

SUPPLEMENTARY MATERIAL

4.1.2.2 KCl salt

Figure S1, S2, S3 and S4 compare the simulated results and measured data of CO₂ solubility in KCl salt systems of 1, 1.942, 2.50, and 4.0 mol/kg, respectively. The developed model's simulated results are consistent with experimental data at low temperatures. The CO₂ solubility is generally less than 1.5 mol/kg at low ionic strength values. As seen in Figure S1, CO₂ solubility increases gradually with pressure and shows a relatively moderate sensitivity to temperature. At 10 MPa, it decreases from 1.1 mol/kg to 0.8 mol/kg when the temperature increases from 323 K to 373°K. A Similar trend of CO₂ solubility occurs at a salinity of 1.942, 2.50, and 4.0 mol/kg from Figure S2, S3 and S4. However, the extent of solubility decrease is higher at this ionic strength relative to the salinity of 1 mol/kg presented in Figure S1. Figure S5 depicts the salting-out phenomenon on a three-dimensional response surface plot. This plot demonstrates the interaction between CO₂ molecules, water, and ions, which leads to a reduction in the solubility of CO₂ in a saline environment as the salinity level rises.

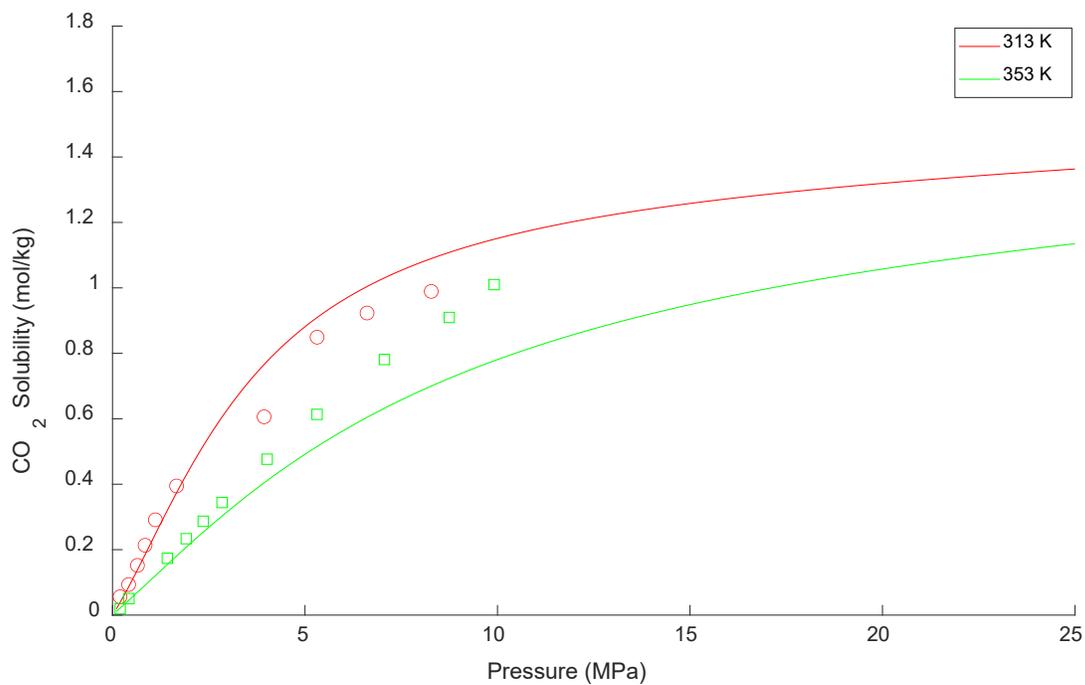


Figure S1. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 1 mol/kg (KCl solution). The experimental data are adopted from Kiepe et al. [1].

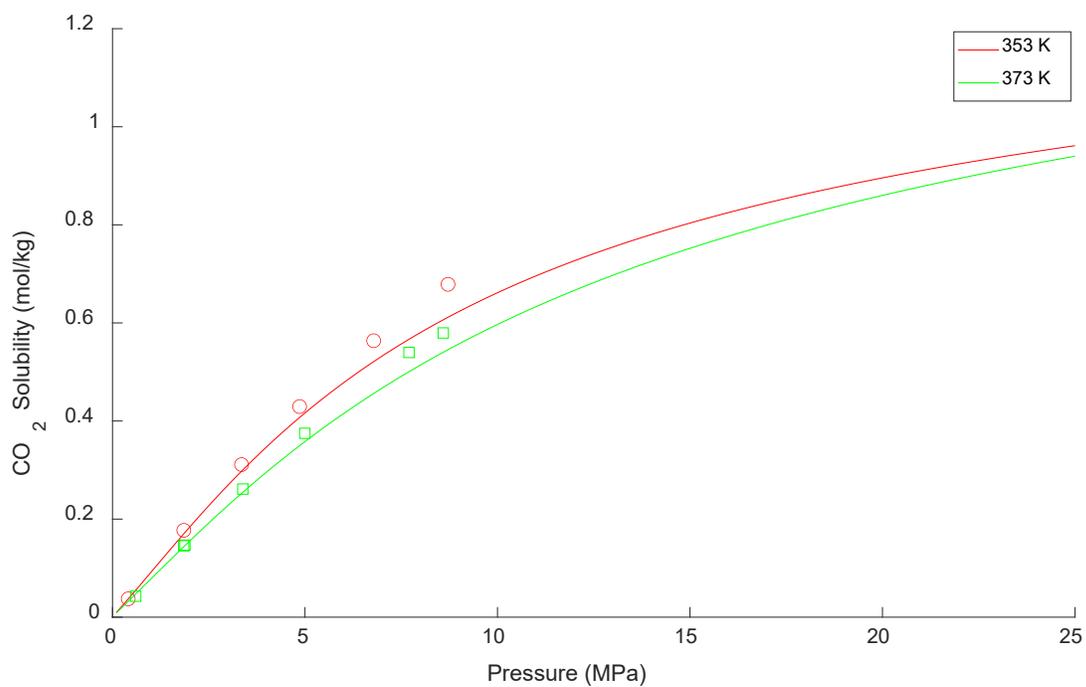


Figure S2 . Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 1.942 mol/kg (KCl solution). The experimental data are adopted from Kamps et al.[2].

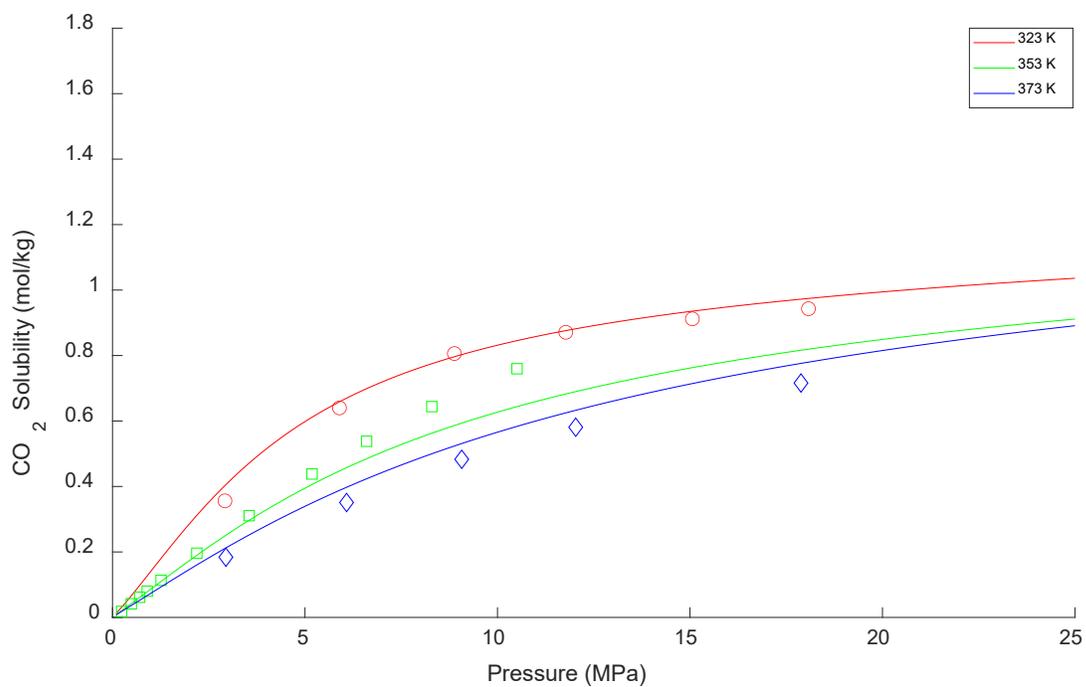


Figure S3. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 2.50 mol/kg (KCl solution). The experimental data are adopted from Hou et al. [3] and Kiepe et al. [1].

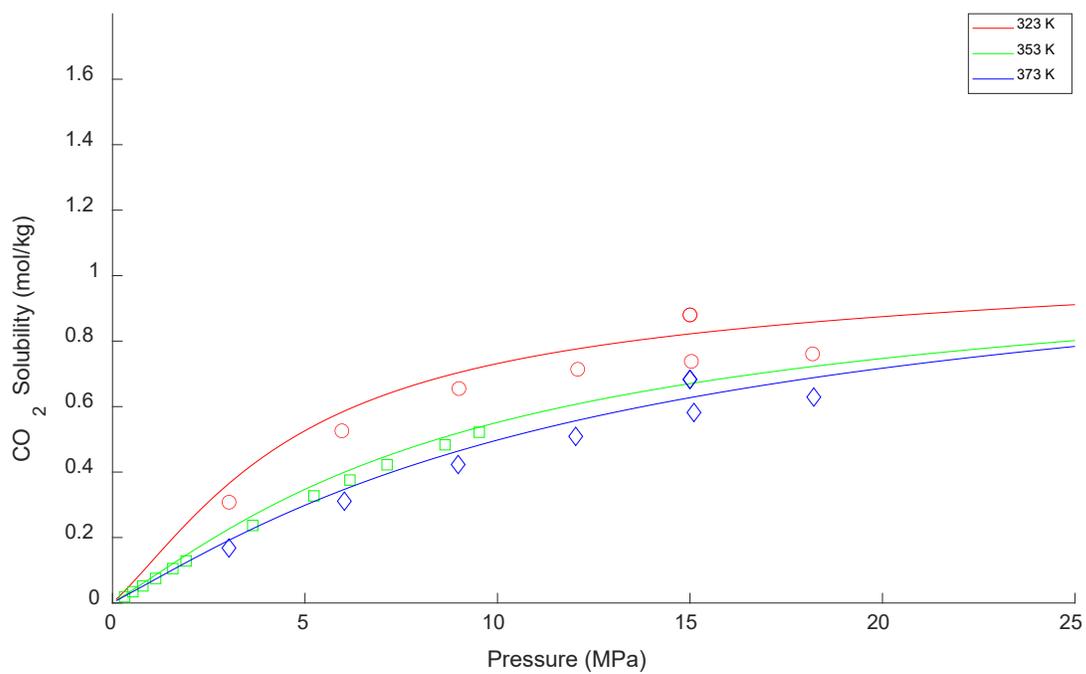


Figure S4 . Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 4.0 mol/kg (KCl solution). The experimental data are adopted from Hou et al. [3], Kiepe et al. [1], Koschel et al. [4] and Zhao et al. [5].

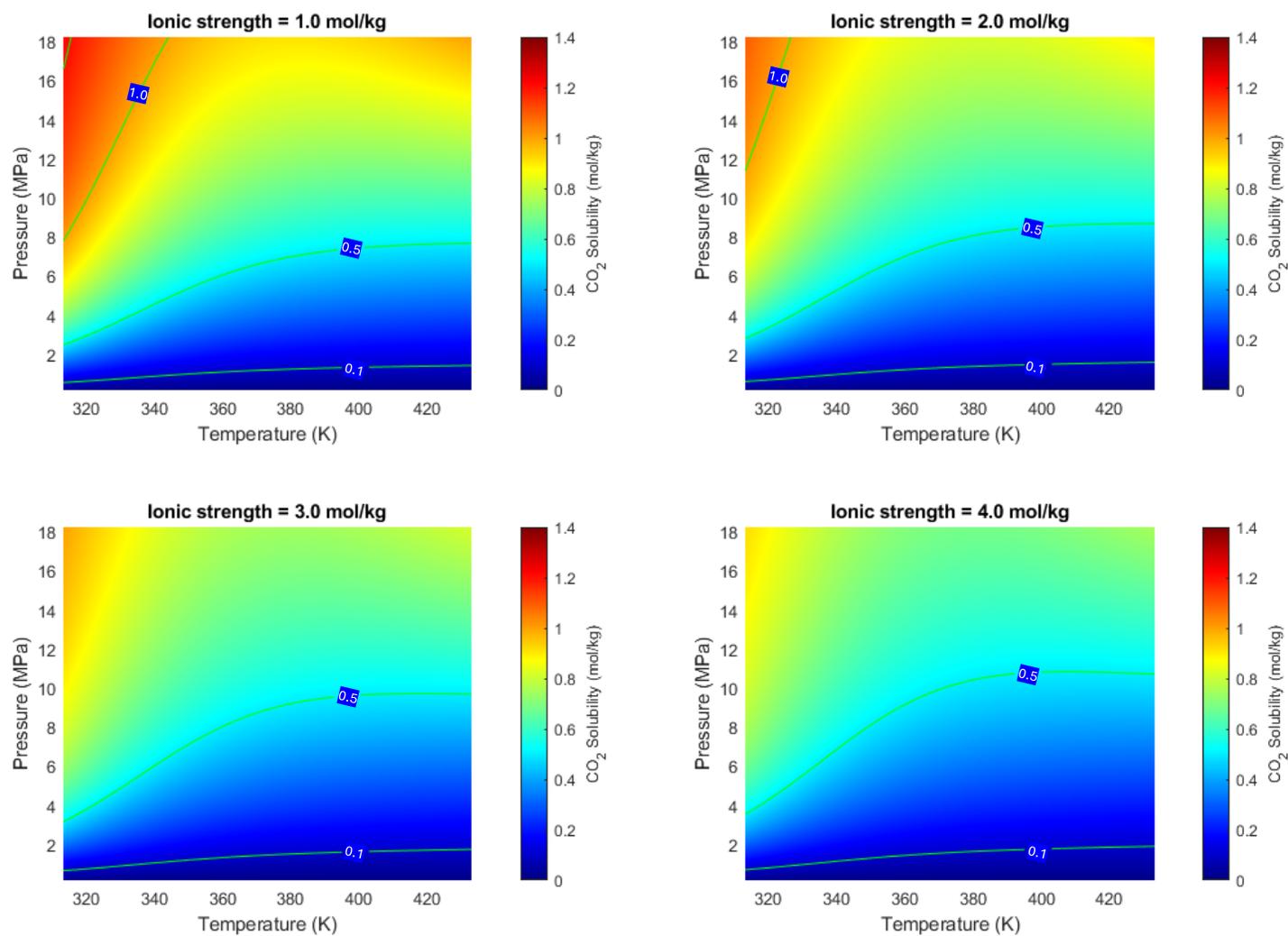


Figure S5. 3D response surfaces of CO₂ solubility (KCl) system at different salinities in terms of ionic strength.

4.1.2.3 NaCl salt

Figure S 6 and Figure S 7 compare the simulated results and measured data of CO₂ solubility in NaCl salt systems. At different temperatures, our model's simulated results are closely consistent with the experimental data. Figure S 6 shows that the CO₂ solubility is generally less than 1.5 mol/kg at an ionic strength value of 1.0 mol/kg for lower temperatures. At elevated pressure (40 MPa) and temperatures (453K), the solubility exceeds 1.5 mol/kg. A similar phenomenon is observed at a higher ionic strength of 6 mol/kg, as seen in Figure S 7; there exists a good agreement between published experimental and model data. At elevated pressure, CO₂ solubility is more sensitive to temperature in NaCl salt systems. As pressure increases, CO₂ solubility increases gradually, but the variation rate decreases. Figure S 8 illustrates the salting-out effect on a 3D response surface plot, which results from the interaction between the CO₂ molecules, water, and solution ions. This interaction is responsible for the decrease in CO₂ solubility in a saline system as the salinity increases.

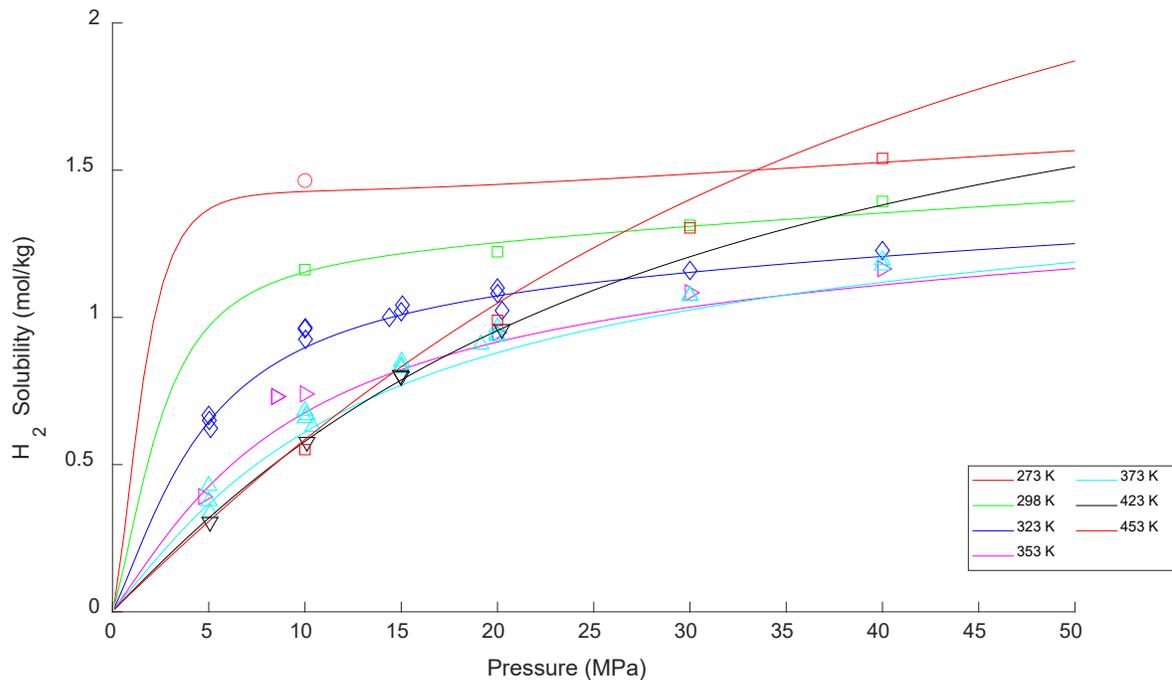


Figure S6. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 1 mol/kg (NaCl solution). The experimental data are adopted from Carvalho et al. [6], Guo et al. [7], Koschel et al. [4], Messabeb et al. [8], Yan et al. [9] and Zhao et al. [10].

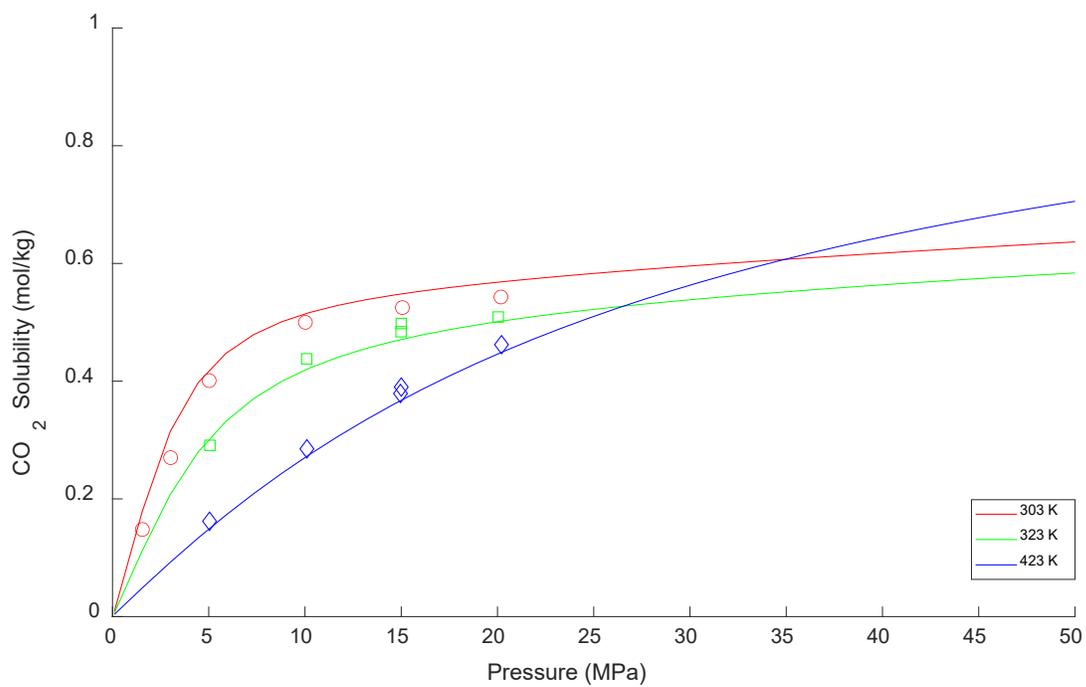


Figure S7. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 6 mol/kg (NaCl solution). The experimental data are adopted from Dos Santos et al. [11], Messabeh et al. [8] and Zhao et al. [10].

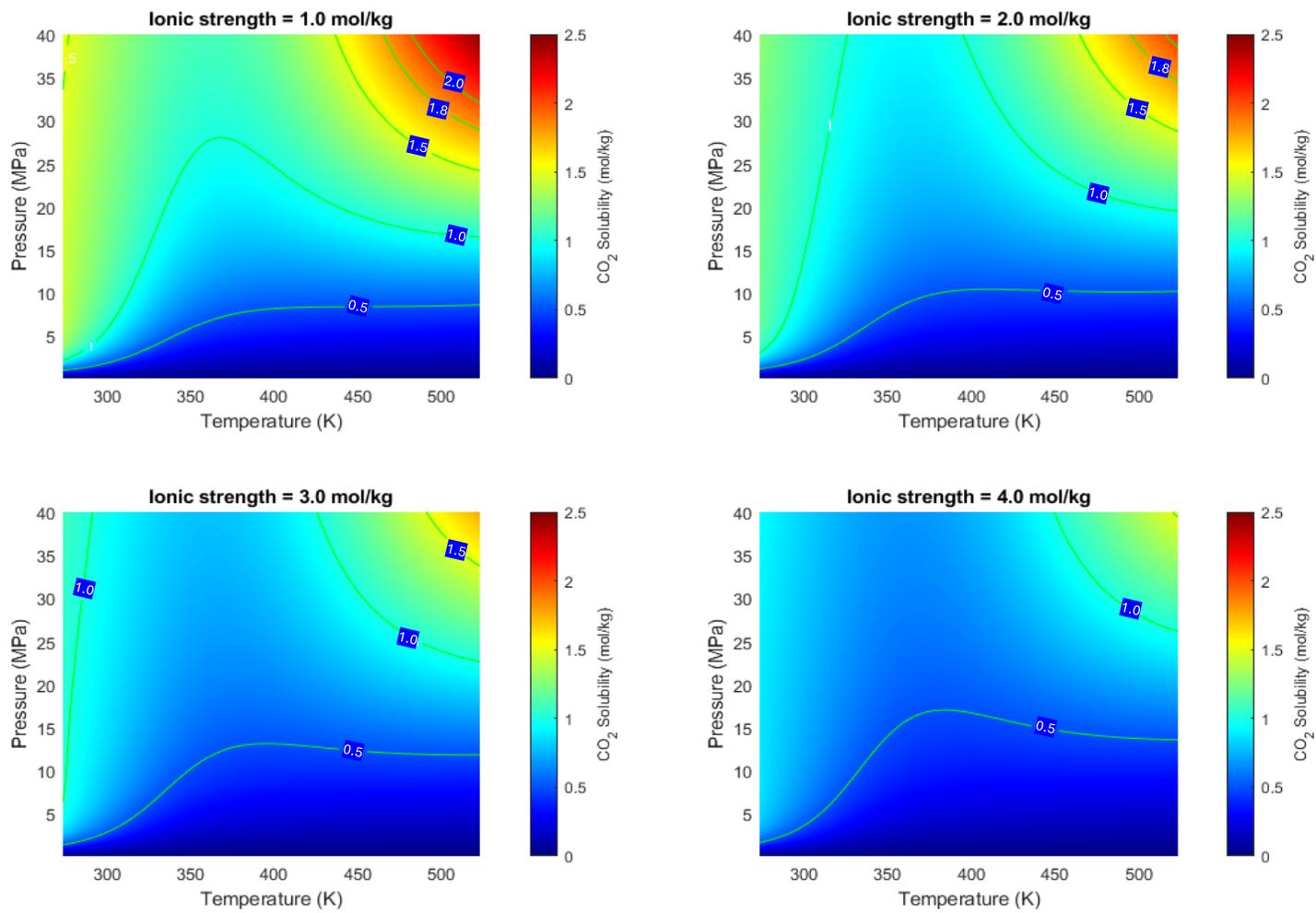


Figure S8. 3D response surfaces of CO₂ solubility (NaCl salt) system at different salinities in terms of ionic strength.

4.1.2.4 Na₂SO₄ salt

Figure S9 and S10 compare the simulated results and measured data of CO₂ solubility in the Na₂SO₄ salt system. The developed model's simulated results are closely consistent with the experimental data at low temperatures. As seen in Figure S9 and S10, the CO₂ solubility at low ionic strength values of 0.747 and 3.0 mol/kg are in good agreement with published experimental and model data. Also, CO₂ solubility increases gradually with pressure and shows a relative medium sensitivity to temperature. Figure S11 depicts the salting-out phenomenon on a 3D response surface plot. This plot demonstrates the interaction between CO₂ molecules, water, and ions, which leads to a reduction in the solubility of CO₂ in a saline environment as the salinity level rises.

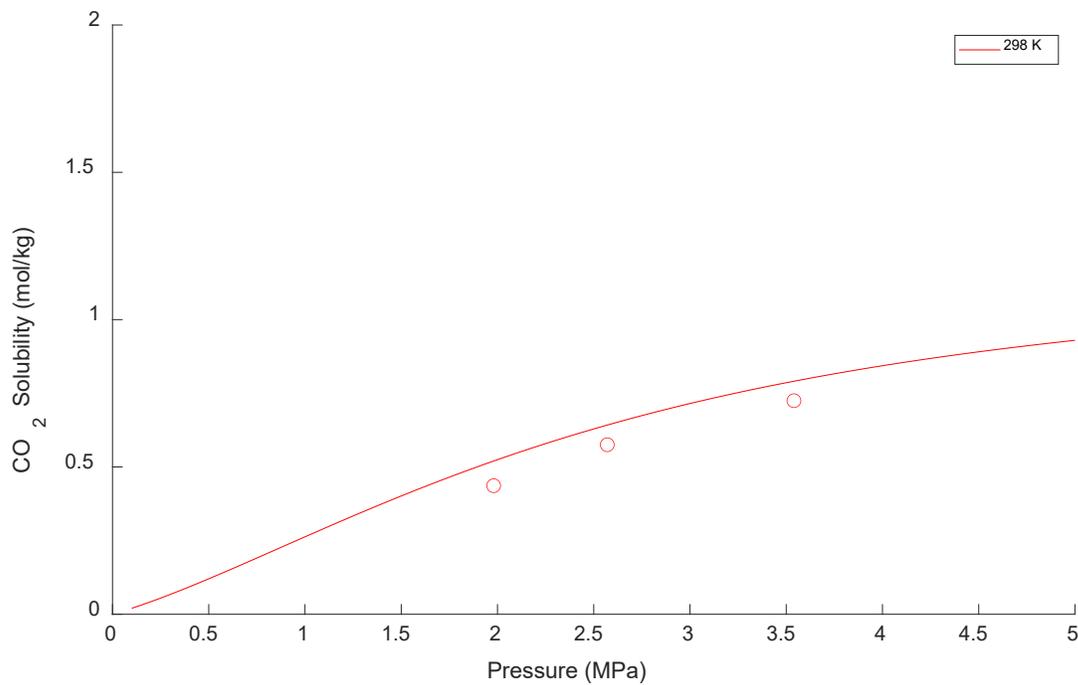


Figure S9. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 0.747 mol/kg (Na₂SO₄ solution). The experimental data are adopted from Bermejo et al. [12].

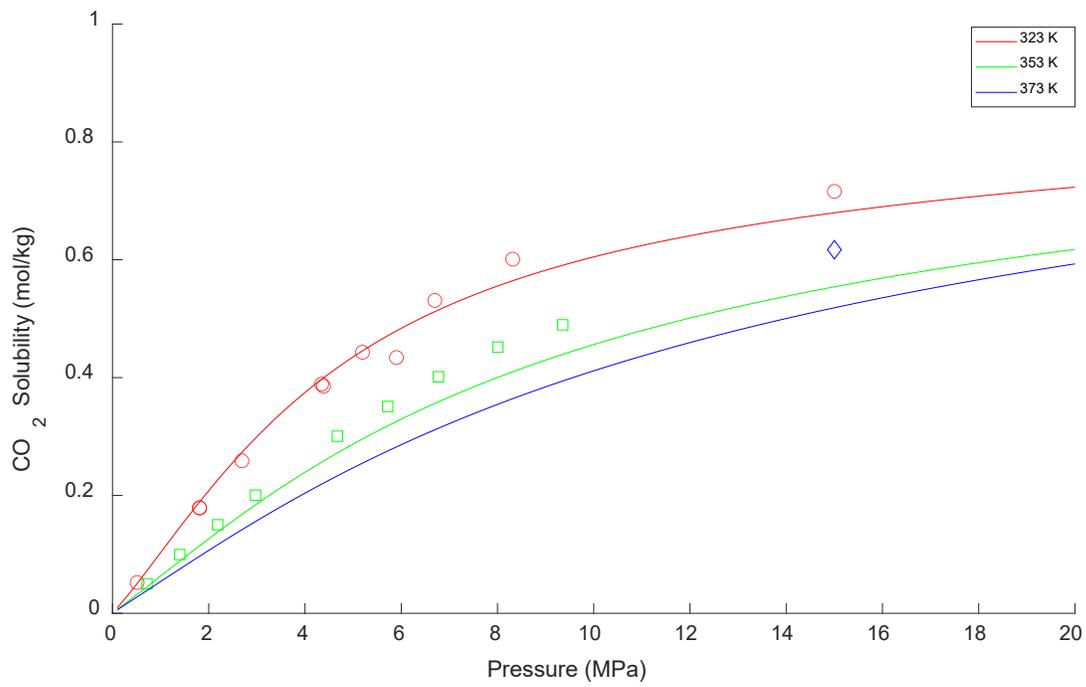


Figure S10. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 3.0 mol/kg (Na₂SO₄ solution). The experimental data are adopted from Bermejo et al. [12], Rumpf and Maurer [13] and Zhao et al. [5].

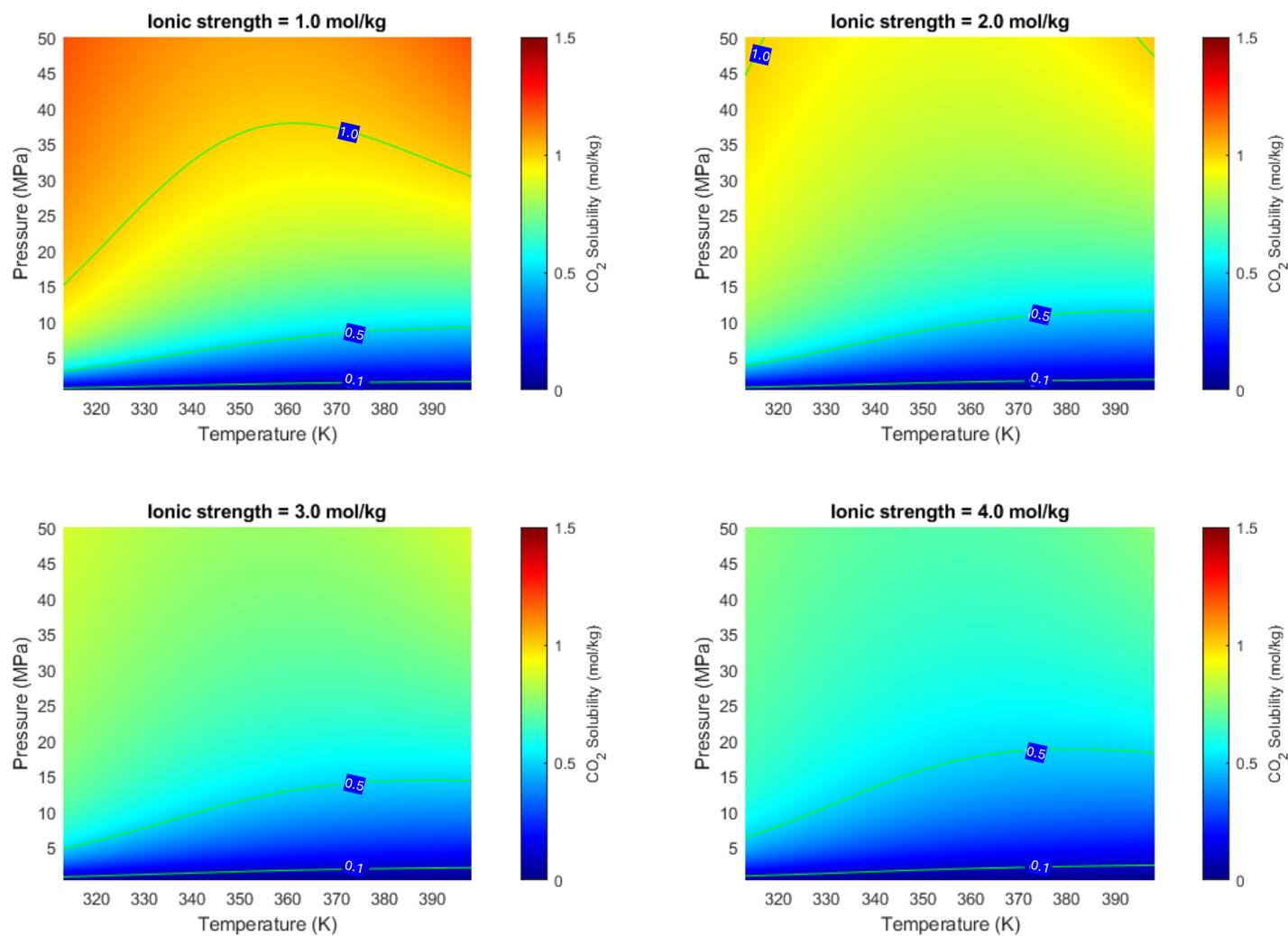


Figure S11. 3D response surfaces of CO₂ solubility (Na₂SO₄) system at different salinities in terms of ionic strength.

4.1.2.5 NaHCO₃ salt

The simulated results and measured data of CO₂ solubility in NaHCO₃ salt systems are compared in Figure S12, S13, and S14. The developed model's simulated results are closely consistent with the experimental data at low temperatures. The CO₂ solubility is generally less than 1.0 mol/kg at low ionic strength values, with a good agreement between published experimental and model data. Moreover, as the ionic strength increased from 0.05 through to 1 mol/kg, the CO₂ solubility decreased more at higher temperatures. An increase in pressure also resulted in a gradual CO₂ solubility increase regardless of the salinity level highlighted. Figure S15 depicts the salting-out phenomenon on a 3D response surface plot. This plot demonstrates the interaction between CO₂ molecules, water, and ions, which reduces the solubility of CO₂ in a saline environment as the salinity level rises.

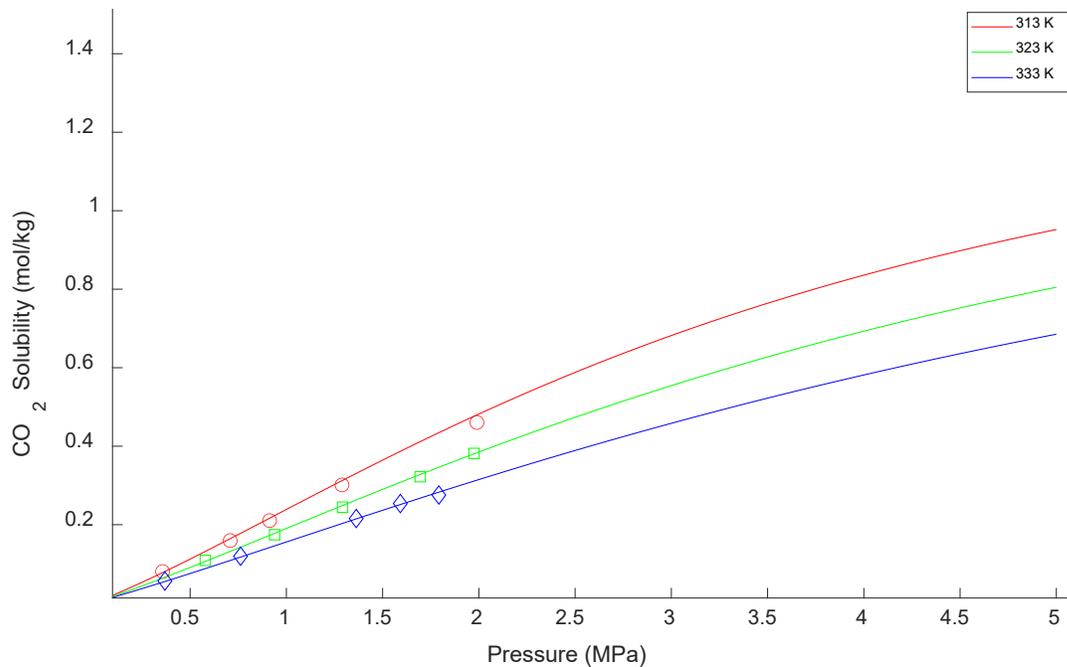


Figure S12. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 0.05 mol/kg (NaHCO₃ solution). The experimental data are adapted from Han et al. [14].

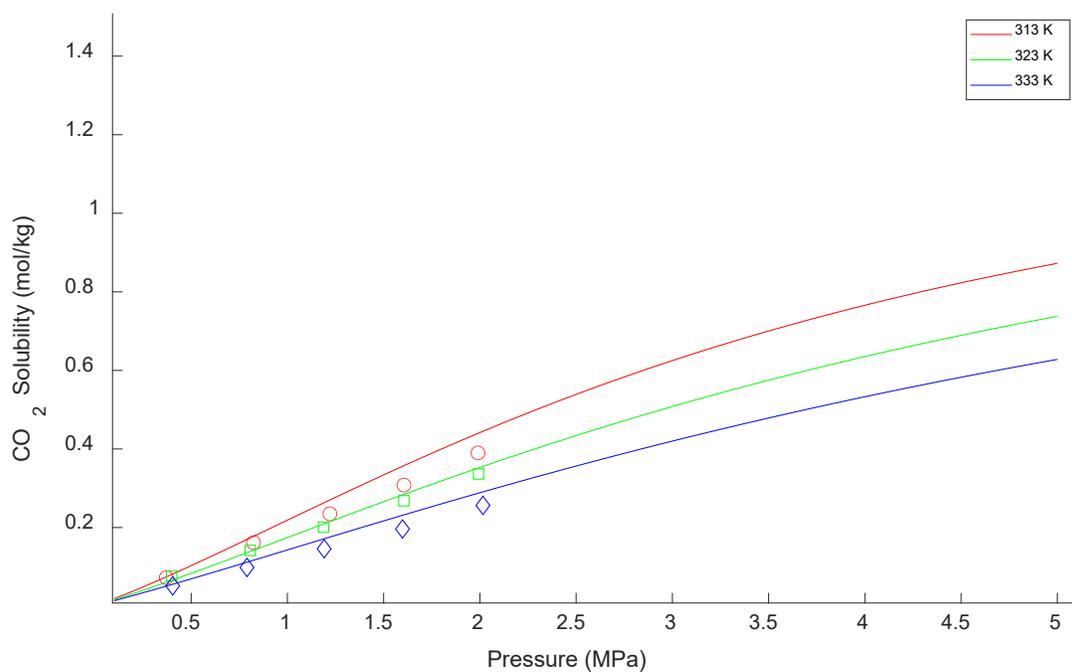


Figure S13. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 0.5 mol/kg (NaHCO₃ solution). The experimental data are adapted from Han et al. [14].

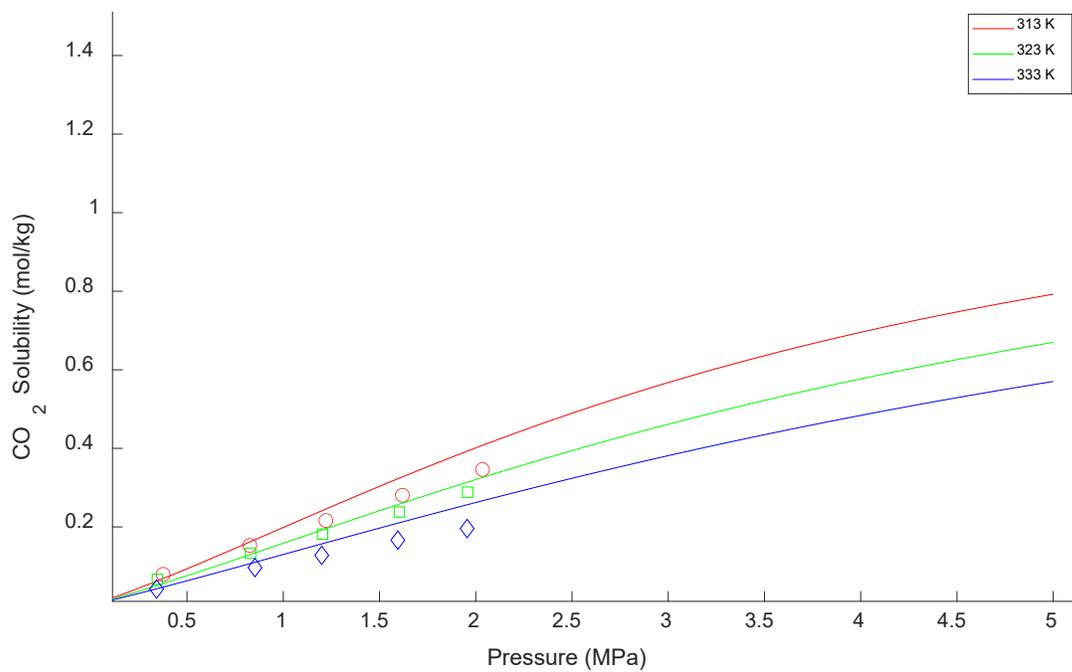


Figure S14. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 1 mol/kg (NaHCO₃ solution). The experimental data are adapted from Han et al. [14].

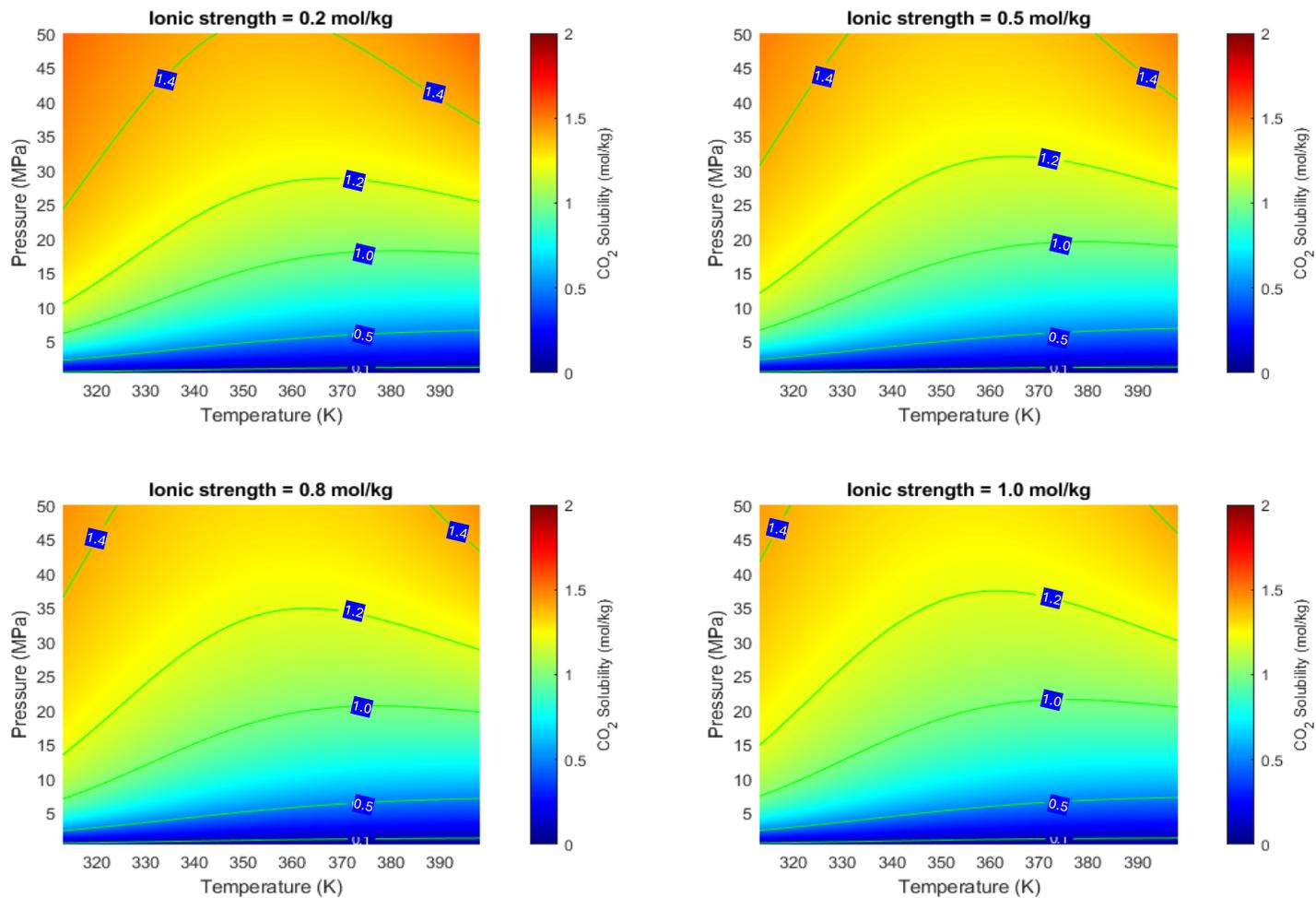


Figure S15. 3D response surfaces of CO₂ solubility (NaHCO₃) system at different salinities in terms of ionic strength.

4.1.2.6 CaCl₂ salt

The simulated results and measured data of the CO₂ solubility of the divalent salts - CaCl₂ system are compared in Figure S16 and S17. Overall, there is a good agreement between the published experimental data and our computed data. The CO₂ solubility is generally less than 1.1 mol/kg at a low ionic strength value of 3.04 mol/kg. At an ionic strength of 11.7 mol/kg, the CO₂ solubility is generally lower than 0.45 mol/kg. Interestingly, as pressure exceeds 20 MPa, higher temperatures begin to improve CO₂ solubility relative to lower temperatures. Figure S18 depicts the salting-out phenomenon on a 3D response surface plot. This plot demonstrates the interaction between CO₂ molecules, water, and ions, which leads to a reduction in the solubility of CO₂ in a saline environment as the salinity level rises.

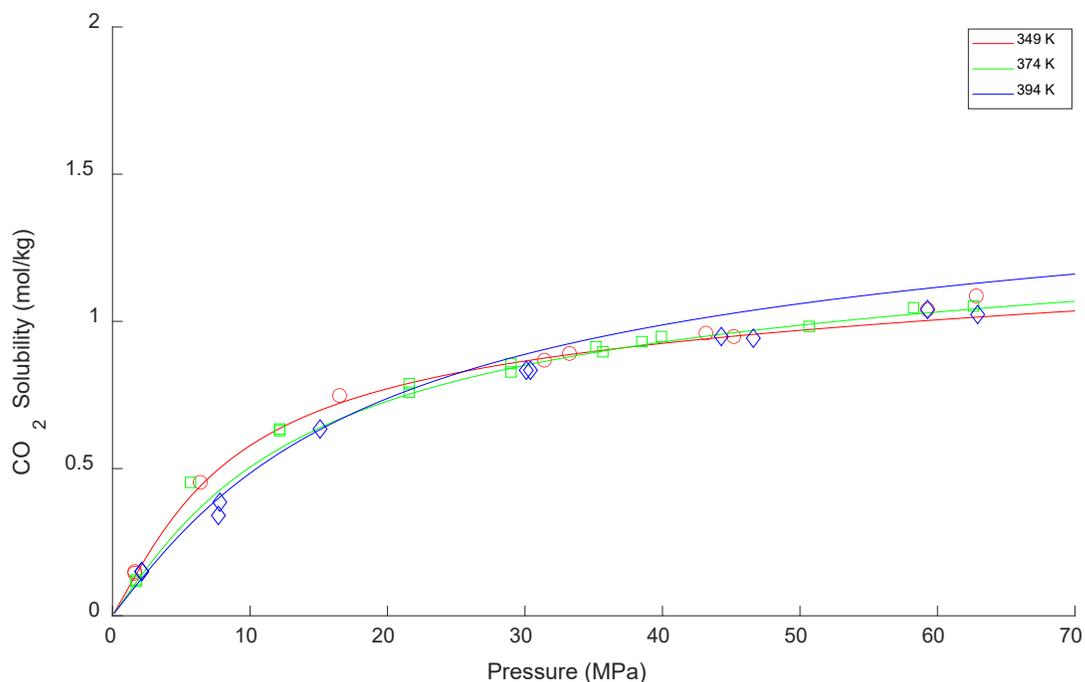


Figure S16. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 3.04 mol/kg (CaCl₂ solution). The experimental data are adapted from Prutton and Savage [15].

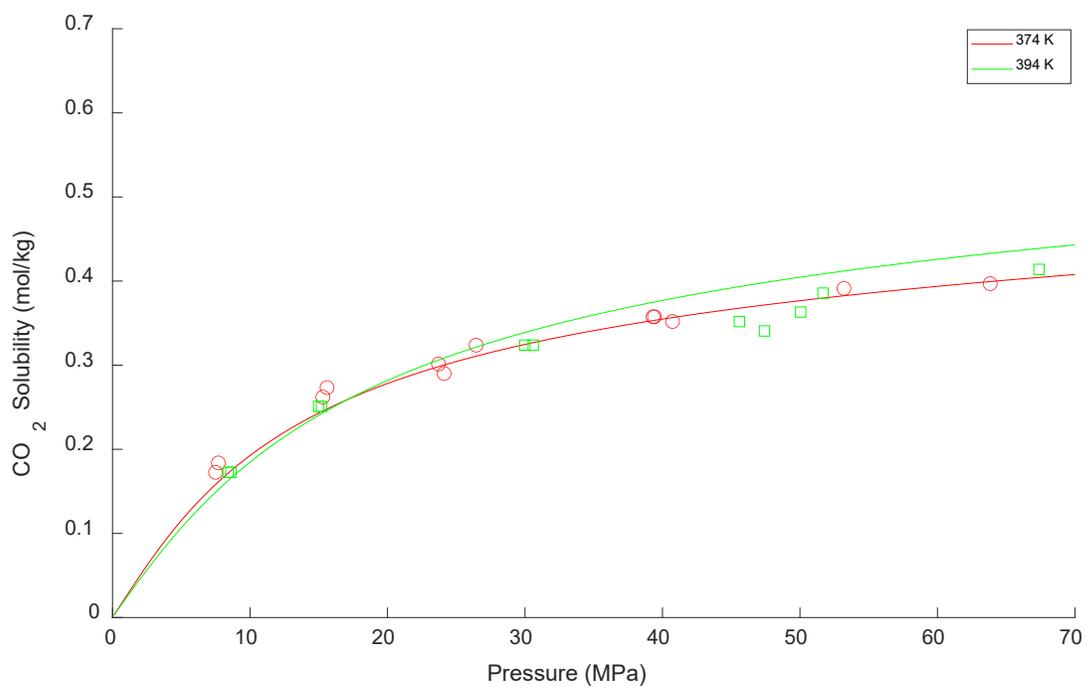


Figure S17. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 11.7 mol/kg (CaCl₂ solution). The experimental data are adapted from Prutton and Savage [15].

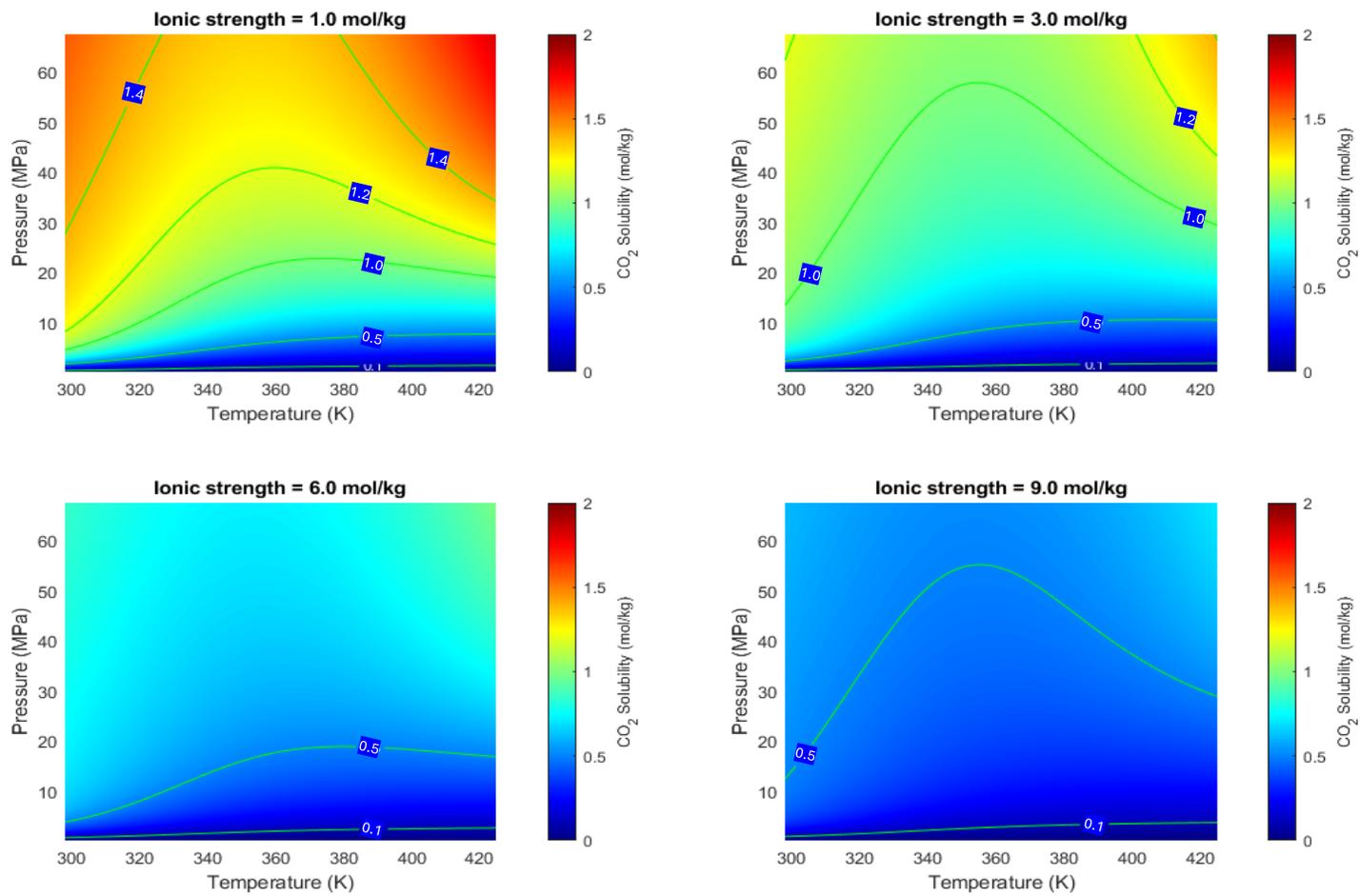


Figure S18 . 3D response surfaces of CO₂ solubility (CaCl₂) system at different salinities in terms of ionic strength.

4.1.2.7 MgCl₂ salt

Figure S19, S20 and S21 compare the simulated results and measured data of the CO₂ solubility of the divalent salts - MgCl₂ system with ionic strength of 0.48, 3, and 15 mol/kg, respectively. Overall, there is a good agreement between the published experimental data and the computed data. The CO₂ solubility is generally less than 2.0 mol/kg at a low ionic strength value of 0.48 mol/kg, with a good agreement between published experimental and model data. At higher ionic strength of 3 and 15 mol/kg, the CO₂ solubility is less than 1 and 0.23 mol/kg, respectively. Again, lower temperatures facilitate more dissolution of CO₂ into MgCl₂ salt relative to higher temperatures at low pressures. As pressure increases, the solubility begins to increase and becomes more reliant on pressure than temperature. Figure S22 depicts the salting-out phenomenon on a 3D response surface plot. This plot demonstrates the interaction between CO₂ molecules, water, and ions, which leads to a reduction in the solubility of CO₂ in a saline environment as the ionic strength increases.

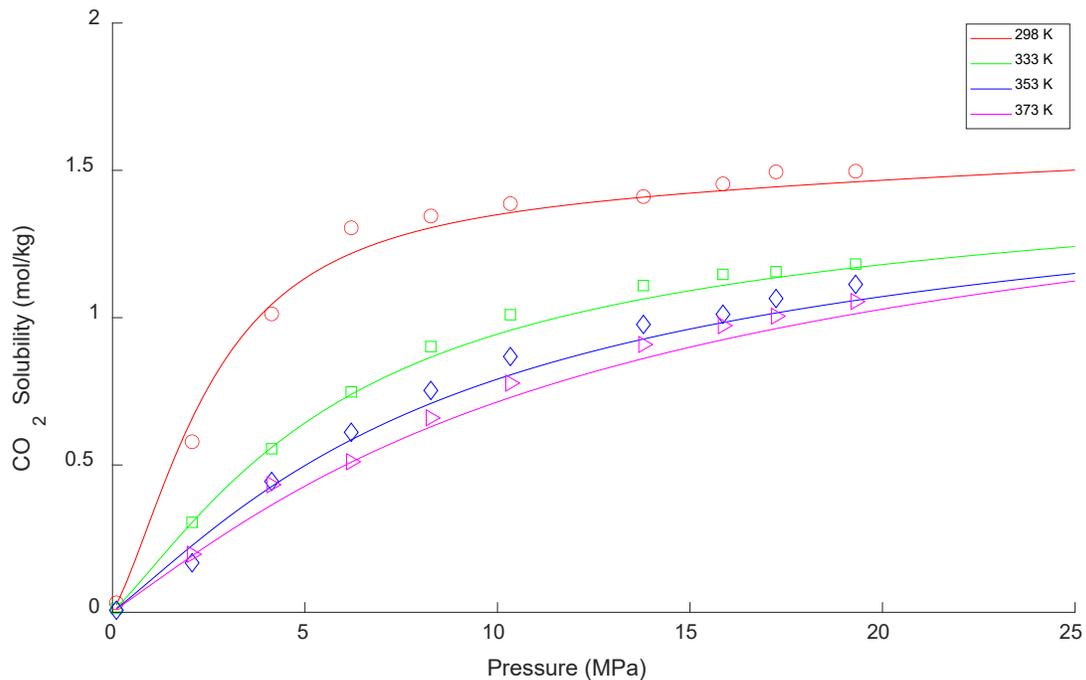


Figure S19. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 0.48 mol/kg (MgCl₂ solution). The experimental data are adapted from Bo Liu et al. [16].

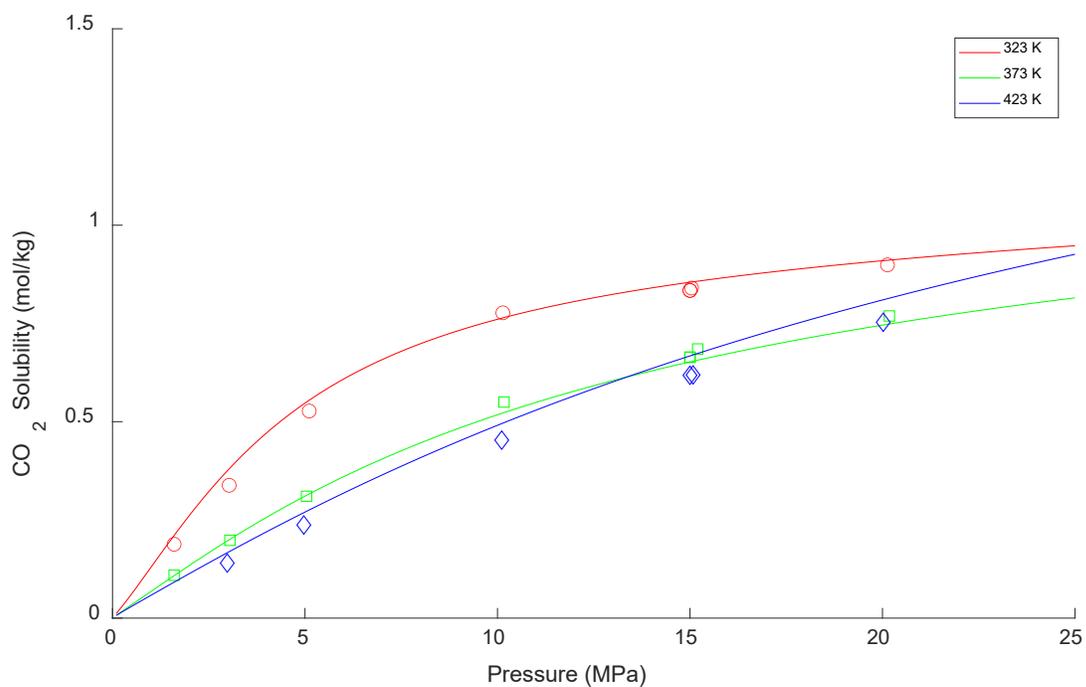


Figure S20. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 3.0 mol/kg (MgCl₂ solution). The experimental data are adapted from Zhao et al. [5], Koschel et al. [4] and Dos Santos et al. [11].

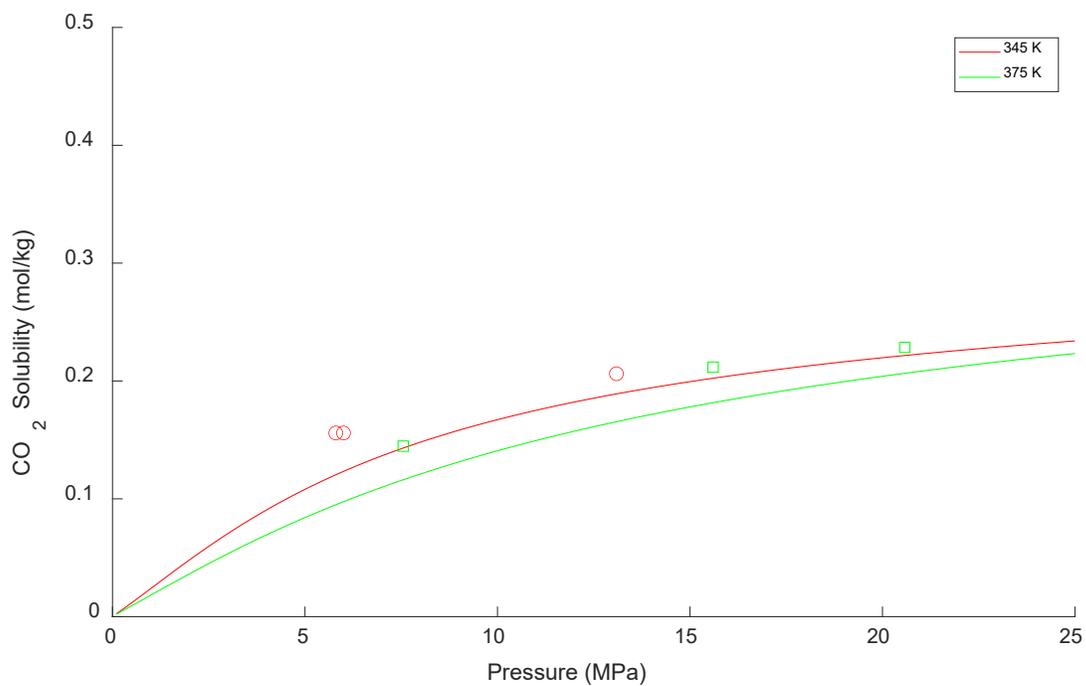


Figure S21. Predicted CO₂ solubility versus experimentally measured data of CO₂ solubility with ionic strength of 15.0 mol/kg (MgCl₂ solution). The experimental data are adapted from Tong et al. [17].

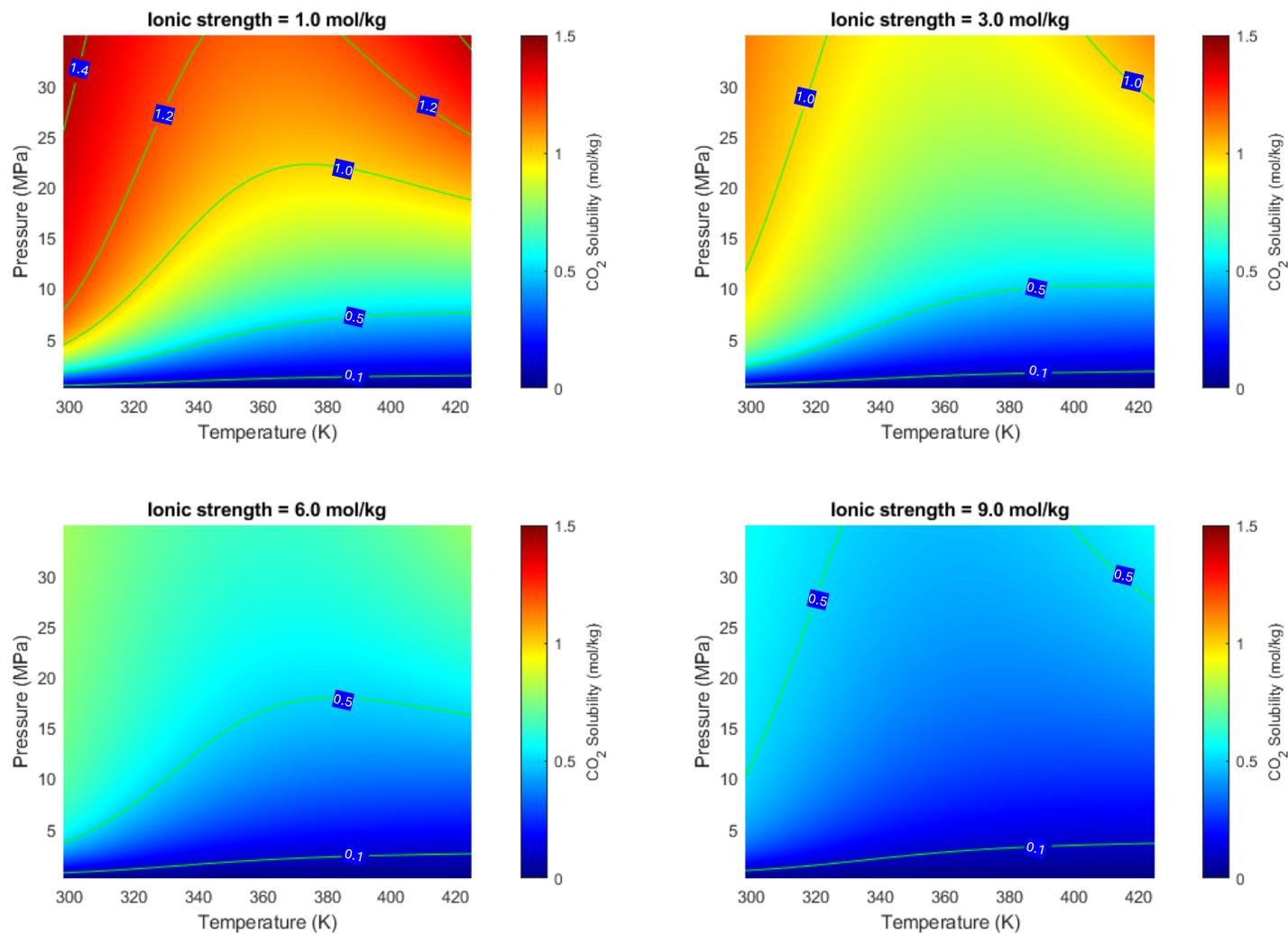


Figure S22. 3D response surfaces of CO₂ solubility (MgCl₂) system at different salinities in terms of ionic strength.

References

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