Memo

User guide

Thermotools
Location:
Trondheim
NORWAY

https://thermotools.github.io/thermopack/index.html

AUTHOR
Vegard Gjeldvik Jervell, Morten Hammer

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1 Introduction

This document is intended for generic user documentation. Also see https://github.com/SINTEF/thermopack/wiki.

2 Phase keys

The phase keys are defined in `src/thermopack_constants.f90`, and are shown in Table 1.

Phase	Key	Description
Two-phase	0	Liquid-vapor two-phase mixture (Code: TWOPH)
Liquid	1	Single phase liquid (Code: LIQPH)
Vapor	2	Single phase vapor (Code: VAPPH)
Minimum Gibbs	3	Single phase root with the minimum Gibbs free energy (Code: MINGIBBSPH)
Single	4	Single phase not identified as liquid or vapor (Code: SINGLEPH)
Solid	5	Single phase solid (Code: SOLIDPH)
Fake	6	In rare cases no physical roots exist, and a fake liquid root is returned (Code: FAKEPH)

Table 1: Phase flags in thermopack.

3 Cubic Equations of State

Name	Key
Van der Waal	VdW
Soave Redlich Kwong	SRK
Peng Robinson	PR
Schmidt-Wensel	SW
Patel Teja	PT
Translated consistent PR	tcPR

Table 2: Cubic Equations of state implemented in ThermoPack and the corresponding keys used for initialization.

3.1 Pure fluid α

Model	Key
Model default*	Classic
Twu-Coon-Bluck-Cunninghan	TWU
Mathias-Copeman	MC
Graboski and Daubert	GD
Redlich-Kwong	RK
Soave	Soave
Peng Robinson 76	PR
UMR α formulation	UMR
Peng Robinson 78	PR78
Van der Waal	VdW
Schmidt-Wensel	SW
Patel Teja	PT

*Will use original α for specified EOS.
E.g. SRK will use Soave α,
Peng-Robinson will use PR α etc.

3.2 α mixing Rules

Name	Key
Van der Waals	Classic or vdW
Wong Sandler	WS
Huron Vidal	HV or HV2
NRTL	NRTL
UNIFAC	UNIFAC

Table 3: Mixing rules and phases available in thermopack, with the corresponding keys used to identify them.

4 Adding new fluids

The fluid database consists of a set of .json -files in the fluids directory. These files are are used to auto-generate the FORTRAN-files compdatadb.f90 and saftvrmie_datadb.f90 by running the respective python scripts compdata.py and saftvrmie.py found in the directory addon/pyUtils/datadb/ . The files are generated in the current working directory and must be copied to the src -directory before recompiling ThermoPack to make the fluids available.

A <fluid>.json file must contain a minimal set of data to be valid. This includes the critical point, accentric factor, mole weight and ideal gas heat capacity.

4.1 Ideal gas heat capacity

Several different correlations for the heat capacity are available, selected by the "correlation"-key in the "ideal-heat-capacity-1" field of the fluid files. These are summarized in Table 4.

Table 4: Ideal gas heat capacity correlations, and the corresponding keys used in the fluid-database.

Key	Correlation	Equation	Unit
1	Sherwood, Reid & Prausnitz[(a)]	$A + BT + CT^2 + DT^3$	$\mathrm{cal\,g^{-1}\,mol^{-1}\,K^{-1}}$
2	API-Project	44	-
3	Hypothetic components	-	-
4	Sherwood, Reid & Prausniz[(b)]	$A + BT + CT^2 + DT^3$	$\mathrm{J\,mol^{-1}\,K^{-1}}$
5	Ici (Krister Strøm)	$A + BT + CT^2 + DT^3 + ET^{-2}$	$\mathrm{J\,g^{-1}\,K^{-1}}$
6	Chen, Bender (Petter Nekså)	$A + BT + CT^2 + DT^3 + ET^4$	$\mathrm{J\,g^{-1}\,K^{-1}}$
7	Aiche, Daubert & Danner[(c)]	$A + B\left[\frac{C}{T}\sinh\left(\frac{C}{T}\right)\right]^2 + D\left[\frac{E}{T}\cosh\left(\frac{E}{T}\right)\right]^2$	$\mathrm{J\,kmol^{-1}\,K^{-1}}$
8	Poling, Prausnitz & O'Connel[(d)]	$\mathrm{R}\left(A + BT + CT^2 + DT^3 + ET^4\right)$	$\mathrm{J\,mol^{-1}\,K^{-1}}$
9	Linear function and fraction	$A + BT + \frac{C}{T+D}$	$\mathrm{J\,mol^{-1}\,K^{-1}}$
10	Leachman & Valenta for H_2	-	-
11	Use TREND model	-	-
12	Shomate equation*	$A + BT_s + CT_s^2 + DT_s^3 + ET_s^{-2}$	$\mathrm{J\,mol^{-1}\,K^{-1}}$

[(a)]3rd ed. [(c)]DIPPR-database
[(b)]4th ed. [(d)]5th ed.
*Note: $T_s = 10^{-3}T$