D 3.2.1
New standard property model for CO_2 mixtures

The IMPACTS project was initiated to understand the impact of impurities in CO_2-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 CO_2 mixtures") the thermodynamics group of RUB (Ruhr-Universität Bochum) is continuously developing an accurate equation of state for CO_2-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 CO_2 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 CO_2 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.

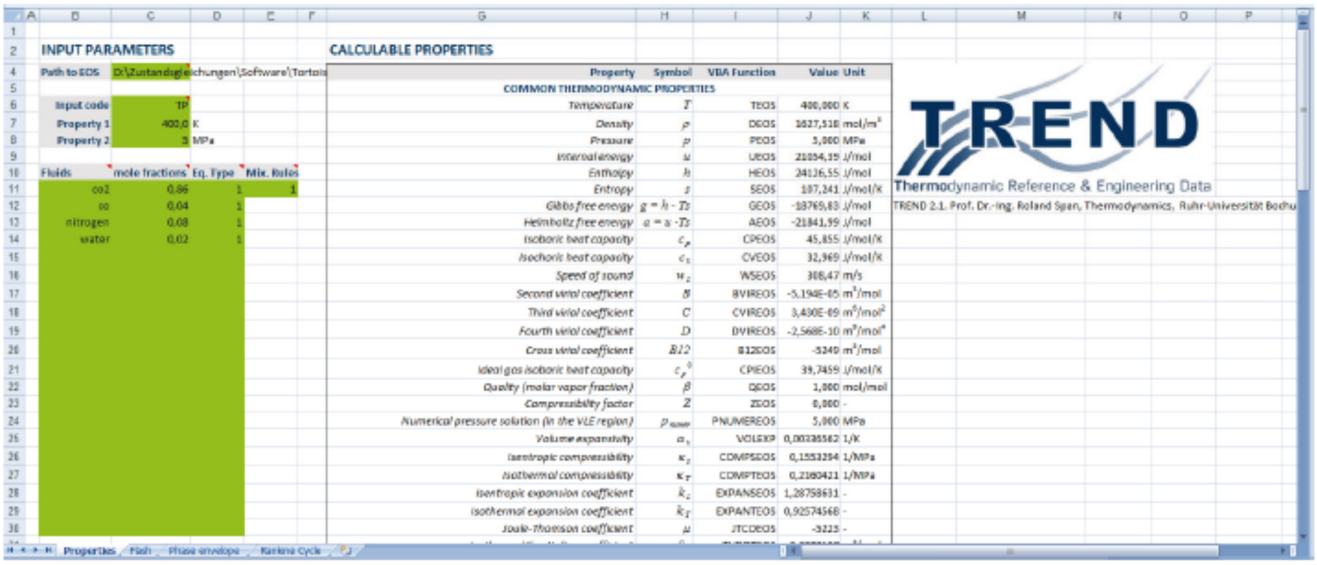

Figure 1: Example calculations of several relevant state properties within the TREND Excel interface for a multicomponent CO_2 -rich mixture at given temperature and pressure.