

Pipeline Safety

NIST CAPABILITIES AND CONSIDERATIONS FOR CO₂ INFRASTRUCTURE

Dash Weeks

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EXPANDING THE CO₂ INFRASTRUCTURE

- The state of the CO₂ equation of state
- Effects of impurities on thermodynamics
- Erosion/corrosion implications
- In-situ mechanical material properties
- NIST involvement overview

EXPANDING THE CO₂ INFRASTRUCTURE

The following may be disturbing to some viewers...

Viewer discretion is advised.

1834

72

There are many more versions and modifications but most are fine for single-phase pure fluids.

The state of the CO₂ Equation of State

STATE OF THE CO₂ EOS

Need:

- Accurate Pressure-Volume-Temperature, enthalpy behavior, and phase equilibria is essential for design.
- Better accuracy than simple cubic equations especially near phase boundaries and critical points.
- Viscosity and thermal conductivity correlations, which require calculating density as a function of temperature and pressure.

Solution:

Current Reference EOS: Span and Wagner (1996)

- Experimentally educated
- Multi-parameter
- Substance-Specific

Incorporated in NIST's REFPROP

The Span and Wagner EOS has 42 terms of different types. It is computationally complex and too slow for some applications. There are numerical problems in mixture models and near critical points.

NIST CO₂ EOS EVOLUTION

- New experimental data is available since 1996; the speed of sound is more accurate than heat capacity which reduces uncertainty.
- We have a better understanding of theoretical constraints, and the model is a better representation of super-critical and high-temperature behavior.
- Can now perform state-of-the-art molecular modelling and calculations for heat capacity, thermal conductivity, and viscosity.
- The latest EOS optimization techniques retain high accuracy with fewer terms and improved computational efficiency (factor 1.5 – 2)

RUHR
UNIVERSITÄT
BOCHUM

This work is part of an international collaboration with Ruhr University in Bochum Germany.

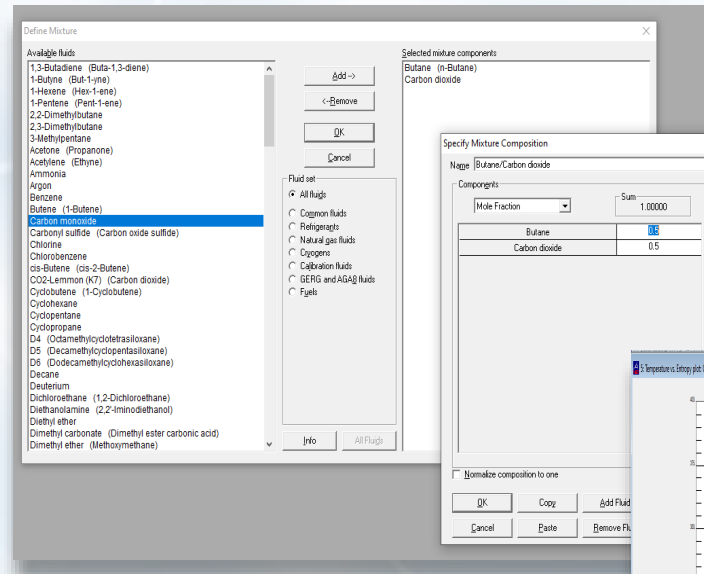
The collaborators are:

- E.W. Lemmon, A.H. Harvey, and I.H. Bell, Applied Chemicals and Materials Division, NIST
- T. Eckermann, R. Span, and M. Thol, Ruhr University Bochum.

REFPROP

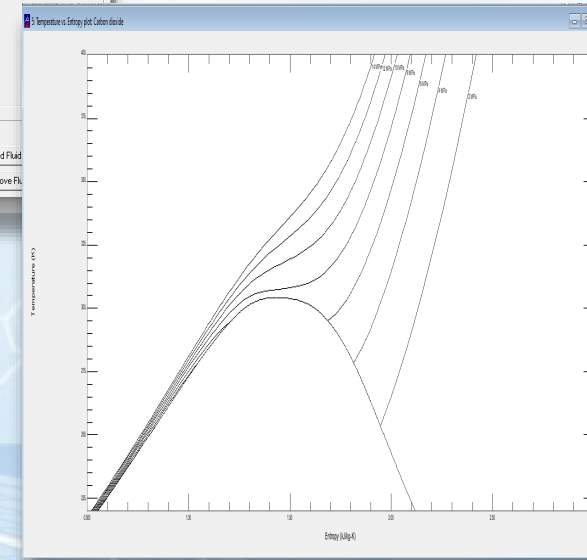
REference Fluid Thermodynamic and Transport PROPERTIES (NIST23)

- REFPROP is a computer program that can provide the thermophysical properties of common industrial fluids and their mixtures, including CO₂ and CO₂ mixtures.
- Computer program sold by NIST Standard Reference Data
<https://www.nist.gov/srd/refprop>
- It may be used on a Windows machine with the graphical user interface (GUI) or one can interface the program with 3rd party software and programs such as Python, Excel, Matlab, Mathematica, etc. using the supplied DLL.



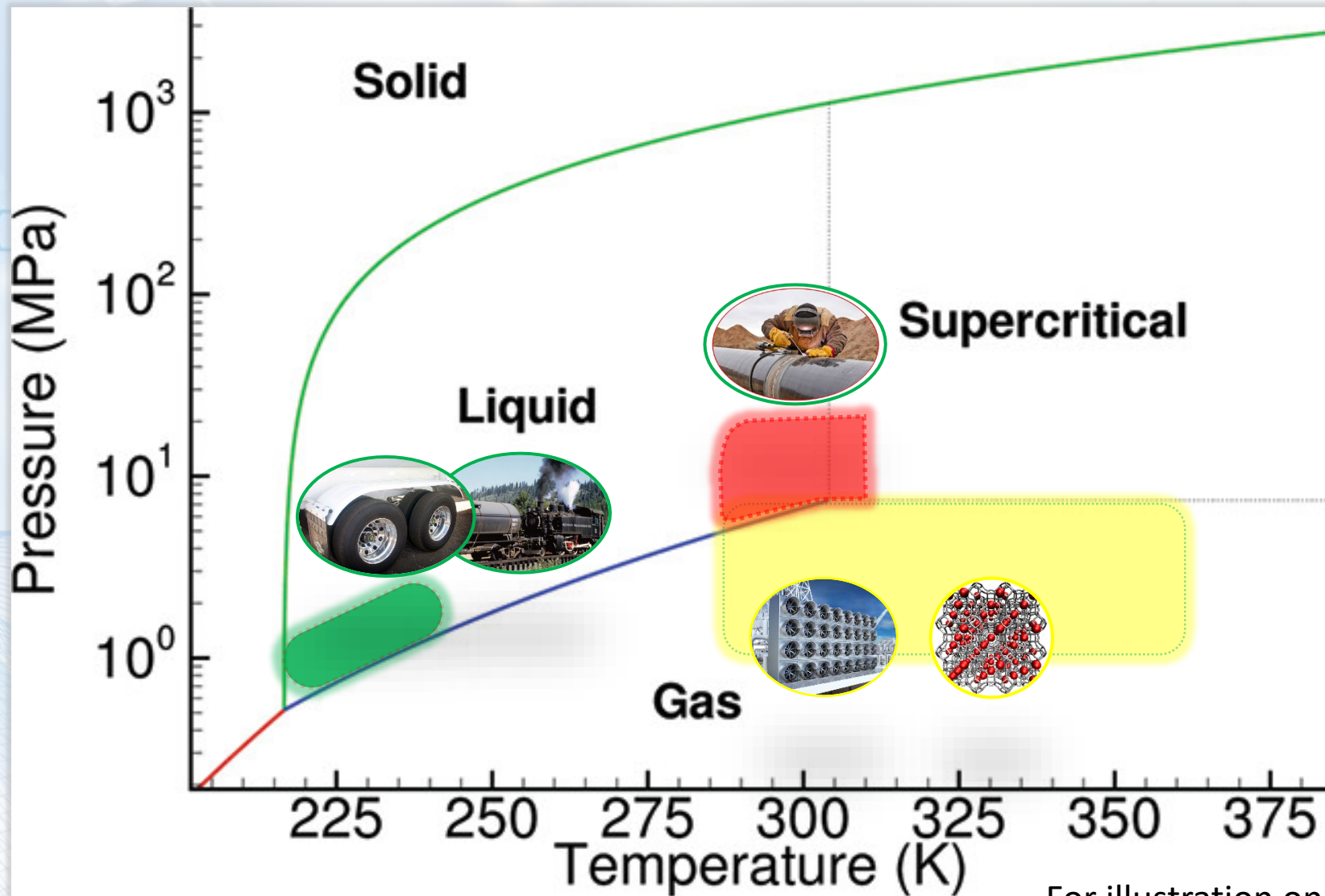
Simple Workflow and GUI

- Select Fluid/Mixture
- Select Units & Properties
- Select calculation(s)
- Plot/Export



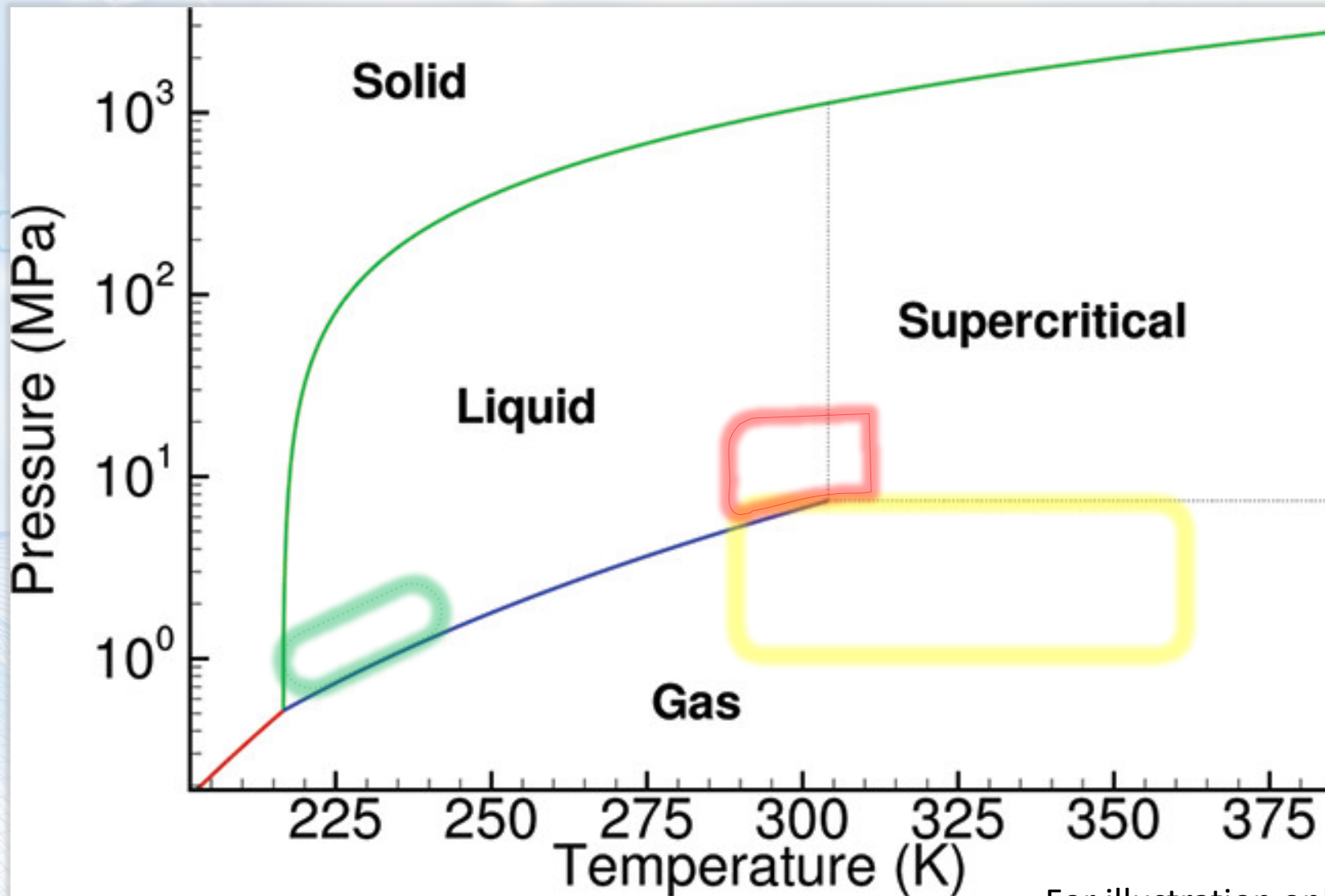
“The NIST REFPROP Database for Highly Accurate Properties of Industrially Important Fluids”, Marcia L. Huber, Eric W. Lemmon, Ian H. Bell, and Mark O. McLinden, Ind. Eng. Chem. Res. 2022, 61, 42, 15449-15472 <https://doi.org/10.1021/acs.iecr.2c01427>

CO₂ PHASE DIAGRAM



For illustration only

CO₂ PHASE DIAGRAM UNCERTAINTY



For illustration only

MIXTURE OR CONTAMINANT (?)

Small concentrations result in small changes in thermodynamic properties

1. What is a significant concentration (change)?
2. What are the limits of detectability?
3. How accurately can we measure concentration?

[CO₂ Measurements and Reference Materials](https://www.nist.gov/programs-projects/carbon-dioxide-measurements-and-reference-materials)

<https://www.nist.gov/programs-projects/carbon-dioxide-measurements-and-reference-materials>



Contaminants also impact:

Mechanical Material Properties

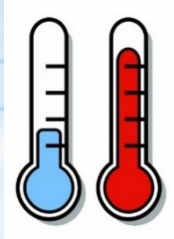
Corrosion/Erosion

Health & Safety

Operations

What are acceptable levels of contaminants to maintain pipeline integrity and public safety?

RANGE OF CONDITIONS IN THE LITERATURE



Temperature
12 °C – 265 °C



Duration
hours → 1 year



Pressure
80 – 240 bar



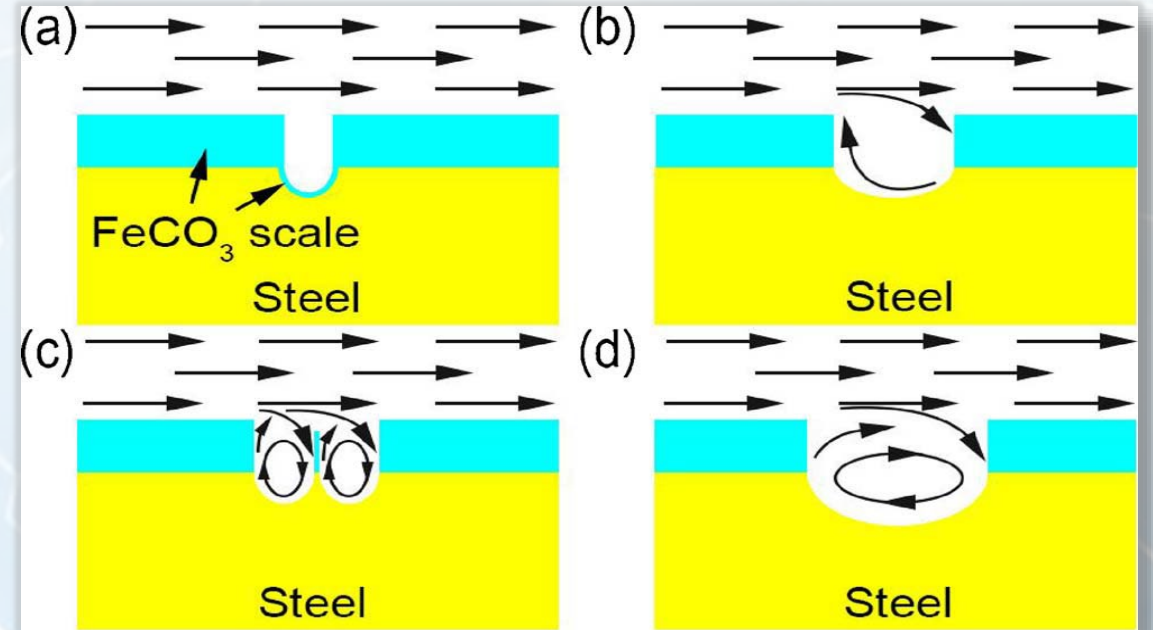
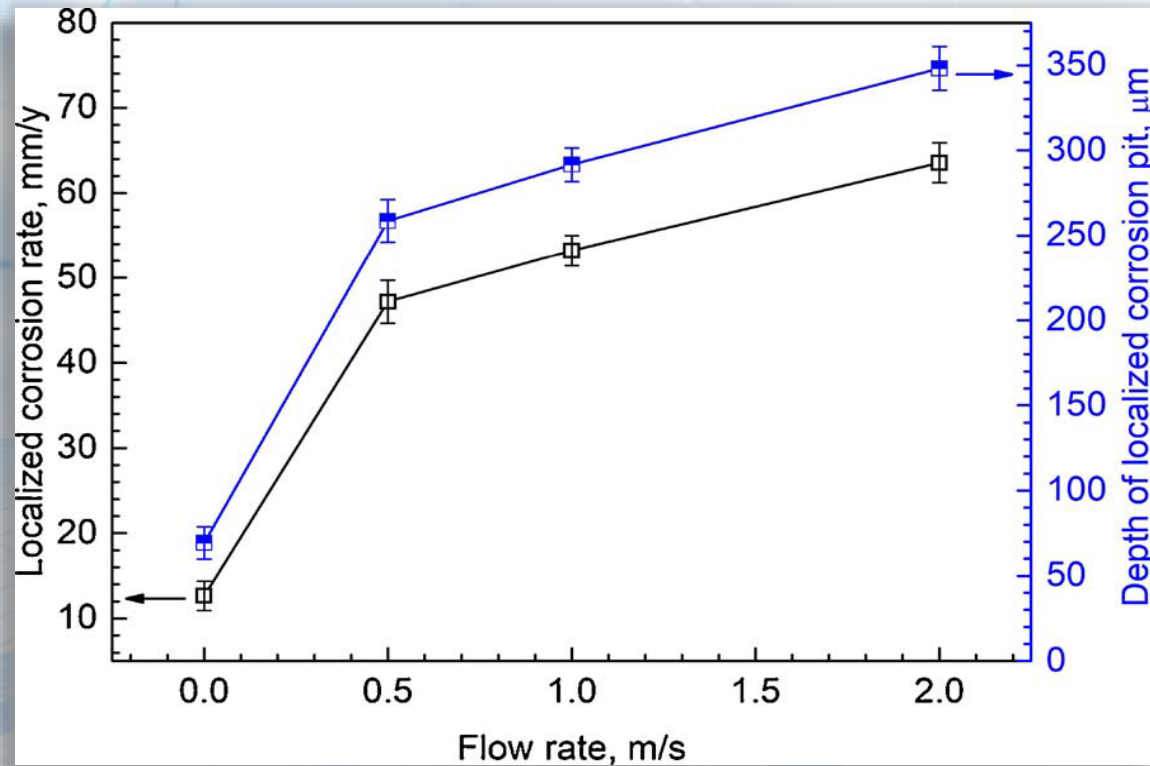
Flow Rate
many static, a few
with flow



Contaminants
H₂O, H₂S, O₂, NO₂, SO₂
(often in combination)

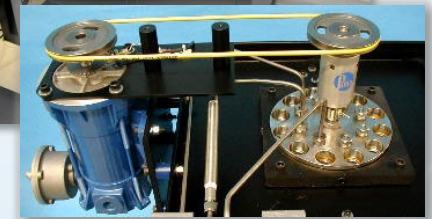
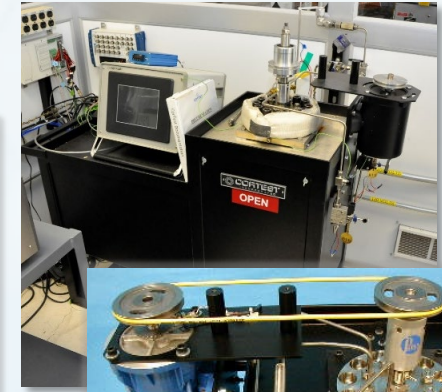
Result: reported corrosion rates **vary over four orders of magnitude** (0.01 – 100 mm/year)

IMPORTANCE OF FLOW RATE



L. Wei, X. Panga, K. Gaoa, *Effect of flow rate on localized corrosion of X70 steel in supercritical CO₂ environments*, *Corr. Sci.* **136** (2018)

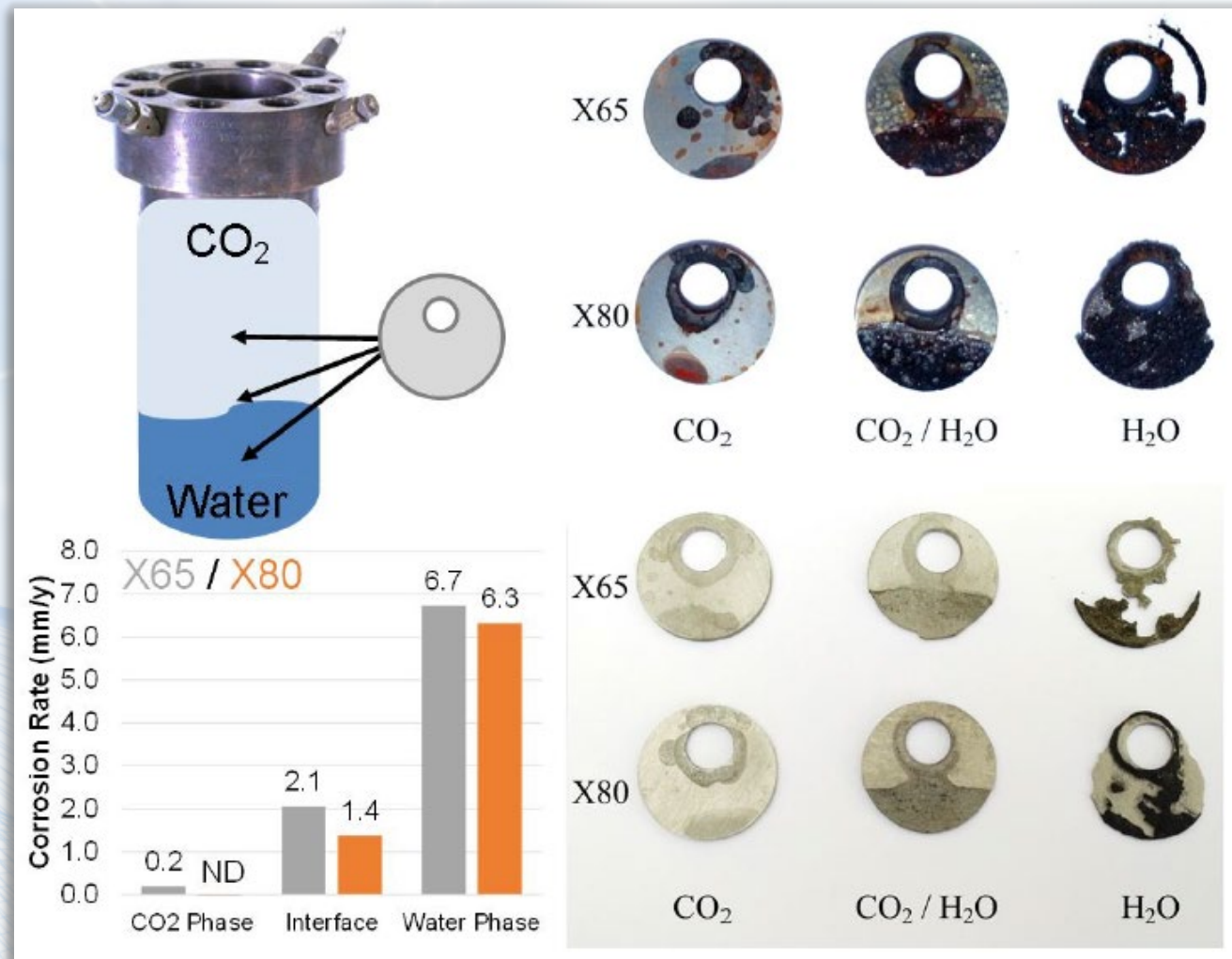
NIST CO₂ TEST FACILITY



- State-of-the-art test facility for SCCO₂ environmental testing within a walk-in fume hood for H₂S testing capability with remote monitoring and continuous data-logging.
- Static and dynamic test applications to evaluate flow-induced damage on multiple alloys simultaneously.
- Multiple autoclaves up to 206 bar and 500 °C
- IGS Analyzer (FTIR) for constituent monitoring

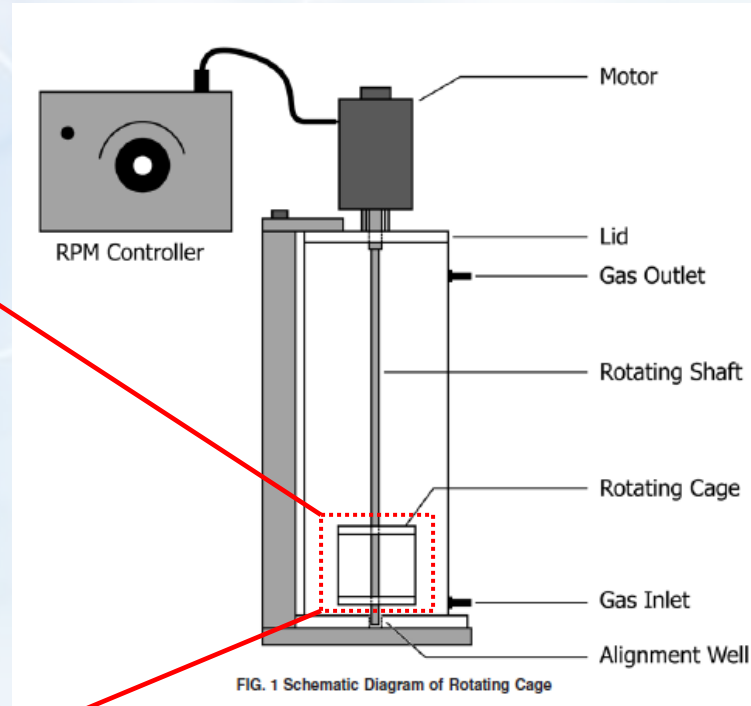
Real conditions include turbulent mixing and contaminants are replenished (locally).
Lab conditions have little to no mixing and a limited contaminant supply (locally).

NIST CO₂ CORROSION TESTS



NACE TM0169
ASTM G31

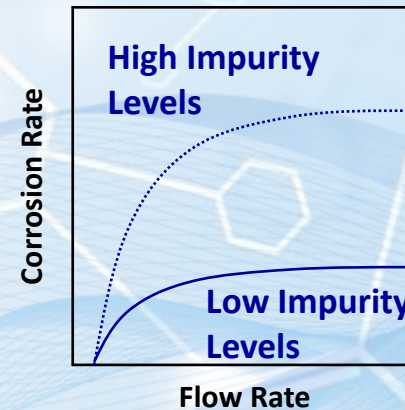
NIST CO₂ FLOW Simulations



Test coupons are 75 x 19 mm and 3 mm thick

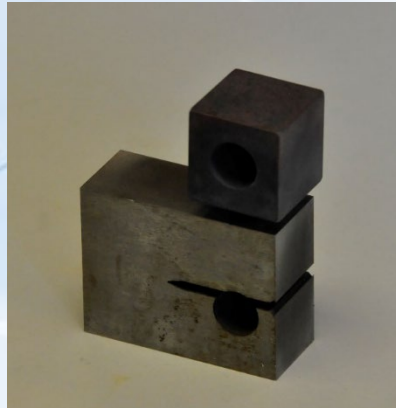
ASTM G184

Concept modified for use in an autoclave with a magnetic drive.



Higher impurity levels are expected to produce thicker corrosion products which could lead to spallation and erosion-corrosion.

NIST CO₂ IN-SITU MECHANICAL TESTS



ASTM E1681

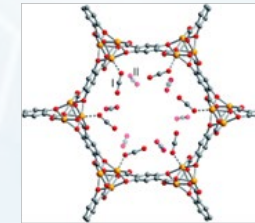


*NACE TM0177
Method B*

Direct Air Capture Sorbent Materials Characterization

Examples of focus areas include:

- [Direct Air Capture Sorbent Materials Characterization](#)
- [Low Carbon Cements and Concretes Consortium](#)
- [Next Generation Seawater CO₂ Reference Materials](#)
- [CO₂ Measurements and Reference Materials](#)
- [Ocean Color Satellite Calibration](#)
- Standards to Underpin MRV
- Standards for Carbon Markets and Accounting
- CO₂ Pipeline Material Reliability
- Convergence with
 - [GHG Measurements](#)
 - [Circular Economy](#)
- NIST collaborates with industry, academia, standards, and government organizations on a broad array of **research, measurements, and standards** to advance CDR, carbon accounting, and decarbonization.

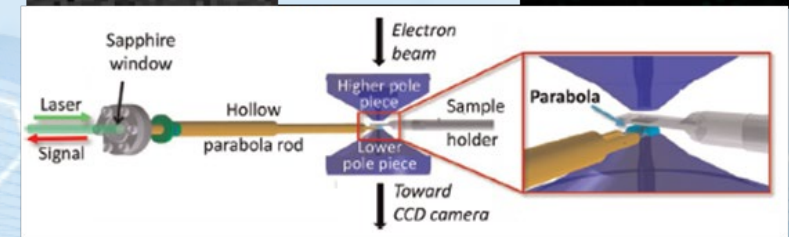
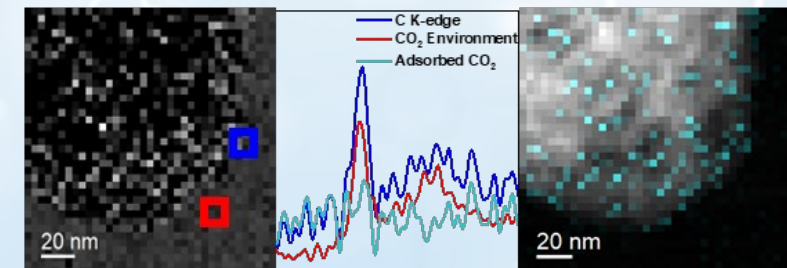


CO₂-MOFs
Structure



[Crystal structures nanosecond dynamics via neutron scattering](#)

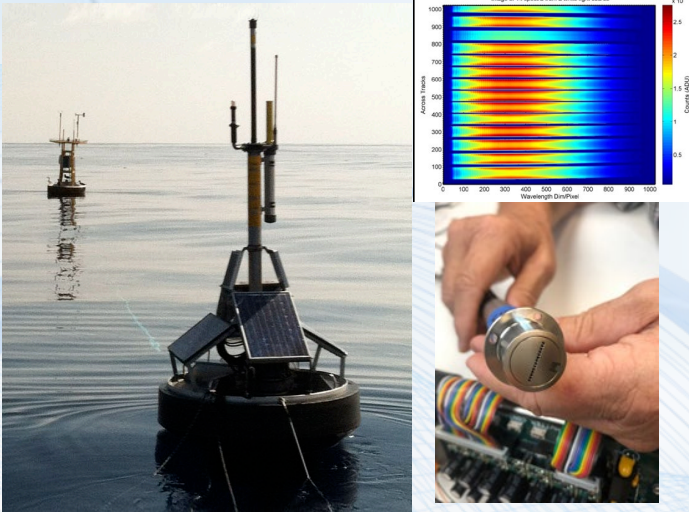
CO₂ adsorption via in-situ STEM-EELS imaging



US Patent US9431211B2 Hybrid electron microscope; Ultramicroscopy 150, 10 (2015), Nature Materials 18 (6), 614-619 (2019) Microscopy and Microanalysis 27 (S1), 800-801 (2021)

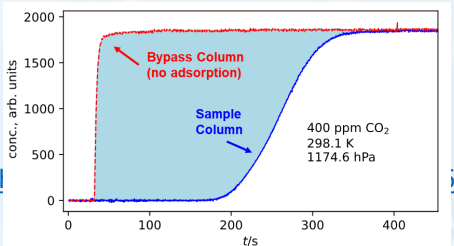
NIST's Mission is to promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.

Technology



Develop critical measurement science to accelerate innovation, scalability, & reduce uncertainties

Benchmark Measurements Data & Materials



Facilitate **rigor and reproducibility** across measurement ecosystems

Documentary Standards



Support industry and Federal use of **voluntary consensus standards**