



the **ENERGY** lab

## PROJECT FACTS

### Hydrogen Turbines

# Thermophysical Properties of CO<sub>2</sub> and CO<sub>2</sub>-Rich Mixtures—National Institute of Standards and Technology

## Background

Carbon capture and storage (CCS) technologies associated with fossil fuel power generation require the handling of significant quantities of carbon dioxide (CO<sub>2</sub>) under a range of application-specific pressure and temperature conditions. These systems typically involve a stream that is mostly CO<sub>2</sub>, with a variety of minor components, including water (H<sub>2</sub>O). Optimization of compressors and other machinery for handling the CO<sub>2</sub> requires knowledge of the thermophysical properties of such mixtures with some precision in order to ensure safe and predictable operation; for example, the H<sub>2</sub>O dew point of the mixture (conditions where liquid water drops out) is significant in order to avoid process conditions where liquid H<sub>2</sub>O condenses in unwanted places, causing mechanical and/or corrosion problems.

There is also growing interest in the use of supercritical CO<sub>2</sub> as a working fluid in power cycles. In this case, it is primarily the properties of pure CO<sub>2</sub> that are of interest. While an equation of state (EOS) exists that describes the thermodynamic properties of pure CO<sub>2</sub> with good accuracy over the relevant range of conditions, the existing correlations for viscosity and thermal conductivity were developed over 20 years ago and have large uncertainties at the high temperatures and pressures relevant for supercritical CO<sub>2</sub> power cycles. In the case of the viscosity, sufficient experimental data are available (or will soon become available) to produce an improved correlation. In the case of the thermal conductivity, experimental data at high temperatures and pressures are largely lacking, and the few data that exist have relatively large uncertainties, so new data are needed in order to produce an improved correlation.

To this end, the National Institute of Standards and Technology (NIST) will develop accurate data and correlations for the dew point of H<sub>2</sub>O in CO<sub>2</sub>/H<sub>2</sub>O mixtures and for viscosity and thermal conductivity for pure CO<sub>2</sub>. This project is managed by the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL). NETL is researching advanced turbine technology with the goal of producing reliable, affordable, and environmentally friendly electric power in response to the nation's increasing energy challenges. With the Hydrogen Turbine Program, NETL is leading the research, development, and demonstration of these technologies to achieve power production from high hydrogen content fuels derived from coal that is clean, efficient, and cost-effective; minimizes carbon dioxide (CO<sub>2</sub>) emissions; and will help maintain the nation's leadership in the export of gas turbine equipment.

## CONTACTS

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## PARTNERS

None

## PROJECT DURATION

Start Date	End Date
10/01/2011	09/30/2014

## COST

**Total Project Value**  
\$600,970

**DOE/Non-DOE Share**  
\$600,970/\$0

## AWARD NUMBER

FE0003931

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U.S. DEPARTMENT OF  
**ENERGY**

## Project Description

NIST will execute experimental and modeling work on the thermodynamics of the CO<sub>2</sub>/H<sub>2</sub>O system, modeling work on the viscosity of pure CO<sub>2</sub>, and experimental and modeling work on the thermal conductivity of pure CO<sub>2</sub>. Specific activities include:

- Perform measurements of dew point for H<sub>2</sub>O in CO<sub>2</sub> at temperatures from approximately 10 degrees Celsius (°C) to approximately 85 °C, at pressures up to about 7 megapascals (MPa). Analyze data to extract thermodynamic parameters such as mixture virial coefficients.
- Develop algorithm for reliable vapor-liquid equilibria (VLE) calculation in CO<sub>2</sub>/H<sub>2</sub>O and similar mixtures. Fit mixture model to available experimental data. Incorporate model and algorithm into NIST REFPROP software.
- Develop new standard viscosity correlation valid to at least 1273 Kelvin (K) and 1000 MPa.
- Using existing apparatus at NIST, measure pure CO<sub>2</sub> thermal conductivity up to 750 K and 70 MPa.
- Develop new standard thermal conductivity correlation valid to at least 1273 K and 100 MPa.

## Goals and Objectives

The overall objective of this effort is to address the critical need to experimentally obtain accurate thermodynamic and physical property data for CO<sub>2</sub> and CO<sub>2</sub>/H<sub>2</sub>O mixtures under specific conditions relevant to advanced power systems (e.g., super-critical CO<sub>2</sub> power cycles) and CCS and, through analysis, develop models based upon the obtained experimental data. The ultimate goal is to provide a standard, validated, high-accuracy set of properties for incorporation into existing public databases.

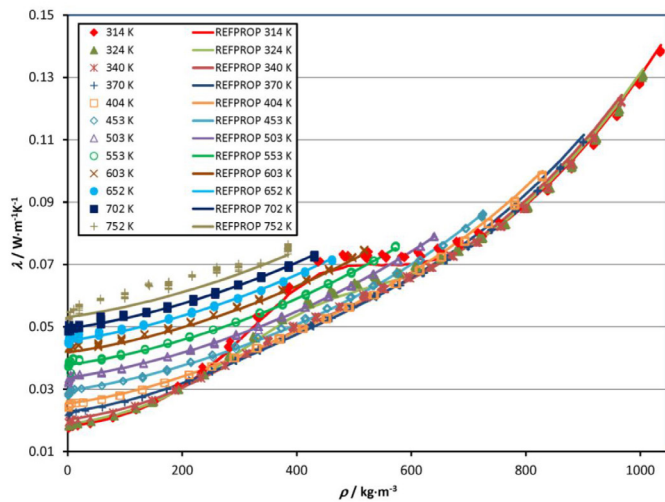


Figure 1. Data obtained in this project for thermal conductivity of pure CO<sub>2</sub> compared with current state-of-the-art correlation.

## Accomplishments

- Completed thermal conductivity measurements of pure CO<sub>2</sub> at temperatures from 220 K to 752 K and pressures up to 69 MPa in the liquid, vapor, and supercritical gas phases with lower uncertainty than existing literature data in most of the region.
- Measurements underway for dew point of H<sub>2</sub>O in compressed CO<sub>2</sub> with four isotherms measured between 10 °C and 40 °C. Uncertainty is much smaller than existing literature data.
- Completed evaluation of literature data for viscosity of pure CO<sub>2</sub> and developed preliminary gas-phase correlation.

## Benefits

This project supports DOE's Hydrogen Turbine Program that is striving to show that gas turbines can operate on coal-based hydrogen fuels, increase combined cycle efficiency by three to five percentage points over baseline, and reduce emissions. Experimental and modeling work by NIST's Thermophysical Properties Division will contribute to the advancement of CCS and facilitate the adoption of novel power cycles and turbo-machinery that have the potential to reduce emissions and increase efficiency.

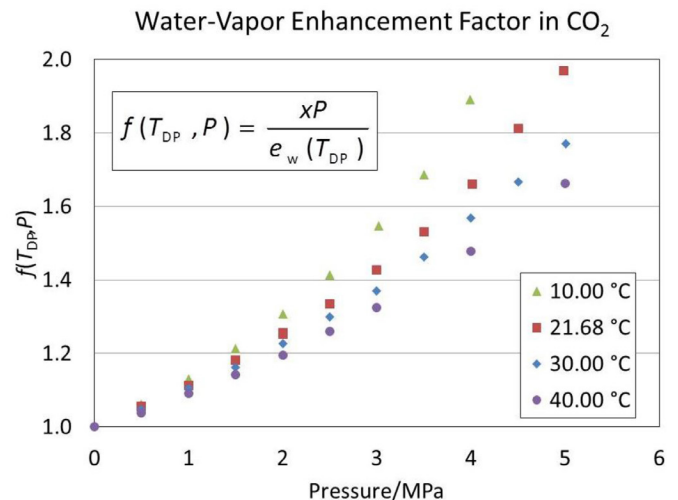


Figure 2. Data obtained so far in this project for enhancement factor, which is the ratio of dew-point water content in the gas to that given by the pure-water vapor pressure alone.