

Supplementary material for:

The use of equations of state of pure fluid components in pore fluid and fluid inclusion research: computer program PURES (software package FLUIDS)

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Figure A.1.

I/O interface of the module "Pressure" with an example of CO₂ illustrating the input possibilities to calculate pressure defined by a temperature and molar

Pressure

Fluid: CO₂ (Span and Wagner, 1996)

Definitions Pressure: ρ is density
 A is Helmholtz energy
 R is the gas constant
 T is temperature

$$p = \rho^2 \frac{\partial A}{\partial \rho}$$

$$p = \rho RT \left[1 + \delta \left(\frac{\partial \alpha}{\partial \delta} \right) \right]$$

δ is the reduced density $\frac{\rho}{\rho_{crit}}$
 τ is the inverse reduced temperature $\frac{T_{crit}}{T}$
 α is the dimensionless Helmholtz energy $\frac{A}{RT}$

Molar Volume cm³/mol Vol. Unit

corresponding density = 880.196 kg/m³ cm³/mol

Temperature °Celsius kg/m³

Kelvin

°Celsius

At selected temperature: molar volume must exceed 226.6161 cm³/mol or be smaller than 56.90489 cm³/mol. Pressure at melting line is 491.5467 MPa, with a corresponding molar volume of 31.00046 cm³/mol.

Pressure 12.21988 MPa

Figure A.2.

I/O interface of the module “Molar Volume” with an example of CH₄ illustrating the input possibilities to calculate the molar volume (or density) defined by a temperature and pressure

Molar Volume

Fluid: CH₄ (Setzmann and Wagner, 1991) clear

Definition Molar Volume: *numerically estimated with the pressure definition*

Pressure MPa Temp. Unit

Temperature Kelvin Kelvin

°Celsius

pressure limits Supercritical fluid. Maximum pressure of model is 1000 MPa. Maximum pressure at melting line is 628.2429 MPa.

Select bracketing limits Root-Finding Method

The complexity of the equation of state can result in a variety of solutions of the molar volume

*automatic** *note: desired result not always obtained

manual: upper value cm³/mol

lower value cm³/mol

Root-Finding method

Sectant method method of analysis

Brent-Dekker's method

Newton-Raphson's method

bracketing low: 215.6882

bracketing up: 22068.82

calculate

Molar Volume	182.7948	cm ³ /mol
Density	87.764	kg/m ³
number of iterations	40 (Sectant)	
slope (dP/dV)	-0.0111837 (stable)	

Figure A.3.

I/O interface of the module “Temperature” with an example of N₂ illustrating the input possibilities to calculate the temperature defined by a molar volume (or density) and pressure.

Temperature

Fluid: N2 (Span et al., 2000) clear

Definition Temperature: *numerically estimated with the pressure definition*

Molar Volume cm³/mol Vol. Unit
 corresponding density = 280.1348 kg/m³ cm³/mol
 kg/m³

Pressure MPa

limits At selected molar volume: pressure at upper temperature limit (726.85 °C) is 118.33 MPa. Minimum temperature at selected pressure is -201.6293 °C.

Select bracketing limits Root-Finding Method

The complexity of the equation of state can result in a variety of solutions of the temperature

automatic* *note: desired result not always obtained

manual upper value °C
 lower value °C

Root-Finding method

sectant method method of analysis

Brent-Dekker's method bracketing low: 71.52075

Newton-Raphson's method bracketing up: 1100

calculate

Temperature 114.7431 °Celsius Temp. Unit
 Kelvin
 °Celsius

number of iterations: 8 (Brent-Dekker)

slope (dP/dT) = 0.1345677

Figure A.4.

I/O interface of the module “Isochore” with an example of C₂H₆ illustrating the input possibilities to calculate an isochore in the homogeneous fluid stability field (liquid or vapour).

Fluid: C₂H₆ (Bücker and Wagner, 2006)
Fluid Inclusions: Isochore Correction

Molar Volume cm³/mol

corresponding density = 300.6904 kg/m³

Vol. Unit

cm³/mol
 kg/m³

Fluid Inclusions: Homogenization conditions

intersection isochore and liquid-vapour curve

homogenization temperature 27.25795 °C
homogenization pressure 4.394866 MPa

Isochore definition

pressure calculation between lower and upper temperature limits

lower temperature °C

upper temperature °C

temperature interval degree

Molar Volume is defined at:

temperature °C

corresponding pressure:

Temperature (°C)	Pressure (MPa)
50	8.912689
100	19.50127
150	30.28094
200	41.04364
250	51.73002
300	62.32398
350	72.82328
400	83.23033

data is available in:
100.txt

Figure. A.5.

I/O interface of the module “*Isotherm*” with an example of C_3H_8 illustrating the input possibilities to calculate an isotherm.

Fluid: C3H8 (Miyamoto, Watanabe, 2000)
Isotherm definition

Temperature °Celsius

Temp. Unit

 Kelvin
 °Celsius

Vol. Unit

 cm³/mol
 kg/m³

pressure calculation between lower and upper molar volume (density) limits

lower molar volume cm³/mol

upper molar volume cm³/mol

molar volume interval

Molar Volume	Density	Pressure (MPa)
60	734.927	572.372
70	629.9374	146.8513
80	551.1952	33.3737
90	489.9513	0.2903621
100	440.9562	-8.111667

data is available in: 298.15.txt

Liquid-Vapour Equilibrium

homogenisation conditions

pressure 0.9522078 MPa

molar volume (liquid) 89.60496 cm³/mol

molar volume (vapour) 2138.796 cm³/mol