

D 3.2.1

New standard property model for CO₂ mixtures

The IMPACTS project was initiated to understand the impact of impurities in CO₂-rich mixtures on the process chain of Carbon Capture and Storage (CCS). This aim requires various interdisciplinary contributions resulting from, e.g., process simulations, geological research, material science, or safety analyses. However, at a certain point all these efforts demand the knowledge of thermodynamic properties of the involved mixtures. Nowadays, the most accurate way to determine these properties is by means of empirical multiparameter equations of state. As a member of Work Package 1.2 (“Thermophysical behavior of CO₂ mixtures”) the thermodynamics group of RUB (Ruhr-Universität Bochum) is continuously developing an accurate equation of state for CO₂-rich mixtures including components found to be relevant in CCS applications. In addition, new algorithms were developed to face the challenges of phase stability analyses and predictions of various phase equilibria including fluid phases as well as hydrates or solids of CO₂ and water. It is not surprising that neither the application of these algorithms nor the calculation of thermodynamic properties from the equation of state can be individually handled by typical users. Consequently, a simple interface is needed that enables straightforward calculations based on these complex thermodynamic models and algorithms. Within Work Package 3.2 (“Technical knowledge base for CO₂ transport and storage”) RUB is providing the software package TREND (see *Span et al., 2015*) to the CCS community. Since 2009, this property package is continuously improved and extended. The latest version 2.0.1 will soon be distributed via the IMPACTS eRoom and is supposed to become an element of the IMPACTS Toolbox.

The screenshot displays the TREND Excel interface, divided into two main sections: INPUT PARAMETERS and CALCULABLE PROPERTIES.

INPUT PARAMETERS:

- Path to EOS: D:\Zustandsgleichungen\Software\Tortoise
- Input code: TP
- Property 1: 400.0 K
- Property 2: 3 MPa
- Fluids: CO₂, Nitrogen, water
- mole fractions: CO₂ (0.96), Nitrogen (0.04), water (0.02)
- Eq. Type: 1
- Mix. Rules: 1

CALCULABLE PROPERTIES:

Property	Symbol	VBA Function	Value	Unit
COMMON THERMODYNAMIC PROPERTIES				
Temperature	T	TEOS	400.000	K
Density	ρ	DEOS	1627.518	mol/m ³
Pressure	p	PEOS	3.000	MPa
Internal energy	u	UEOS	21094.29	J/mol
Enthalpy	h	HEOS	24126.55	J/mol
Entropy	s	SEOS	187.241	J/mol/K
Gibbs free energy	$g = h - Ts$	GEOS	-18769.83	J/mol
Helmholtz free energy	$a = u - Ts$	AEOS	-21841.99	J/mol
Isobaric heat capacity	c_p	CPEOS	45.855	J/mol/K
Isochoric heat capacity	c_v	CVEOS	32.969	J/mol/K
Speed of sound	w_s	WSEOS	368.47	m/s
Second virial coefficient	B	BVREOS	-5.194E-05	m ³ /mol
Third virial coefficient	C	CVREOS	3.430E-09	m ³ /mol ²
Fourth virial coefficient	D	DVREOS	-2.568E-10	m ³ /mol ³
Cross virial coefficient	B_{12}	B12EOS	-5249	m ³ /mol
Ideal gas isobaric heat capacity	c_p^0	CPEOS	39.7459	J/mol/K
Quality (molar vapor fraction)	β	QEOS	1.000	mol/mol
Compressibility factor	Z	ZEOS	0.980	-
Numerical pressure solution (in the VLE region)	p_{numer}	PNUMEROS	3.980	MPa
Volume expansivity	α_v	VOLEXP	0.00285862	1/K
Isobaric compressibility	κ_T	COMPTEOS	0.1553294	1/MPa
Isothermal compressibility	κ_T	COMPTEOS	0.2180421	1/MPa
Isentropic expansion coefficient	β_s	EXPANSEOS	1.28758631	-
Isothermal expansion coefficient	β_T	EXPANTEOS	0.92574568	-
Joule-Thomson coefficient	μ	JTCDEOS	-3223	-

TREND
Thermodynamic Reference & Engineering Data
TREND 2.1, Prof. Dr.-Ing. Roland Span, Thermodynamics, Ruhr-Universität Bochum

Figure 1: Example calculations of several relevant state properties within the TREND Excel interface for a multicomponent CO₂-rich mixture at given temperature and pressure.