An Open-Source Platform for Industrial Collaboration on CO_2-Impurity Studies

Introduction

Transportation is an essential yet challenging part of Carbon Capture and Storage (CCS). The captured CO_2 can rarely be stored near the capture site, so it must be transported by ship or pipeline to an underground storage reservoir. CO_2 from capture processes inevitably contains impurities (e.g., SO_x, NO_x, O_2, H_2S, H_2O), which, depending on conditions and concentrations, can react with each other or with CO_2 to form corrosive compounds (Sonke et al., 2024). Extra complexity arises when streams from multiple emitters are mixed, as this can affect impurity combinations and the potential to form corrosive sulfuric or nitric acids. If the produced quantities result in a separate phase, it poses a real corrosion and subsequent containment risk. Unfortunately, the current understanding of complex impurity interactions and their influence on corrosion is limited.

To accelerate research on CO_2 impurities, a new open-source platform, called AcidWatch, was launched. It enables researchers and engineers to run multiple models to evaluate acid-forming potential and compare the results with available laboratory data directly in the browser.

Open development model is a key feature of AcidWatch: the web application is freely accessible at `acidwatch.radix.equinor.com`, and the source code is available at `https://github.com/equinor/acidwatch`. To promote collaboration, the platform facilitates the addition of new models and laboratory data. This openness and transparency promote engagement with the research community and enable reproducibility by providing a common platform for running models, benchmarking results, and converging on best practices.

Method

As of February 2026, AcidWatch has five computational models and laboratory results from open publications for verification and benchmarking. The platform is actively developed, and changes to the user interface and the included models are to be expected. The user interface as of February 2026 is presented in Figure 1.

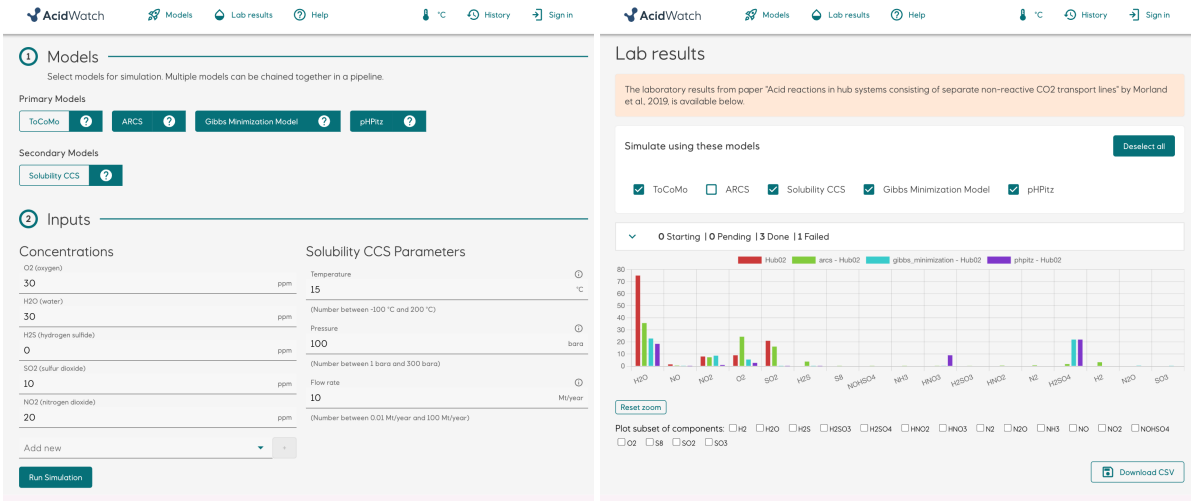

Figure 1: The AcidWatch platform: running a reactive and solubility model on the left, comparing laboratory results from publication with model runs view on the right.

Available open laboratory data

Laboratory experiments are essential for validating numerical models and for testing hypotheses. To facilitate systematic comparisons, we started compiling a database of relevant laboratory results from published papers, for example (Morland et al., 2019; Svenningsen & Morland, 2024; Svenningsen et al., 2024). Comparing model outputs with the experimental dataset provides a rigorous means of determining which models perform best under specific conditions, which is why we continue to expand the database with openly available laboratory results.

Available models

- **ARCS**
  To predict possible chemical reactions for a given set of initial impurity concentrations, we employ the Automated Reactions for CO_2 Storage (ARCS) model. ARCS combines first-principles calculations (density functional theory, DFT) with Monte Carlo sampling to model possible reactions under a given set of conditions. The ARCS model currently assumes full thermodynamic equilibrium for a given reaction, with Gibbs Free Energies ($\Delta G_{reac.}$) calculated within the gas phase approximation. Source code available at `https://github.com/badw/arcs`.
- **ToCoMo**
  A conservative total-consumption model that is useful for quick evaluations. Allows only the five most common impurities (H_2O, SO_2, H_2S, NO_2, O_2) and runs a predefined set of reactions until full consumption of one of the reactants:
  1. $H_2S + 3\,NO_2 \longrightarrow SO_2 + H_2O + 3\,NO$
  2. $2\,NO + O_2 \longrightarrow 2\,NO_2$
  3. $NO_2 + SO_2 + H_2O \longrightarrow NO + H_2SO_4$
  4. $3\,NO_2 + H_2O \longrightarrow 2\,HNO_3 + NO$
  5. $2\,NO_2 + H_2O \longrightarrow HNO_3 + HNO_2$
  6. $8\,H_2S + 4\,O_2 \longrightarrow 8\,H_2O + S_8$

  Source code available at `https://github.com/equinor/tocomo`.
- **Gibbs Minimization Model**
  The model predicts the equilibrium state by minimizing the system's total Gibbs free energy at a given temperature and pressure, without specifying individual reactions. The model is built on top of another open library, called NeqSim (`https://github.com/equinor/neqsim`).
- **pHPitz**
  A thermodynamic model that estimates chemical reactions in a CO_2-rich phase. It uses a standard Equation of State (EoS) to calculate fugacity and the Gibbs minimization principle to predict final compound concentrations. The model also predicts whether a separate acidic phase was formed.
- **SolubilityCCS**
  The model predicts the solubility of nitric and sulfuric acids in CO_2 and the formation of a separate acidic phase. Phase equilibrium is computed based on SRK-CPA (Soave-Redlich-Kwong Cubic Plus Association) equation of state and developed activity model (Kontogeorgis et al., 2006).
  Source code is available at `https://github.com/equinor/solubilityCCS`.

Platform usage

The AcidWatch project started in November 2024, and we are seeing growing interest from the research community and companies. Figure 2 shows the total number of page visits per day and their distribution by country in the period from 23rd of November 2025 till 20th of February 2026.

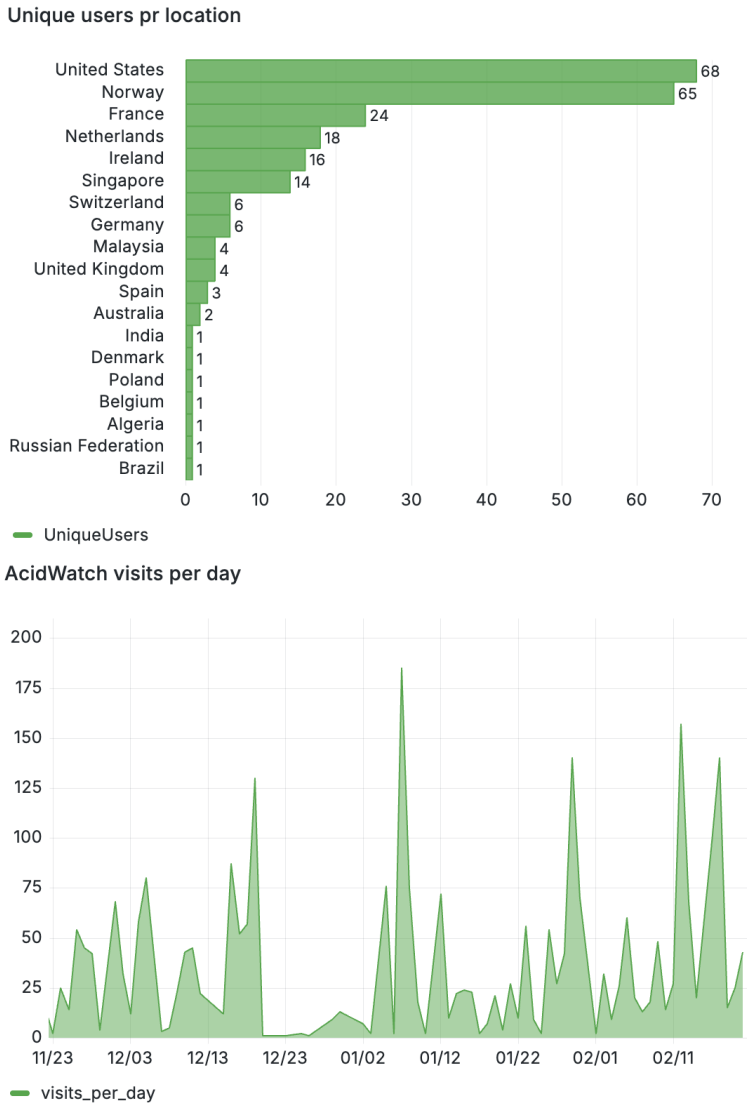

Figure 2: AcidWatch unique users per location (top) and number of non-unique page visits per day (bottom) in the period from 23rd of November 2025 till 20th of February 2026.

Conclusion

We introduced an open-source platform for studying chemical processes in an impure CO_2 stream, called AcidWatch. Designed to support researchers investigating CO_2 impurities, AcidWatch allows running several models, comparing their results against each other and against experimental data, all directly in the browser: `https://acidwatch.radix.equinor.com/`.

The presented usage data shows strong community interest, confirming the demand for accessible and comprehensive tools for the CCS industry. We note, however, that the platform is intended for research use, as the currently available models have not reached a maturity level sufficient to serve as the basis for decision-making.

In the future, we plan to mature both the platform and the available models, adding new features (such as kinetics) and improving modeling accuracy using new experimental data. Moreover, the platform's openness and modularity enable community contributions. We welcome collaboration to extend, validate, and apply the platform.

Source code available at `https://github.com/equinor/acidwatch`.

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References

Kontogeorgis, G. M., Michelsen, M. L., Folas, G. K., Derawi, S., Von Solms, N., & Stenby, E. H. (2006). Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 1. Pure compounds and self-associating systems. *Industrial & engineering chemistry research*, *45*(14), 4855–4868.

Morland, B. H., Tjelta, M., Norby, T., & Svenningsen, G. (2019). Acid reactions in hub systems consisting of separate non-reactive CO_2 transport lines. *International Journal of Greenhouse Gas Control*, *87*, 246–255.

Sonke, J., Morland, B., Moulie, G., & Franke, M. (2024). Corrosion and chemical reactions in impure CO_2. *International Journal of Greenhouse Gas Control*, *133*, 104075.

Svenningsen, G., & Morland, B. H. (2024). Experimental Testing of CO_2 Specifications Under Simulated Ship Transport Conditions. In *Proceedings of the 17th Greenhouse Gas Control Technologies Conference (GHGT-17) 20-24 October 2024.*

Svenningsen, G., Morland, B. H., & Solberg, K. (2024). Impurity reactions in subsea CO_2 pipelines. In *Proceedings of the 17th Greenhouse Gas Control Technologies Conference (GHGT-17) 20-24 October 2024.*