Geological Carbon Sequestration Research Publications

Chen Zhu, Indiana University

CO_2 and Co-injectant Solubility (impurities in CO_2 streams)

- Ji X and **Zhu** C (2013) Predicting possible effects of H_2S impurity on CO_2 transportation and geological storage. ***Environmental Science & Technology*** 47: 55-62, dx.doi.org/10.1021/es301292n.
- Ji X and **Zhu** C (2012) A SAFT Equation of State for the Quaternary H_2S-CO_2-H_2O-NaCl system. ***Geochimica et Cosmochimica Acta*** 91: 40–59, doi.org/10.1016/j.gca.2012.05.023.
- Ji, X. and **Zhu**, C. (2010) Modelling of phase equilibria in the H_2S-H_2O system with statistical associating fluid theory. ***Energy & Fuels*** v. 24, 6208-6213. DOI:10.1021/ef100847j.
- Hu, J, Duan, Z, **Zhu, C.**, and Chou, I., (2007) PVTx properties of the CO_2-H_2O and CO_2-H_2O-NaCl systems below 647K: Assessment of experimental data and thermodynamic models. ***Chemical Geology***, v. 238, p.249-267.
- Duan, Z., Sun, R, Liu, R, and **Zhu**, C. (2007) Accurate thermodynamic model for H_2S solubility in pure water and brines. ***Energy & Fuels***, v. 21, 2056-2065.
- Duan, Z., Sun, R., **Zhu, C.** and Chou, I., (2006) An improved model for the calculation of CO_2 solubility in aqueous solutions containing Na^+, K^+, Ca^{2+}, Mg^{2+}, Cl^-, and SO_4^{2-}. ***Marine Chemistry***. v.98, 131-139.

Geochemical Modeling of CO_2 Reactions with Reservoir and Cap Rocks

- Zhang GR, [*]Lu P, Huang Y, Li GH, [*]**Zhu** C (2021) Investigation of mineral trapping processes based on coherent front propagation theory: A dawsonite-rich natural CO_2 reservoir as an example. ***International Journal of Greenhouse Gas Control*** v110, 103400, https://doi.org/10.1016/j.ijggc.2021.103400.
- [‡]Zhang GR, [‡]Lu P, [‡]Zhang YL, Wei XM, [*]**Zhu C** (2016) Impacts of mineral reaction kinetics and regional groundwater flow on long-term CO_2 fate at Sleipner. ***Energy & Fuel*** 30(5): 4159-4180, doi: 10.1021/acs.energyfuels.5b02556s
- **Zhu C**, [‡]Zhang GR, [‡]Lu P, [‡]Meng LF, Ji X (2015) Benchmark modeling of the Sleipner CO_2 plume: Calibration to seismic data for the uppermost layer and model sensitivity analysis. ***The International Journal of Greenhouse Gas Control*** 43: 233-246, doi: 10.1016/j.ijggc.2014.12.016
- Zhang GR, [‡]Peng L, [‡]Zhang YL, Wei XM, [*]**Zhu C** (2015) Effects of rate law formulation on predicting CO_2 sequestration in sandstone formations. *International Journal of Energy Research* 39(14): 1890-1908, doi: 10.1002/er.3374.
- Liu, Faye (Yifei), P. Lu, C. **Zhu**, Y. Xiao (2011) Coupled reactive transport modeling of CO_2 Sequestration in the Mt. Simon Sandstone Formation, Midwest U.S.A. ***The International Journal of Greenhouse Gas Control***, DOI: 10.1016/j.ijggc.2010.08.008.
- Strazisar, B. R., **Zhu, C.**, and Hedges, S. W., (2006) Preliminary modeling of the long-term fate of CO_2 following injection into deep geological formations. ***Environmental Geosciences*** v.13, no.1, 1-15, 2006.

Mineralogical or above Ground Carbon Sequestration (U.S. Patent 7922792 "Method for Sequestration of CO_2 and SO_2 Utilizing a Plurality of Waste Streams")

- Dilmore, R., Lu, P., Soong, Y. , Allen, Hedges, H., Fu, J. K., Dobbs, C., Degalbo, A., **Zhu, C.** , (2008) Sequestration of CO_2 in mixtures of bauxite residue and saline waste water. ***Energy & Fuels***, v 22, No.1, p.343-353.

Laboratory Experiments on Host Rock Reactivity and Caprock Integrity

- Lu P, Fu Q, Seyfried Jr. WE, Jones K., and Zhu C (2013) Coupled alkali feldspar dissolution and secondary mineral precipitation in batch systems: 2 Effects of CO_2 and implications for carbon sequestration. ***Applied Geochemistry*** 30: 75-90, Doi10.1016/j.apgeochem.2012.04.005
- Liu, Faye (Yifei), P. Lu, C. Griffth, S.a W. Hedges, C. **Zhu** (2012) CO_2-caprock-brine interaction: Reactivity Experiments on Eau Claire Shale and a review of literature. ***The International Journal of Greenhouse Gas Control*** 7: 153–167, doi.org/10.1016/j.ijggc.2012.01.012.
- Lu, P, Fu, Q., Seyfried, W.E. Jr, Hereford, A.G., **Zhu**, C. (2010) Navajo Sandstone-Brine-CO_2 interaction: Implications for Geological Carbon Sequestration. ***Environmental Earth Sciences***, 62 (1): 101-118doi:10.1007/s12665-010-0501-y

Single Mineral Reaction Kinetics with Applications to CCUS (last five years)

- ‡Kang JT, Bracco JN, Rimstidt JR, Zhu GH, Huang F, *__Zhu__ C (2022). Ba attachment and detachment fluxes to and from barite surfaces in ^{137}Ba-enriched solutions with variable $[Ba^{2+}]/[SO_4^{2-}]$ ratios near solubility equilibrium. *Geochimica et Cosmochimica Acta*. v317, 180-200, doi.org/10.1016/j.gca.2021.11.008.
- **Zhu C**, ‡Zhang YL, Rimstidt JD, Gong L, ‡Burkhart, JA, Chen KY, Yuan HL (2021) Testing hypotheses of albite dissolution mechanisms at near-equilibrium using Si isotope tracers. ***Geochimica et Cosmochimica Acta*.** v303, 15-37. doi.org/10.1016/j.gca.2021.03.023.
- **Zhu C,** Rimstidt JD, ‡Zhang YL, ‡Kang JT, Schott J, Yuan HL (2020) Decoupling feldspar dissolution and precipitation rates at near-equilibrium with Si isotope tracers: Implications for modeling silicate weathering. ***Geochimica et Cosmochimica Acta***. v271, 132-153. DOI: 10.1016/j.gca.2019.12.024.
- Gong L, Rimstidt JD†, ‡Zhang YL, Chen KY, ***Zhu C** (2019) Unidirectional kaolinite dissolution rates at near-equilibrium and near-neutral pH conditions. ***Applied Clay Science*** v182, doi.org/10.1016/j.clay.2019.105284;
- Zhang YL, Gong L, Chen KY, ‡Burkhart J, Yuan HL, *__Zhu C__ (2020) A method for Si isotope tracer kinetics experiments: Using Q-ICP-MS to obtain $^{29}Si/^{28}Si$ ratios in aqueous solutions. ***Chemical Geology*** v531, Doi: 10.1016/j.chemgeo.2019.119337;
- Rimstidt, JD, ‡Zhang Y, *__Zhu C__ (2016) Rate equations for sodium catalyzed amorphous silica dissolution. ***Geochimica et Cosmochimica Acta*** 195: 120-125. doi.org/10.1016/j.gca.2015.07.030
- **Zhu C**, ‡Liu ZY, ‡Wang C, ‡Schaefer A, ‡Lu P, ‡Zhang GR, ‡Zhang YL, Georg RB, Rimstidt JD, Yuan HL (2016) Measuring silicate mineral dissolution rates using Si isotope doping. ***Chemical Geology***, 445: 146-163, doi:10.1016/j.chemgeo.2016.02.027

Geochemical Modeling Tools

- Lu P, Zhang GR, Apps J, *__Zhu__ C. (2022) Comparison of thermodynamic data files for PHREEQC. ***Earth-Science Reviews***, https://doi.org/10.1016/j.earscirev.2021.103888..
- Zhang GR, Lu P, ‡Zhang YL, ‡Tu K, *__Zhu C__ (2020) SupPHREEQC: A program to generate customized PHREEQC thermodynamic database based on Supcrtbl. ***Computers & Geosciences***. v143. doi.org/10.1016/j.cageo.2020.104560.
- ‡Zhang YL, ‡Hu B, Teng YG, *__Zhu C__ (2019) A library of BASIC scripts of reaction rates for geochemical modeling using PHREEQC. ***Computers & Geosciences***, v133, doi.org/10.1016/j.cageo.2019.104316;
- ‡Zimmer K, ‡Zhang YL, ‡Lu P, ‡Chen YY, ‡Zhang GR, *__Zhu C__ (2016) SUPCRTBL: A revised and extended thermodynamic dataset and software package of SUPCRT92. ***Computers & Geosciences*** 90: 97-111, doi:10.1016/j.cageo.2016.02.013.

Online Geochemical Modeling Tools (3000 visits between 9/20 and 11/21)

- CO_2 Solubility Calculator: Users input temperature, pressure, and NaCl molality, and the online tool generates CO_2 solubility.

- H_2S Solubility Calculator: H_2S is a common impurity in CO_2 streams in CCUS. Users input temperature, pressure, NaCl molality, and H_2S and CO_s mole fractions, the online tool generates H_2S solubility.

- Online PHREEQC: We developed an online version of the US Geological Survey modeling software for speciation – solubility reaction path, and one-dimensional coupled reactive transport modeling.

- Online SUPCRTBL: An online version of SUPCRT that is dynamically linked to a MySQL database to make preparation of input files easier.