];
T1 = [T1,'|',num2str(pH,'%3f'),'|',num2str(-log10(HT),'%3f'),'|',num2str(-log10(Hsws),'%3f'),'|',num2str(-
log10(OH),'%3f')];
T1 = [T1,'|',num2str(H2CO3*1000,'%4f'),'|',num2str(HCO3*1000,'%3f'),'|',num2str(CO3*1000,'%4f')];
T1 = [T1,'|',num2str(DIC,'%3f'),'|'];
if Ca>0.01;T1 = [T1, num2str(Ca*1000,'%3f')];else;T1 = [T1, num2str(Ca*1000,'%4f')];endif
T1 = [T1,'|',num2str(Alk,'%3f'),'|',num2str(CaCO3,'%3f'),'|',num2str(OverSatCal,'%3f')];
T1 = [T1,'|',num2str(OverSatAra,'%3f'),'|',num2str(exp(LnpH2O),'%4f'),'|',num2str(Cout,'%2f')];
disp(T1);
++j;
endfor
disp(T2);

```