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Research article

ANN prediction of the CO_2 solubility in water and brine under reservoir conditions

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Appendix

Table A1. Pure water experimental solubility data.*

Temperature	Pressure	Solubility	Temperature	Pressure	Solubility
273.15	10	0.028943	323.20	6.06	0.0161
273.15	20	0.036002	323.20	7.08	0.0176
273.15	30	0.037789	323.20	8.08	0.019
273.15	40	0.038887	323.20	9.09	0.02
273.15	50	0.041325	323.20	10.09	0.0205
274.14	0.19	0.00262	323.20	11.1	0.021
274.83	1.201	0.0142	323.20	12.1	0.0214
276.74	1.327	0.0142	323.20	14.11	0.0217
278.15	10	0.031009	328.15	2.86	0.008322
278.15	20	0.03389	328.15	4.37	0.011859
278.15	30	0.035232	328.15	6.11	0.015005
278.15	40	0.036487	328.15	8.48	0.017963
278.22	0.228	0.00262	328.15	9.99	0.019171
278.22	0.501	0.00585	328.15	12.2	0.020556
278.22	0.755	0.00852	328.15	13.19	0.021034
278.22	1.016	0.01111	328.15	15.23	0.021295

278.22	1.322	0.01403	330.60	0.913	0.00262
278.22	1.674	0.01747	333.15	10	0.018669
278.22	2.031	0.02015	333.15	20	0.02233
278.74	1.426	0.0142	333.15	30	0.023893
283.15	10	0.028943	333.15	30	0.025075
283.15	20	0.031634	333.15	50	0.027736
283.15	30	0.032966	333.15	60	0.030146
283.15	30	0.034344	333.15	90	0.033907
283.15	50	0.036571	333.15	120	0.035216
283.38	1.732	0.0142	333.20	4.05	0.0096
284.27	0.287	0.00262	333.20	5.06	0.0121
284.37	3.938	0.02488	333.20	6.06	0.0138
288.15	10	0.0276	333.20	7.08	0.0157
288.15	20	0.030079	333.20	8.08	0.0166
288.15	30	0.031499	333.20	9.09	0.0179
288.15	30	0.032662	333.20	10.09	0.0186
288.26	0.496	0.00401	333.20	11.1	0.0195
288.26	1.103	0.00867	333.20	12.1	0.0201
288.26	1.941	0.01434	333.20	14.11	0.0208
288.26	2.777	0.01882	341.24	1.086	0.00262
288.26	3.719	0.02343	351.31	1.243	0.00262
288.26	4.601	0.02673	353.10	4.05	0.008
288.26	5.059	0.02797	353.10	6.06	0.0114
288.41	0.329	0.00262	353.10	7.08	0.0128
289.20	2.062	0.0142	353.10	8.08	0.014
289.62	4.844	0.02488	353.10	9.09	0.0151
292.35	5.172	0.02488	353.10	10.09	0.016
293.01	2.349	0.0142	353.10	11	0.0172
293.15	20	0.028417	353.10	12.1	0.0176
293.15	30	0.029808	353.10	13.1	0.0184
293.15	30	0.031246	353.15	10	0.015714
293.15	50	0.033336	353.15	20	0.021107
293.15	60	0.035299	353.15	30	0.023241
293.15	120	0.041953	353.15	30	0.024801
293.34	0.385	0.00262	353.15	50	0.026629
298.15	10	0.025126	353.15	60	0.028909
298.15	20	0.027447	353.15	90	0.03384
298.15	30	0.028841	353.15	120	0.035417
298.15	30	0.030265	373.15	20	0.020486
298.15	50	0.032325	373.15	30	0.023516
298.28	0.504	0.00314	373.15	30	0.024989
298.28	1.007	0.00614	373.15	50	0.027226
298.28	1.496	0.00887	373.15	60	0.029909
298.28	2.483	0.01356	373.15	90	0.034679
298.28	3.491	0.01772	373.15	120	0.037138
298.28	4.492	0.02089	393.15	10	0.013056

298.28	5.524	0.02323	393.15	20	0.020555
298.40	2.78	0.0142	393.15	30	0.023927
299.06	1.008	0.0059	393.15	30	0.026254
299.32	0.452	0.00262	393.15	50	0.028637
303.99	0.499	0.00262	393.15	60	0.031617
308.15	2.1	0.009329	393.15	90	0.037389
308.15	4.09	0.015731	393.15	120	0.039983
308.15	6.08	0.02034	413.15	20	0.021245
308.15	8.09	0.022383	413.15	30	0.025332
308.15	10.08	0.023125	413.15	30	0.028434
308.15	12.05	0.023737	413.15	50	0.031229
308.15	14.01	0.024525	413.15	60	0.03488
308.15	15.83	0.02492	413.15	90	0.039735
308.20	0.579	0.00276	413.15	120	0.044326
308.20	1.889	0.00856	433.15	10	0.012583
308.20	2.95	0.01212	433.15	20	0.021435
308.20	3.029	0.01259	433.15	30	0.027124
308.20	4.005	0.01563	433.15	30	0.031229
308.20	4.985	0.01837	433.15	50	0.034746
308.20	5.949	0.02033	433.15	60	0.038887
308.20	6.077	0.02066	433.15	90	0.045197
308.20	6.972	0.02229	433.15	120	0.050565
308.20	6.986	0.02152	453.15	20	0.023069
308.20	7.029	0.02221	453.15	30	0.029299
308.20	7.963	0.02304	453.15	30	0.034864
310.86	7.309	0.02017	453.15	50	0.038887
311.62	0.63	0.00262	453.15	60	0.043075
313.15	120	0.037222	453.15	90	0.052023
313.15	10	0.021693	453.15	120	0.059676
313.15	20	0.02451	473.15	10	0.012512
313.15	30	0.025827	473.15	20	0.023825
313.15	30	0.027089	473.15	30	0.032679
313.15	50	0.029808	473.15	30	0.039818
313.15	60	0.030586	473.15	50	0.044967
313.15	90	0.035567	473.15	60	0.050954
313.36	4.119	0.0142	473.15	90	0.063243
318.15	2.08	0.007485	473.15	120	0.070297
318.15	4.1	0.013046	493.15	20	0.025161
318.15	6.09	0.017103	493.15	30	0.035802
318.15	8.11	0.02021	493.15	30	0.044737
318.15	10.08	0.021686	493.15	50	0.052087
318.15	12.06	0.022296	493.15	60	0.059978
318.15	14.11	0.022644	493.15	90	0.07703
318.15	15.86	0.02295	493.15	120	0.0868
318.23	0.465	0.00182	513.15	10	0.011915
318.23	1.045	0.00394	513.15	20	0.027089

318.23	1.863	0.0068	513.15	30	0.040481
318.23	1.984	0.0073	513.15	30	0.051699
318.23	2.97	0.01036	513.15	50	0.061883
318.23	3.001	0.01018	513.15	60	0.071369
318.23	3.969	0.01293	513.15	90	0.097554
318.23	3.977	0.01259	513.15	120	0.11212
318.23	4.952	0.01508	533.15	20	0.028298
318.23	4.982	0.01532	533.15	30	0.04408
318.23	5.976	0.0172	533.15	30	0.060836
318.23	5.992	0.01726	533.15	50	0.073475
318.23	6.923	0.01895	533.15	60	0.092157
318.23	6.984	0.01905	533.15	90	0.126882
318.23	7.933	0.02031	533.15	120	0.149522
321.64	0.779	0.00262	553.15	10	0.008866
321.97	5.216	0.0142	553.15	20	0.0284
322.14	9.333	0.02017	553.15	30	0.048304
323.15	2.1	0.006816	553.15	30	0.071012
323.15	4.11	0.01169	553.15	50	0.088702
323.15	6.12	0.015689	553.15	60	0.122497
323.15	8.1	0.018136	573.15	10	0.005406
323.15	10.1	0.019993	573.15	20	0.028366
323.15	12.04	0.02086	573.15	30	0.053621
323.15	15.99	0.021599	573.15	30	0.084211
323.20	4.05	0.0109	573.15	50	0.119786
323.20	5.06	0.0137			

Note: *Data source literature: [20,22,41–43].

Table A2. Brine experimental solubility data.*

Temperature	Pressure	Salinity	Solubility	Temperature	Pressure	Salinity	Solubility
273.15	10	1	0.02525	373	1.7	1	0.00237
273.15	10	3	0.01691	373	5.05	1	0.0068
278.15	10	1	0.02424	373	9.97	1	0.01137
278.15	10	3	0.01601	373	15	1	0.0147
283.15	10	1	0.02304	373	19.96	1	0.01667
283.15	10	3	0.01533	373	30	1	0.01897
288.15	10	1	0.02191	373	6.05	1.13	0.0075
293.15	10	1	0.02091	373	15.19	1.13	0.0136
293.15	10	3	0.01417	373	19.2	1.13	0.0157
293.17	3.34	0.5	0.017	373	5.74	2.5	0.00545
298.15	10	1	0.02013	373	11.87	2.5	0.00911
298.15	10	1	0.02013	373	14.92	2.5	0.01039
298.15	20	5	0.01055	373	18.01	2.5	0.01139
313	0.46	4	0.00095	373	5	3	0.00417
313	0.56	4	0.00101	373	10	3	0.00834

313	0.84	4	0.00149	373	20.06	3	0.01129
313	2.34	4	0.00403	373	30	3	0.01357
313	4.03	4	0.00657	373	5	5	0.00383
313	5.09	4	0.0081	373	10	5	0.00697
313	6.88	4	0.00975	373	15	5	0.00859
313	0.61	6	0.001	373	20	5	0.01031
313	1.28	6	0.002	373	4.68	6	0.00333
313	2.36	6	0.004	373	12.06	6	0.00654
313	6.79	6	0.008	373	20.59	6	0.00846
313	1.89	4	0.00363	373	10.05	1	0.01188
313	1.25	4	0.00222	373	6.82	1	0.00833
313	3.16	4	0.00556	373	15.02	1	0.01507
313	5.98	4	0.00898	373	3.11	1.13	0.0039
313	4.46	6	0.006	373	19.15	3	0.01117
313.28	1.81	0.25	0.007	373	10	5	0.00652
323	5.07	1	0.01102	373	20	5	0.00975
323	10.15	1	0.01621	373.15	15	3	0.01044
323	14.29	1	0.01748	373.15	15	4	0.00877
323	15	1	0.01803	373.15	15	6	0.00689
323	20.01	1	0.0187	373.2	30	1	0.01897
323	30	1	0.02046	373.2	40	1	0.02107
323	5.35	1.13	0.0103	373.2	30	5	0.0114
323	10.04	1.13	0.0151	393	5	1	0.00617
323	14.51	1.13	0.01701	393	10	1	0.01071
323	5.74	2.5	0.00875	393	20	1	0.01603
323	11.77	2.5	0.01238	393	1.2	4	0.00093
323	15.02	2.5	0.01293	393	2.33	4	0.00186
323	18.21	2.5	0.01335	393	7.65	4	0.00561
323	4.87	3	0.0077	393	10	4	0.00667
323	10.08	3	0.01122	393	20	4	0.00996
323	14.38	3	0.0123	393	0.151	6	0.00001
323	20.12	3	0.01296	393	1.42	6	0.00093
323	5	5	0.00602	393	5.94	6	0.0037
323	15	5	0.00987	393	9.14	6	0.00546
323	20	5	0.00997	393	9.33	4	0.00654
323	30	5	0.01077	393	5	4	0.00389
323	3.58	6	0.00418	393	4.74	4	0.00374
323	8.97	6	0.0076	393.15	20	3	0.01133
323	24.58	6	0.00939	413	5	1	0.00552
323	7.56	1.13	0.0129	413	15	1	0.01476
323	8.73	2.5	0.01146	413	20	1	0.01704
323	5.05	3	0.0082	413	10	3	0.00745
323	15.04	3	0.01227	413	20	3	0.01213
323	10	5	0.00876	413	30	3	0.01356
323.15	15	4	0.01035	413	1.39	4	0.00091
323.15	15	6	0.00802	413	2.55	4	0.00182

323.2	40	1	0.02163	413	8.67	4	0.00586
323.2	40	5	0.01165	413	5	5	0.00342
333	9.88	1	0.01481	413	10	5	0.0058
333	19.94	1	0.01779	413	15	5	0.00825
333	20	1	0.01784	413	20	5	0.00954
333	30	1	0.01954	413	1.66	6	0.00092
333	9.81	2	0.01245	413	3.2	6	0.00184
333	19.97	2	0.01455	413	6.29	6	0.00368
333	29.43	2	0.01596	413	9.2	6	0.00515
333	1.33	4	0.00193	413	20	1	0.01655
333	2.51	4	0.00345	413	5.04	4	0.00364
333	3.52	4	0.0046	413	10	1	0.01054
333	4.74	4	0.00591	413	10	5	0.00617
333	9.64	4	0.0094	413.15	30	5	0.01073
333	19.93	4	0.01108	413.2	30	1	0.02187
333	29.44	4	0.01159	413.2	40	1	0.02261
333	0.82	6	0.00095	423	4.94	1	0.00567
333	3.66	6	0.00378	423	9.98	1	0.01035
333	6.84	6	0.00606	423	15.05	1	0.01427
333	8.67	6	0.00709	423	20.01	1	0.01699
333	10	1	0.01514	423	4.97	2	0.00469
333	29.42	1	0.01984	423	15	2	0.01112
333	2.87	4	0.00392	423	19.99	2	0.01377
333	7.3	4	0.00799	423	29.98	2	0.01684
333	9.81	4	0.00895	423	15	3	0.00957
333	1.68	6	0.00188	423	4.95	4	0.00354
333.15	20	1	0.01753	423	9.97	4	0.00632
333.15	20	3	0.0122	423	15	4	0.00829
342.81	7.26	3.01	0.0088	423	20	4	0.01003
342.82	3.04	3.01	0.00441	423	29.98	4	0.01248
342.82	10.1	3.01	0.01057	423	5.04	6	0.00291
353	10	1	0.01314	423	10.1	6	0.0051
353	20	1	0.01678	423	14.96	6	0.00678
353	30	1	0.01914	423	20.21	6	0.00827
353	10	3	0.00922	423	15	5	0.00721
353	20	3	0.01236	423	10.01	2	0.00852
353	30	3	0.01386	423	5.03	1	0.00546
353	1.64	4	0.00182	423	10.04	1	0.01017
353	5.59	4	0.00552	433	10	3	0.00715
353	6.94	4	0.00643	433	20	3	0.01214
353	9.64	4	0.00824	433	30	3	0.015
353	3.39	4	0.00364	433	1.66	4	0.00096
353	8.337	4	0.00735	433	5.9	4	0.00393
353.05	7.78	0.5	0.012	433	9.09	4	0.00586
353.12	3.96	0.5	0.007	433	10	5	0.00601
353.14	5.72	2	0.007	433	20	5	0.00957

353.15	10	5	0.00703	433	30	5	0.012
353.16	14.29	2	0.013	433	1.88	6	0.00096
353.18	12.53	0.5	0.017	433	3.4	6	0.0019
363	9.8	1	0.01217	433	6.62	6	0.00375
363	19.93	1	0.01605	433	8.99	6	0.00499
363	29.4	1	0.01866	453.15	10	1	0.00958
363	9.84	2	0.01042	453.15	20	1	0.0172
363	19.97	2	0.01324	453.15	30	1	0.02254
363	29.44	2	0.01516	453.15	40	1	0.02651
363	9.84	4	0.00741	453.15	10	3	0.0068
363	19.92	4	0.01035	453.15	20	3	0.0117
372.39	2.56	3.01	0.00292	453.15	30	3	0.01507
372.45	22.982	3.01	0.01337	453.15	40	3	0.01742

Note: *Data source literature: [21,27,30,44–46].

Table A3. Validation set of the ANN predictions on CO_2 solublity in water based on comparisons between literature reported data and the predicted solubility data.

Temperature (K)	Pressure	Actual Solubility	Predicted Solubility	Percentage Error (%)
278.15	20	0.03389	0.033463	1.260748
278.15	40	0.036487	0.036972	1.329639
283.15	20	0.031634	0.031214	1.328938
288.26	2.777	0.01882	0.018424	2.104706
288.26	5.059	0.02797	0.025831	7.647223
288.41	0.329	0.00262	0.00282	7.623903
293.15	20	0.028417	0.028359	0.204124
293.34	0.385	0.00262	0.003152	20.29977
298.15	20	0.027447	0.027122	1.18309
298.28	5.524	0.02323	0.023239	0.036649
298.28	1.007	0.00614	0.006072	1.106928
298.28	2.483	0.01356	0.013151	3.015233
299.06	1.008	0.0059	0.005959	1.003378
299.32	0.452	0.00262	0.003163	20.7205
308.2	5.949	0.02033	0.020229	0.496873
308.2	1.889	0.00856	0.008604	0.519767
313.15	60	0.030586	0.031125	1.759592
313.15	30	0.027089	0.025581	5.568723
318.23	3.001	0.01018	0.010226	0.450706
318.23	4.952	0.01508	0.014714	2.424333
318.23	3.969	0.01293	0.012436	3.820877
318.23	1.045	0.00394	0.004061	3.064352
318.23	5.976	0.0172	0.016723	2.775468
323.2	10.09	0.0205	0.020093	1.985359
323.2	7.08	0.0176	0.017171	2.438658
333.2	6.06	0.0138	0.013851	0.372514

333.2	14.11	0.0208	0.0204	1.921327
341.24	1.086	0.00262	0.002527	3.562063
353.1	7.08	0.0128	0.01305	1.949852
353.1	10.09	0.016	0.015879	0.753726
353.15	60	0.028909	0.029008	0.342841
373.15	90	0.034679	0.034166	1.480612
393.15	20	0.020555	0.020115	2.140782
393.15	50	0.028637	0.029022	1.342924
413.15	20	0.021245	0.020336	4.278199
413.15	30	0.025332	0.026778	5.710113
413.15	120	0.044326	0.043773	1.248116
433.15	10	0.012583	0.012113	3.736293
433.15	90	0.045197	0.044983	0.471978
433.15	50	0.034746	0.035202	1.312322
433.15	30	0.031229	0.028773	7.864495
433.15	120	0.050565	0.050901	0.664742
473.15	120	0.070297	0.072138	2.6192
473.15	10	0.012512	0.013105	4.734776
473.15	50	0.044967	0.044564	0.895979
493.15	30	0.044737	0.039814	11.00548
513.15	20	0.027089	0.026839	0.925405

Table A4. Validation set of the ANN predictions on CO_2 solublity in brine based on comparisons between literature reported data and the predicted solubility data.

Temperature	Pressure	Salinity	True Solubility	Predicted Solubility	Percentage Error (%)
298.15	10	1	0.02013	0.020121	0.044188
298.15	20	5	0.01055	0.010611	0.581637
313	1.89	4	0.00363	0.003474	4.297016
313	1.25	4	0.00222	0.00238	7.221207
313	3.16	4	0.00556	0.005594	0.619806
313	5.98	4	0.00898	0.008987	0.078866
313	4.46	6	0.006	0.005879	2.020286
323	7.56	1.13	0.0129	0.013455	4.304295
323	8.73	2.5	0.01146	0.011717	2.242575
323	5.05	3	0.0082	0.008127	0.894103
323	15.04	3	0.01227	0.012477	1.689677
323	10	5	0.00876	0.008535	2.564373
333	10	1	0.01514	0.015253	0.744657
333	29.42	1	0.01984	0.019633	1.043465
333	2.87	4	0.00392	0.003896	0.60761
333	7.3	4	0.00799	0.00812	1.626852
333	9.81	4	0.00895	0.009322	4.153227
333	1.68	6	0.00188	0.001733	7.837346
333.15	20	1	0.01753	0.017807	1.582695
333.15	20	3	0.0122	0.012578	3.100203

353	3.39	4	0.00364	0.003608	0.876351
353	8.337	4	0.00735	0.007445	1.289414
373	10.05	1	0.01188	0.01201	1.096367
373	6.82	1	0.00833	0.008744	4.973985
373	15.02	1	0.01507	0.014965	0.695243
373	3.11	1.13	0.0039	0.00414	6.146058
373	19.15	3	0.01117	0.011435	2.373812
373	10	5	0.00652	0.006811	4.464882
373	20	5	0.00975	0.009742	0.084237
393	9.33	4	0.00654	0.006659	1.81657
393.15	20	3	0.01133	0.011669	2.989284
393	5	4	0.00389	0.004118	5.854842
393	4.74	4	0.00374	0.00392	4.805166
413	20	1	0.01655	0.017234	4.133501
413	5.04	4	0.00364	0.003885	6.731723
413	10	1	0.01054	0.010855	2.987497
413	10	5	0.00617	0.006114	0.912848
423	10.01	2	0.00852	0.008754	2.744774
423	5.03	1	0.00546	0.005856	7.256617
423	10.04	1	0.01017	0.010733	5.537895

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