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TREND

Thermodynamic Reference & Engineering Data

TREND User Manual for the Microsoft Excel Interface

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Thermodynamic property calculation

The TREND.DLL was wrapped in VBA code within the TREND.xlam add-in in order to make the dll functions available in Excel. The thermodynamic property function TRENDEOS has the following calling sequence:

Property = TRENDEOS(CALCTYPE;INPUT;PROP1;PROP2;FLUIDS;MOLES;EOSTYPE;MIXTYPE;PATH;UNIT; SHOWERRORCODE)

PATH, UNIT, and SHOWERRORCODE are optional Excel arguments. Detailed descriptions including the default settings are given in Table 1.

Table 1: Optional arguments of TREND Excel functions.

Variable	Type	Description
PATH	Character(255)	Path to the directory, where the FLUIDS and BINARY_MIX_FILES folders are located. By default, TREND search in the same directory where the ExcelSheet is located.
UNIT	Character(20)	Defines the units of the input properties and the resulting properties. Available units are specific, molar, and reduced. Using molar and specific units, all input and output properties (including mole fraction) are given in the corresponding molar or specific SI units. Exceptions are: - Pressure-related units in MPa - Surface tension in 10^3 N/m By default, TREND is set to molar units.
SHOWERRORCODE	Boolean	Controls the error handling in Excel. In case an error occurs in a routine, either the Excel error (FALSE) or the TREND error (TRUE) can be returned. By default, Excel errors are returned.

An overview of all available CALCTYPEs is given in Table 2. The other input parameters correspond to the definitions made in the main Trend Manual. The unit of each property is obtained with the function

Unit = PROPUNIT(CALCTYPE;UNIT; SHOWERRORCODE)

Table 2: Calculable properties with TRENDEOS, the corresponding Calctype, and their input parameters. Examples are given for molar units. All units are given as SI units except for pressure-related properties, which are given in MPa. For further information on the specific units, see the main Trend Manual.

Input parameters: CALCTYPE;INPUT;PROP1;PROP2;FLUIDS;MOLES;EOSTYPE;MIXTYPE;PATH;UNIT; SHOWERRORCODE			
Property	**Symbol**	**Unit = molar**	**Calctype**
Temperature	T	K	T
Density	ρ	mol/m^3	D
Pressure	p	MPa	P
Internal energy	u	J/mol	U
Enthalpy	h	J/mol	H
Entropy	s	J/mol/K	S
Gibbs free energy	$g = h - Ts$	J/mol	G
Helmholtz free energy	$a = u - Ts$	J/mol	A
Isobaric heat capacity	c_p	J/mol/K	CP

Isochoric heat capacity	c_v	J/mol/K	CV
Speed of sound	w_s	m/s	WS
Second virial coefficient	B	m^3/mol	BVIR
Third virial coefficient	C	m^6/mol^2	CVIR
Forth virial coefficient	D	m^9/mol^4	DVIR
1st derivative of *B* wrt. temperature	$\mathrm{d}B/\mathrm{d}T$	m^3/mol/T	DBDT
1st derivative of *C* wrt. temperature	$\mathrm{d}C/\mathrm{d}T$	m^6/mol^2/T	DCDT
Second cross virial coeffcient	B_{12}	m³/mol	B12
Ideal gas isobaric heat capacity	c_p^{o}	J/mol/K	CP0
Quality (molar vapor fraction)	q	mol/mol	Q
Compressibility factor	Z	-	Z
Numerical solution for $p(T,\rho)$	p_{numer}	MPa	PNUM
Numerical speed of sound solution $w(p,s)$	$w_{s,\mathrm{numer}}$	m/s	WSNUM
Volume expansivity	α_v	1/K	VEXP
Isothermal compressibility	κ_T	1/MPa	COMPS
Isentropic compressibility	κ_s	1/MPa	COMPT
Isothermal expansion coefficient	k_T	-	EXPT
Isentropic expansion coefficient	k_s	-	EXPS
Joule-Thomson coefficient	μ	K/MPa	JTCO
Isothermal throttling coefficient	δ_T	m³/mol	THROT
Grueneisen coefficient	Γ	-	GRUEN
Phase Identification parameter	Π	-	PIP
Density of spinodal for given T	$\rho_{\mathrm{Spin,vap/liq}}$	mol/m^3	DSPIN
First derivative of u wrt. v at const. T	$(\partial u/\partial v)_T$	J/mol/m³	DUDV
Riemann scalar curvature	$RIEM$	-	RIEM
Phasetype	PHT	-	PHASE
1st derivative of pressure wrt temperatur	$(\partial p/\partial T)_\rho$	MPa/K	DPDT
1st derivative of pressure wrt density	$(\partial p/\partial \rho)_T$	MPa/(mol/m³)	DPDD
2nd derivative of pressure wrt temperatur	$(\partial^2 p/\partial T^2)_\rho$	MPa/K^2	D2PDT2
2nd derivative of pressure wrt density	$(\partial^2 p/\partial \rho^2)_T$	MPa/(mol/m³)²	D2PDD2
2nd derivative of pressure wrt temperature and density	$(\partial^2 p/\partial \rho \partial T)$	MPa/(mol/m³)/K	D2PDDT
Fundamental derivative of gas dynamics	γ_{GD}	-	GAMMAGD
Boyle temperature	T_{BL}	K	TBOYLE
Joule inversion temperature	T_{JT}	K	TJINV
Joule-Thomson inversion temperature	T_{JTI}	K	TJTINV

RESIDUAL PROPERTIES & HELMHOLTZ DERIVATIVES

Input parameters:

Same as above

Residual pressure	p^{r}	MPa	PR
Residual isochoric heat capacity	c_v^{r}	J/mol/K	CVR
Residual internal energy	u^{r}	J/mol	UR
Residual enthalpy	h^{r}	J/mol	HR
Residual entropy	s^{r}	J/mol/K	SR
Residual chemical potential	μ^r	J/mol	CPOTR
Reduced residual Helmholtz energy	α^r	-	A00
1st derivative of α^r w.r.t δ, multiplied with δ	$\delta \cdot \alpha^r_\delta$	-	A01
1st derivative of α^r w.r.t τ, multiplied with τ	$\tau \cdot \alpha^r_\tau$	-	A10
2nd derivative of α^r w.r.t δ and τ multiplied with $\delta * \tau$	$\delta\tau \cdot \alpha^r_{\delta\tau}$	-	A11
2nd derivative of α^r w.r.t δ, multiplied with δ^2	$\delta^2 \cdot \alpha^r_{\delta\delta}$	-	A02

2nd derivative of α^r w.r.t τ, multiplied with τ^2	$\tau^2 \cdot \alpha^r_{\tau\tau}$	-	A20
3rd derivative of α^r w.r.t τ, δ, and δ, multiplied with $\tau * \delta^2$	$\tau\delta^2 \cdot \alpha^r_{\tau\delta\delta}$	-	A12
3rd derivative of α^r w.r.t τ, τ, and δ, multiplied with $\delta * \tau^2$	$\tau^2\delta \cdot \alpha^r_{\tau\tau\delta}$	-	A21
3rd derivative of α^r w.r.t δ, multiplied with δ^3	$\delta^3 \cdot \alpha^r_{\delta\delta\delta}$	-	A03
3rd derivative of α^r w.r.t τ, multiplied with τ^3	$\tau^3 \cdot \alpha^r_{\tau\tau\tau}$	-	A30
Excess volume	v^E	m³/mol	VE
Excess enthalpy	h^E	J/mol	HE
Excess Gibbs energy	g^E	J/mol	GE

PHYSICAL PROPERTIES

Input parameters:

Same as above

Surface tension	σ	mN/m	ST
Dielectric constant	ε	-	DE
Dynamic viscosity	η	µPa s	ETA
Thermal conductivity[1]	λ	W/m/K	TCX
Acentric factor	ω	-	AF

[1]Differences in the thermal conductivity compared to TREND 4.0 are attributable to updated viscosity models

The fluid specifications bulk function is only depending on the composition, the chosen equation type, the mixing rule, and the unit system. It provides, e.g., the range of validity of an equation of state, the molar mass of a substance or mixture, or the acentric factor. The calling sequence for this function is:

Specification = TRENDSPECEOS(FLUIDS;MOLFRACTIONS;EOSTYPE;MIXTYPE;PATH;UNIT;SHOWERRORCODE SPECPROP;FLUIDNR)

The grey colored arguments SPECPROP and FLUIDNR are optional. Depending on the number of components (ncomps) in the mixture, a range of 12 ROWS and ncomps + 3 COLUMNS must be selected to obtain all information of each fluid and the mixture specifications, if the optional arguments are not entered. If for example SPECPROP is "MW" and FLUIDNR is not given, the molar mass of the mixture will be the result. If FLUIDNR is provided, the molar mass of the corresponding substance in the mixture will be displayed. See Table 3 for the complete list of possible inputs for SPECPROP.

Table 3: Fluid and mixture specific information provided by TRENDSPECEOS.

BULK FUNCTION FOR FLUID AND MIXTURE SPECIFIC INFORMATION

Input parameters:

FLUIDS; MOLFRACTIONS; EOSTYPE; MIXTYPE; PATH; UNIT; SHOWERRORCODE; SPECPROP; FLUIDNR

Property	Symbol	Unit = molar	SPECPROP
Molecular weight	M	kg / mol	MW
Triple point temperature (pure fluids only)	T_{tr}	K	Ttrip
Triple point pressure (pure fluids only)	p_{tr}	MPa	ptrip
Critical temperature (pure fluids only)	T_c	K	Tcrit
Critical pressure (pure fluids only)	p_c	MPa	pcrit
Critical density (pure fluids only)	ρ_c	mol / m³	Dcrit
Acentric factor	ω	-	af
Minimum temperature (pure fluid)	T_{min}	K	Tmin

Maximum temperature (pure fluid)	T_{max}	K	Tmax
Maximum pressure (pure fluid)	p_{max}	MPa	pmax
Maximum density (pure fluid)	ρ_{max}	mol / m³	Dmax

The subroutine ALLEOS has the following call:

ALLEOS (INPUT;PROP1;PROP2;FLUIDS;MOLFRACTIONS;EOSTYPE;MIXTYPE;PATH;UNIT; SHOWERRORCODE)

In order to use the ALLEOS routine, a range of 15 cells needs to be selected. A click on the *fx* button after typing "ALLEOS(" opens the optional context menu (see Figure 1). After finishing the inputs **Ctrl+Shift+ Enter** need to be pushed at the time instead of just Enter or clicking ok. The 15 selected cells will then be filled with *T, D, P, U, H, S, G, A, CP, CV, WS, B, C, CP0*, and *Q*, respectively.

SUBROUTINE FOR THE CALCULATION OF ALL COMMON THERMODYNAMIC PROPERTIES

Input parameters:

INPUT; PROP1; PROP2; FLUIDS; MOLFRACTION; EOSTYPE; MIXTYPE; PATH; UNIT; SHOWERRORCODE

Property	Symbol	Unit = molar	
Temperature	T	K	ALLEOS
Density	ρ	mol/m^3	
Pressure	p	MPa	
Internal energy	u	J/mol	
Enthalpy	h	J/mol	
Entropy	s	J/mol/K	
Gibbs free energy	$g = h - Ts$	J/mol	
Helmholtz free energy	$a = u - Ts$	J/mol	
Isobaric heat capacity	c_p	J/mol/K	
Isochoric heat capacity	c_v	J/mol/K	
Speed of sound	w_s	m/s	
Second Virial coefficient	B	m^3/mol	
Third Virial coefficient	C	m^6/mol^2	
Ideal gas isobaric heat capacity	c_p^0	J/mol/K	
Quality (molar vapor fraction)	β	mol/mol	

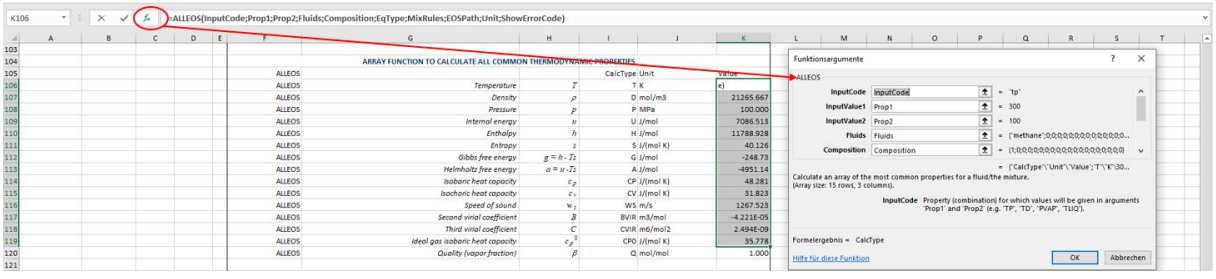

Figure 1: ALLEOS routine.

Instead of specifying the path, hard-coded parameters from the DLL can also be used by setting the path to "HC". For further information see main TREND manual.

The input code indicates the thermodynamic input properties for the calculation. The TREND property package can handle input combinations as indicated in Table 4. The Inputs may depend on the specified UNIT system.

Table 4: Input combinations of thermodynamic properties for the property functions

Input code	PROP1	PROP2	Comment
"TD" [1)]	Temperature [K]	Density UNIT=molar[mol/m³] UNIT=specific[kg/m³]	
"TP" [1)]	Temperature [K]	Pressure [MPa]	
"PH" [1)]	Pressure [MPa]	Enthalpy UNIT=molar[J/mol] UNIT=specific[J/kg]	
"PS" [1)]	Pressure [MPa]	Entropy UNIT=molar[J/mol/K] UNIT=specific[J/(kg K)]	
"PVAP"	Pressure [MPa]	- [2)]	Calculation of the saturated vapor at given pressure
"PLIQ"	Pressure [MPa]	- [2)]	Calculation of the saturated liquid at given pressure
"TVAP"	Temperature [K]	- [2)]	Calculation of the saturated vapor at given temperature
"TLIQ"	Temperature [K]	- [2)]	Calculation of the saturated liquid at given temperature
"TSUBV+"	Temperature [K]	- [2)]	Calculation of the resublimation curve at given temperature. Only possible for pure substances.
"TSUBS+"	Temperature [K]	- [2)]	Calculation of the sublimation curve at given temperature. Only possible for pure substances.
"PSUBV+"	Pressure [MPa]	- [2)]	Calculation of the resublimation curve at given pressure. Only possible for pure substances.
"PSUBS+"	Pressure [MPa]	- [2)]	Calculation of the sublimation curve at given pressure. Only possible for pure substances.
"TMLTL+"	Temperature [K]	- [2)]	Calculation of the freezing curve at given temperature. Only possible for pure substances.
"TMLTS+"	Temperature [K]	- [2)]	Calculation of the melting curve at given temperature. Only possible for pure substances.
"PMLTL+"	Pressure [MPa]	- [2)]	Calculation of the freezing curve at given pressure. Also implemented for mixtures.
"PMLTS+"	Pressure [MPa]	- [2)]	Calculation of the melting curve at given pressure. Only possible for pure substances.

[1)] The combination of PROP1 and PROP2 in the input code is arbitrary, e.g.: "TD" works as well as "DT" (the first letter always indicates PROP1, the second PROP2).

[2)] PROP2 must be an arbitrary value larger than zero. It will be ignored by the routines.

Using the input combinations as indicated in Table 3, the given limits of the equation of state (e.g., T_{min}, T_{max}, p_{max}, etc.) will be taken into account. For calculations outside the range of validity, a “&” has to be used at the end of the input code (e.g., “TD&” or “TP&”).

When choosing the inputs "TP+", "PH+", or "PS+", solid phases and equilibria of up to three phases are considered. "TD+" is not implemented yet. Note that for the inputs without an additional "+" only two-phase equilibria are considered, even if all phases are fluid phases.

In principle, there are two ways to set the needed input. It can be directly entered as seen in Figure 2.

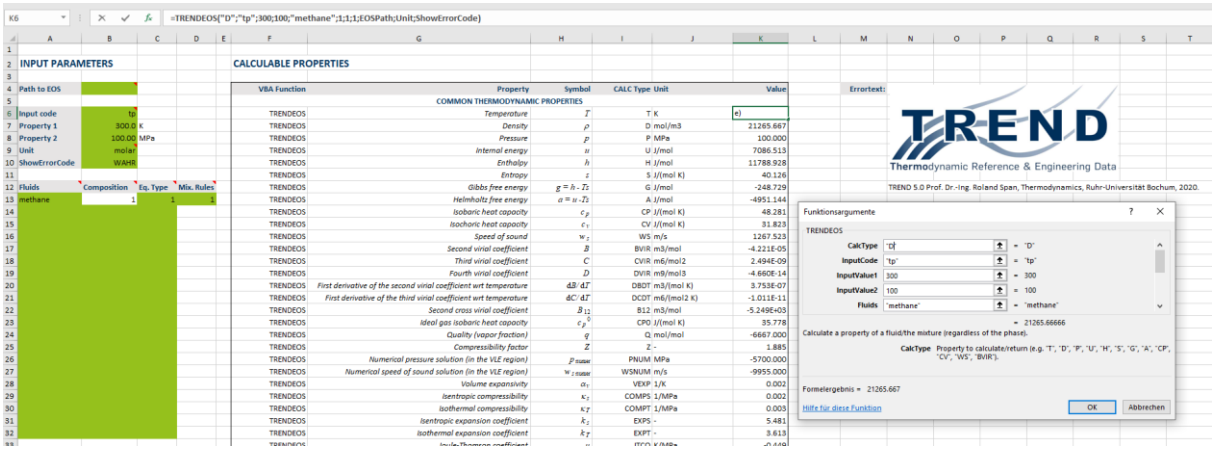

Figure 2: Direct input.

Alternatively, cells and ranges of cells can be given that hold the required information (Figure 3).

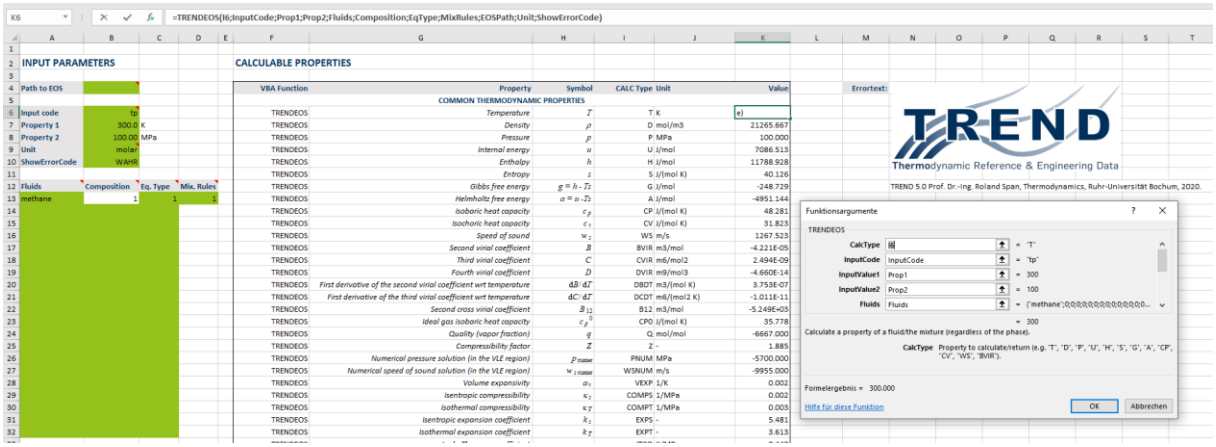

Figure 3: Input in cells and ranges of cells.

For further details on the routines and inputs please see the general TREND manual.

In addition to the calculation with the regular TRENDEOS function, saturation properties can also be calculated with ancillary equations. Ancillary equations are NOT fundamental equations of state! The ancillary equations are used to generate starting values for the iteration of saturation properties with equations of state. With lower accuracy requirements, they enable an estimation of saturation properties with reduced computing time. The function ANC_EQ calculates saturation properties for pure fluids based on ancillary equations. The calling sequence for this function is:

Property = ANC_EQ(CALCTYPE;INPUT;PROP1;PROP2,FLUIDS,MOLEFRACTIONS;EOSTYPE;MIXTYPE; PATH;UNIT)

Table 5: Calculable properties with ANC_EOS and their corresponding CALCTYPE.

Input parameters: CALCTYPE;INPUT;PROP1;PROP2;FLUIDS;MOLES;EOSTYPE;MIXTYPE;PATH;UNIT;SHOWERRORCODE			
Property	**Symbol**	**Unit = molar**	**Calctype**
Melting temperature	T_{melt}	K	TMELT
Melting pressure	p_{melt}	MPa	PMELT
Sublimation temperature	T_{sub}	K	TSUB
Sublimation pressure	p_{sub}	MPa	PSUB
Saturated liquid density	ρ_{liq}	mol/m^3	DLIQ
Saturated vapor density	ρ_{vap}	mol/m^3	DVAP
Vapor pressure	p_{vap}	MPa	PVAP

The function GAMMATFEOS calculates the thermodynamic factor according to Kooijman and Taylor (see general TREND manual). The calling sequence for this function is:

Specification =
GAMMATFEOS (INPUT;PROP1;PROP2,FLUIDS;MOLFRACTIONS;EOSTYPE;MIXTYPE;PATH)

Input parameters are defined as described in Table 2 in the general TREND manual. An output example for a mixture of ten components is given in the TREND.xlsx.

The function FUGCOEFFEOS calculates the fugacity coefficients for pure fluids or for each component in a mixture. The calling sequence for this function is:

Specification =
FUGCOEFF_EOS (INPUT;PROP1;PROP2,FLUIDS;MOLFRACTIONS;EOSTYPE;MIXTYPE;PATH;)

Input parameters are defined as described in Table 2 in the general TREND manual. An output example for a mixture of ten components is given in the TREND.xlsx.

Flash calculation

The calculation of a two-phase or three-phase flash is carried out by the subroutine FLASH. This subroutine has the common calling sequence according to Table 2 in the general TREND manual:

FLASHEOS(INPUT;PROP1;PROP2;FLUIDS;MOLFRACTIONS;EOSTYPE;
MIXTYPE;PATH;UNIT;SHOWERRORCODE)

The FLASH subroutine returns the following output parameters (for details see Table 6 and Figure 4):

PROP_PHASE; PROP_OVERALL; X_PHASE; PHASEFRAC

Table 6: Return parameters of the FLASH subroutine.

Parameter	Type	Comment
PROP_PHASE	Double Array, length {30,5}	Properties of the phases. First index is the property: T, p, ρ, u, h, s, g, a, c_p, c_v, w, hydration number, hydration structure, overall small cage occupancy, overall large cage occupancy, molecular weight Second index: indicates the phase, see phasetype
PROP_OVERALL	Double Array, length 30	Overall properties of the mixture: T, p, ρ, u, h, s, g, a, c_p, c_v, w, molecular weight
PHASEFRAC	Double Array, length 5	Molar phase fraction of the phase. For phase indicator explanation, see phasetype
X_PHASE	Double Array, length {30,5}	Molar composition of the phases in equilibrium First index: mole fraction of the component in the mixture Second index: indicates the phase, see phasetype

In order to use the FLASH routine, 9 columns and 38 rows need to be selected. A click on the *fx* button after typing "FLASHEOS(" opens the optional context menu. After finishing the inputs **Ctrl+Shift+ Enter** need to be pushed at the time instead of just Enter or clicking ok. The selected cells will then be filled as shown in Figure 4.

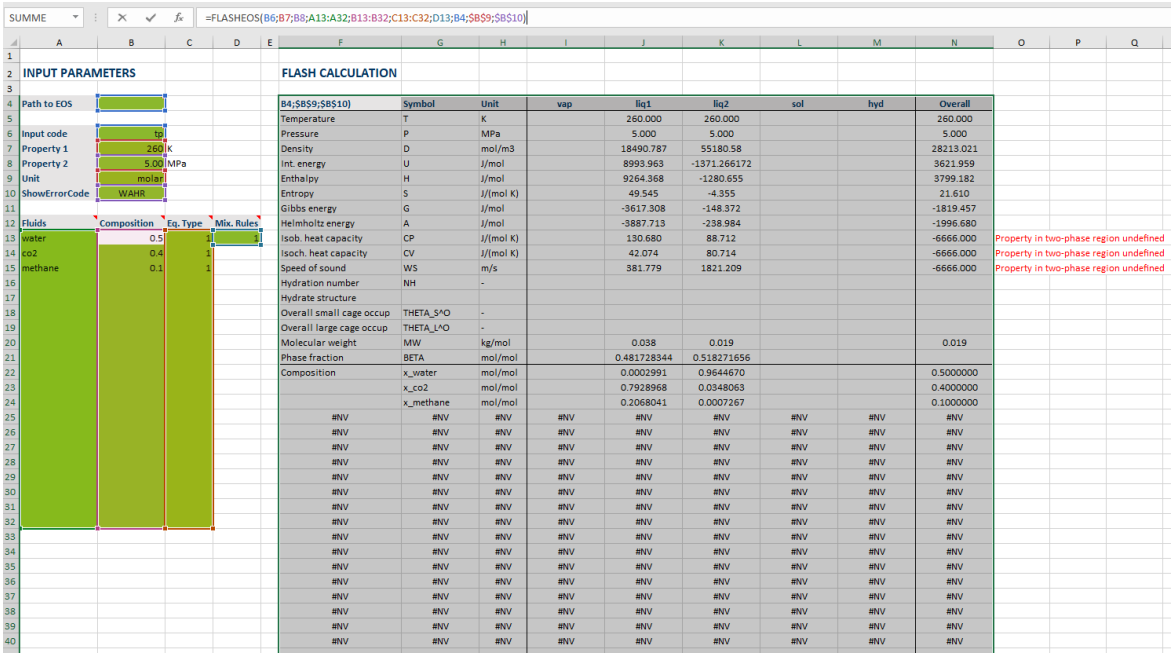

Figure 4: Flash routine

In the subroutine FLASH, a stability analysis determines if the given mixture is stable or if it decomposes into two or three phases. If the mixture is found to be unstable, the mole fractions of the split phases are calculated subsequently.

Calculations with seawater

In TREND, seawater is handled as a pseudo pure fluid. Only the 'tp' input is implemented for seawater or seawater mixtures. The model for seawater is based on the IAPWS standard. For using the model in TREND, the input for the fluids has to be set to 'seawater', which has to be followed by 'salinity'. Otherwise, an error will be returned. Equation type for salinity is the same as for the other components. If only seawater is present, the fraction of seawater has to be set to 1. The salinity, which is defined as mass fraction of salt in the liquid seawater, must always be given as mass fraction of salt in seawater. The seawater model is also implemented for mixtures with other fluid phases. At the moment, only the Mixtype 1 is supported (Helmholtz mixtures). An input example for a seawater+CO_2 mixture is given in Figure 5. In mixtures, the sum of water and salt has to be given as "seawater" followed by the salinity (mass fraction) of salt in liquid seawater. For the proper calculation of mixtures with seawater present, the seawater has to be given as first entry in the fluid list, followed by salinity. For mixtures, only fluid phases are supported with the input 'tp'. Further information are given in the general TREND manual.

Seawater is supported in the following routines:

TRENDEOS, FLASH3, TRENDSPEC

The range of validity as given in the IAWPS release allows the calculations in the following areas:

$0 \leq S \leq 0.12\ \mathrm{kg\,kg^{-1}}$;	$261\ \mathrm{K} \leq T \leq 353\ \mathrm{K}$;	$0.101325\ \mathrm{MPa} \leq p \leq 100\ \mathrm{MPa}$
$0 \leq S \leq 0.042\ \mathrm{kg\,kg^{-1}}$;	$T_f \leq T \leq 313\ \mathrm{K}$;	$p^{\mathrm{vap}} \leq p \leq 0.101325\ \mathrm{MPa}$
$0 \leq S \leq 0.12\ \mathrm{kg\,kg^{-1}}$;	$T_f \leq T \leq 353\ \mathrm{K}$;	$p = 0.101325\ \mathrm{MPa}$

S is the absolute Salinity, T_f is the freezing temperature and p^{vap} is the vapor pressure.

Fluids	mole fractions	Eq. Type	Mix. Rules
seawater	0.5	1	1
salinity	0.035	1	
co2	0.5	1	

Figure 5:Example for fluid and composition input for a mixture with seawater and carbon dioxide.

NaCl-Brine

Similar to the seawater implementation, the brine is handled as pseudo-pure component. Next to the mass or mol fraction of the brine, the molality (mol_{NaCl}/kg_{H2O}) of NaCl has to given as input. The molality always needs to be given as moles of NaCl per kg of water in the solution (mol_{NaCl}/kg_{H2O}). An input example for a 2 *m* brine is given in Figure 6. At the moment, only properties for a NaCl-brine is implemented, calculations for other salts or mixtures with other components like CO_2 are not supported in this version. Possible input combinations are: 'tp', 'tp+' and pmltl+ for the calculation of freezing temperatures of the brine. The fluids always have to be given as 'water' and 'nacl' as shown in the example below. In contrast to the other components, the Eq. Type for the salt has to be set to 15, while the Mix Rule has to remain 1. Up to now, the brine model is only available in combination with Helmholtz equations of state for the solvent water.

Calculations are possible from the freezing point up to T = 373.15 K, pressures up to p = 50 MPa and molalities up to m = 6 mol_{NaCl}/kg_{H2O}.

The brine model is supported in the functions FLASH3 and TRENDEOS for the properties shown in the provided FLASH map of the Excel Spreadsheet.

Path to EOS			
Input code	tp+		
Property 1	298.15	K	
Property 2	0.10	MPa	
Unit	molar		
ShowErrorCode	WAHR		
Fluids	**Composition**	**Eq. Type**	**Mix. Rules**
water	1	1	1
nacl	2	15	

Figure 6:Example for the input for the calculation of thermodynamic properties for a 2 m NaCl brine.

Phase Envelope Calculation

The subroutine PTDIAGEOS calculates points on the phase envelope (bubble and dew points at constant composition) for a given mixture. If a pure fluid is passed to the routine, it returns the vapor-pressure curve. In addition to the temperature and pressure for each point, the routine returns the densities of the original and the incipient phase, the composition of the incipient phase and a point ID number. The subroutine has the following calling sequence:

PTDIAGEOS(ENV_PV;FLUIDS;MOLFRACTIONS;EOSTYPE;MIXTYPE;T_SPEC;P_SPEC;PATH;SHOWERRORCODE)

In addition to the input parameters FLUIDS, MOLFRACTIONS, PATH, EOSTYPE, and MIXTYPE, which are already described in Table 2 of the general TREND manual, the input parameters for this routine are:

Table 7: Additional input parameters for the routine PTDIAGEOS

Parameter	Type	Comment
ENV_PV	Integer	Toggle to set whether pressure (1) or volume-based (2) phase-envelope calculation is used.
T_SPEC	Double	Specified temperature [K] for which a point on the phase envelope is calculated. If no temperature is specified, this parameter has to be set to zero!
P_SPEC	Double	Specified pressure [MPa] for which a point on the phase envelope is calculated. If no pressure is specified, this parameter has to be set to zero!

The PTDIAGEOS subroutine returns the following output (for details see Table 8 and Figure 4):

T_PTS;P_PTS;RHOLIQ_PTS; RHOVAP_PTS;POINTID;X_PTS.

Table 8: Output parameters of the routine PTDIAGEOS

Parameter	Type	Comment
T_PTS	Double Array, length 400	Array with the temperatures of the calculated saturation points.
P_PTS	Double Array, length 400	Array with the pressures of the calculated saturation points.
RHOLIQ_PTS	Double Array, length 400	Array with the densities of the incipient phase of the calculated saturation points.
RHOVAP_PTS	Double Array, length 400	Array with the densities of the original phase of the calculated saturation points.
POINTID	Long Array, length 400	Array with the point IDs for each saturation point. The point IDs are: 0: Normal point on the phase envelope 1: Critical point (interpolated) 2: Maximum temperature (cricondentherm) 3: Maximum pressure (cricondenbar) 4: Specified temperature 5: Specified pressure
X_PTS	Double Array, length {400,30}	Array with the composition of the incipient phase of the calculated saturation points.

In order to use the PTDIAGEOS routine, 26 columns and 203 rows need to be selected. A click on the *fx* button after typing "PTDIAGEOS(" opens the optional context menu. After finishing the inputs **Ctrl+Shift+ Enter** need to be pushed at the time instead of just Enter or clicking ok. The selected cells will then be filled as shown in the Figure 7.

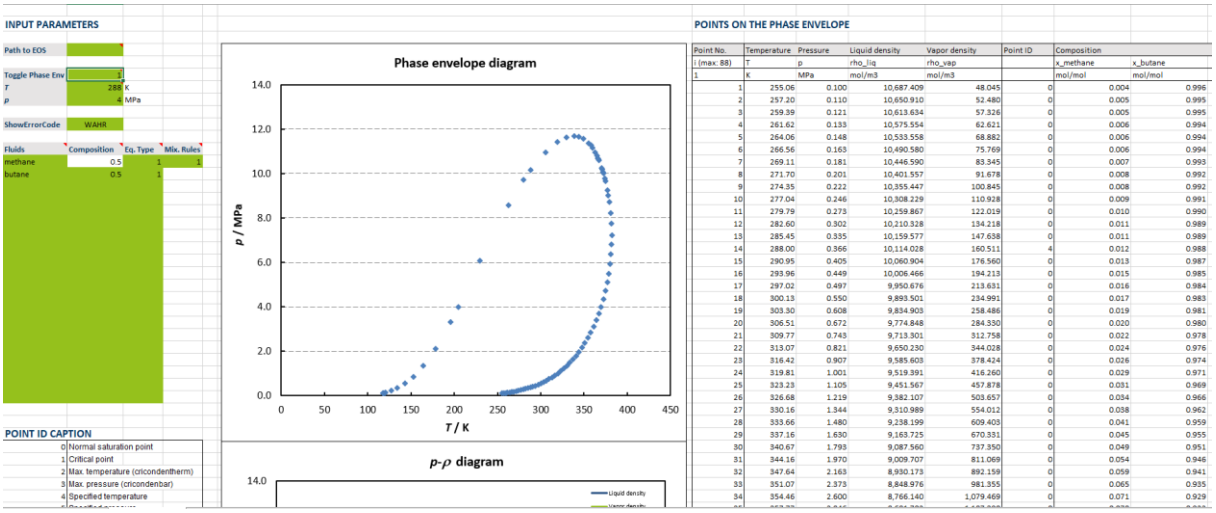

Figure 7: Phase Envelope calculated by PTDIAGEOS

Composition Calculation

The subroutine COMP converts the composition of a mixture to a molar or a specific basis. The subroutine has the following calling sequence:

COMP(FLUIDS; MOLES, EOSTYPE; MIXTYPE; UNIT; PATH;SHOWERRORCODE)

Please note, that in the array MOLES the input composition must be given, which can be either molar or specific. Furthermore, the given input array must be fully molar or fully specific. A mixed input is not supported.

p-x Diagram and *T-x* Diagram Calculation

The subroutine PTXDIAGEOS calculates bubble and dew lines for a given binary mixture in a *p-x* diagram or a *T-x* diagram. If INPUT is set to “TLIQ” or “TVAP” a *p-x* diagram is plotted at constant temperature. To calculate a *T-x* diagram at constant pressure INPUT has to be set to “PLIQ” or “PVAP”. The returned parameters are the number of calculated points, temperature and pressure as well as the compositions and densities for each phase. The subroutine has the following calling sequence:

PTXDIAGEOS (INPUT;PROP;FLUIDS;EOSTYPE;MIXTYPE;PATH;SHOWERRORCODE)

The PTXDIAGEOS subroutine returns the following output (for details see Table 7 and Figure 4):

TPTS;PPTS;XPTS;RHOLIQPTS;RHOVAPPTS;POINTS

Table 9: Output parameters of the routine PTXDIAGEOS.

Parameter	Type	Comment
TPTS	Double Array, length 300	Array with the temperatures of the calculated saturation points.
PPTS	Double Array, length 300	Array with the pressures of the calculated saturation points.
XPTS	Double Array, dimension {300;4}	Array with the composition of the vapor and liquid phases.
RHOLIQPTS	Double Array, length 300	Array with the densities of the liquid phase.
RHOVAPPTS	Double Array, length 300	Array with the densities of the vapor phase. In case of a liquid-liquid equilibrium this might also contain the densities of the second liquid phase.
POINTS	Long	Number of calculated points.

To use the PTXDIAGEOS routine, 9 columns and 303 rows need to be selected. A click on the *fx* button after typing “PTXDIAGEOS(“opens the optional context menu. After finishing the inputs **Ctrl+Shift+ Enter** need to be pushed at the time instead of just Enter or clicking ok. The selected cells will then be filled as shown in the Figure 8.

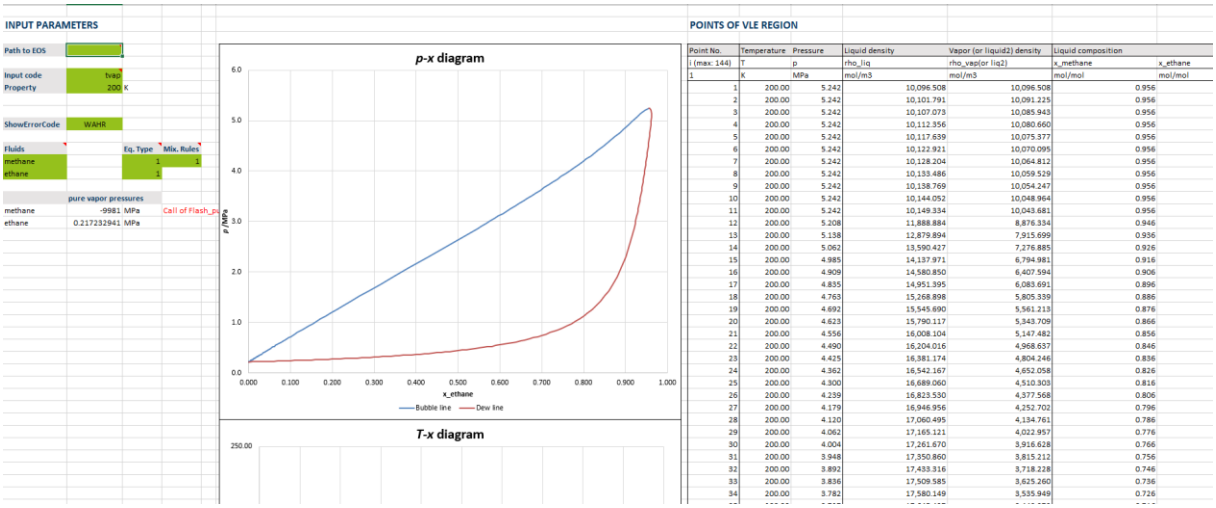

Figure 8: *p-x* Diagram calculated by PTXDIAGEOS

Ternary Diagram Calculation

The subroutine TERNARY_DIAGEOS calculates bubble and dew lines for a given ternary mixture at constant temperature and pressure. The routine returns the compositions and densities for each phase. So far, the routine covers three independent two phase regions starting at each of the binary mixtures. No INPUT is needed because the phase diagram is always calculated at constant temperature PROP1 and constant pressure PROP2. The subroutine has the following calling sequence:

TERNARY_DIAGEOS (PROP1;PROP2;FLUIDS;EOSTYPE;MIXTYPE;PATH;SHOWERRORCODE)

The TERNARY_DIAGEOS subroutine returns the following output (for details see Table 10 and Figure 4):

XPTS;RHOLIQPTS;RHOVAPPTS;POINTS

Table 10: Return parameters of the routine TERNARY_DIAGEOS.

Parameter	Type	Comment
XPTS	Double Array, dimension {300;18}	Array with the compositions of the vapor and liquid phases.
RHOLIQPTS	Double Array, dimension {300;3}	Array with the densities of the liquid phase.
RHOVAPPTS	Double Array, dimension {300;3}	Array with the densities of the vapor phase. In case of a liquid-liquid equilibrium this might also contain the densities of the second liquid phase.
POINTS	Long	Number of calculated points.

To use the TERNARY_DIAGEOS routine, 25 columns and 304 rows need to be selected. A click on the *fx* button after typing "TERNARY_DIAGEOS" opens the optional context menu. After finishing the inputs **Ctrl+Shift+ Enter** need to be pushed at the same time instead of just Enter or clicking ok. The selected cells will then be filled as seen in the Figure 9.

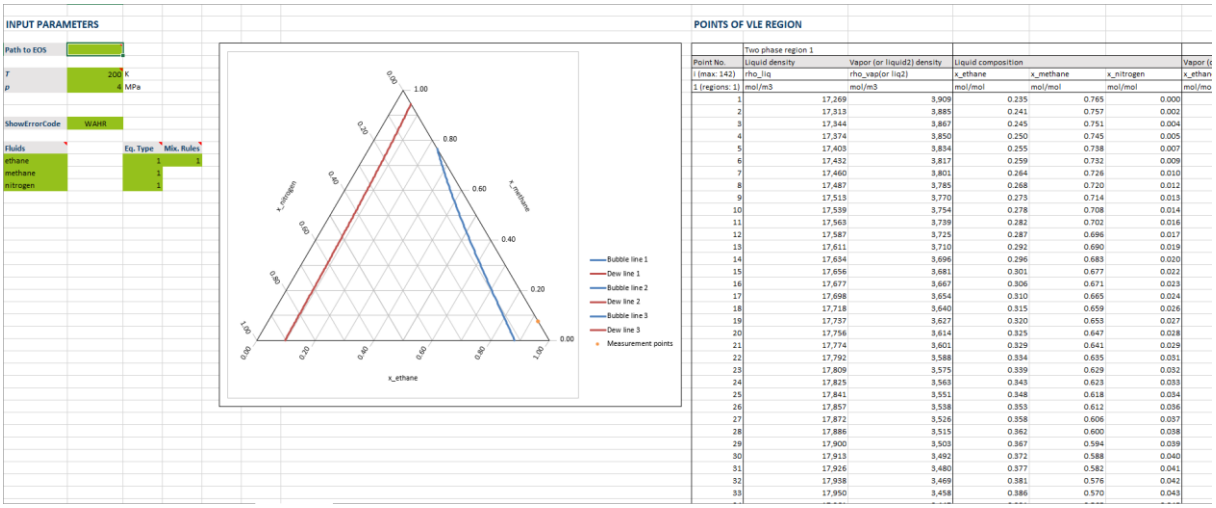

Figure 9: Ternary phase diagram calculated by TERNARY_DIAGEOS

Custom DLL Path

In the TREND Excel sheet, the function “CustomDLLDir” can be used to set a custom directory the VBA code looks for a TREND DLL. This might be useful when the TREND Excel-Addin is used or the TREND Excel sheet is saved at a location different from the TREND DLL directory. The message “Custom DLL Path in this Excel File” will appear in the Cell where the function was used.

Error Codes

Error code	Comment
-1111	MIX: Wrong input(s) to a routine. These are internal errors, for example negative temperatures, wrong iFlash values etc. are caught
-1234	PURE: PhaseDet, p(rho_it,T_it)
-1235	PURE: Temperature iteration T(p,h) failed
-1444	Function Fug_DryIce: FUGCOPURE_CALC: Exponent > 700. Argument to exponential function too big in dry ice fugacity calculation
-2111	PHASEDET: Subroutine RachRiche error during generation of startvalues
-2211	Subroutine PHASEDET_PURE: Flash calculation did not converge
-2212	Subroutine MAXWELL: Flash calculation with MAXWELL did not converge
-2222	FLASH: Flash calculation did not converge
-2223	Function TSUB_EQ: SUBLIMATION TEMPERATURE iteration did not converge (ancillary equation)
-2224	PHASEDET_SOL: MELTING TEMPERATURE iteration did not converge (ancillary equation)
-2225	PHASEDET_SOL: SUBLIMATION PRESSURE calculation failed
-2226	PHASEDET_SOL: MELTING PRESSURE calculation failed
-2230	PHASEDET_SOL: MELTING LINE: Given pressure not valid
-2231	PHASEDET_SOL: MELTING LINE: Given temperature not valid
-2232	PHASEDET_SOL: SUBLIMATION LINE: Given pressure not valid
-2233	PHASEDET_SOL: SUBLIMATION LINE: Given temperature not valid
-2408	Internal Error in Flash_Pure_PhaseBoundary (found same density roots)
-2908	cubic, LKP or generalized equation: No cp0 parameters set
-3333	MIX: Step size reduction error in flash algorithm (step size becomes too small)
-4321	MIX: Flash algorithm converged to unreasonable temperatures
-4322	Subroutine FLASH_PHASEBOUNDARY_CALC: MIX flash algorithm converged to unreasonable pressures
-4323	MIX: Flash algorithm converged to two phases with the same compositions
-4401	Subroutine FLASH_PHASEBOUNDARY: MIX p,x(liq)-flash failed: no bubble point found
-4402	Subroutine FLASH_PHASEBOUNDARY: MIX p,x(vap)-flash failed: no dew point found
-4403	Subroutine FLASH_PHASEBOUNDARY: MIX t,x(liq)-flash failed: no bubble point found
-4404	Subroutine FLASH_PHASEBOUNDARY: MIX t,x(vap)-flash failed: no dew point found
-4405	MIX: ph-flash internal error
-4406	Subroutine PHASEDET_PS: MIX ps-flash internal error
-4407	MIX: td-flash internal error
-4408	CRITICAL POINT FOR MIXTURES: internal error
-4409	Calculation of Henry constant not possible because temperature is lower than triple point temperature or higher than critical temperature
-4444	MIX: LUDECOMP failed to invert matrix
-5211	Surface tension not implemented for mixtures
-5222	Surface tension not defined in the homogeneous region
-5223	Property for mixtures not implemented
-5234	No model for this property and fluid available

-5235	Dielectric constant models cannot be mixed with model DE2
-5242	Error in viscosity calculation
-5243	Existing model for the viscosity not implemented yet
-5244	Existing model for the thermal conductivity not implemented yet
-5245	No viscosity model exists, which is needed for the calculation of the critical enhancement of the thermal conductivity
-5246	VS7 model is treated as VS9 model. Rename it to VS7 and adjust the format in the FLD file.
-5247	Literature reference only available for pure fluids and binary mixtures
-5248	Property only available for mixtures
-5249	Property only available for binary mixtures
-5250	Quality not implemented as input parameter for mixtures
-5251	This diagram is not defined for the specified number of fluids
-5300	ECS: invalid reference fluid
-5301	ECS: internal error
-5302	ECS: iteration failed
-5400	Internal error while iterating the melting temperature
-5501	Creation of four points at low pressures failed: generation of starting point failed. Stability analysis failed.
-5502	Phase envelope: generation of start values failed
-5503	Phase envelope: generation of start values failed
-5504	Successive substitution routine failed
-5507	Subroutine PHASENV: MIX: phase envelope calculation failed (step reduction becomes too large)
-5508	Subroutine PHASENV: MIX: phase envelope calculation failed
-5509	Subroutine PHASENV_pbased or PHASENV_vbased: MIX: phase envelope calculation failed
-5511	p_min for "normal" phase env. OR p_max for open phase env. reached OR exit if the specified point is found and the routine is called from the phase boundary flash algorithm OR one of these variables does not change any more: T, p, rho_vap
-5520	Subroutine PHASENV: MIX: too many points found -> exceeds the vector storage capacity
-5530	Subroutine pxdiag: T is larger than tc(1) and tc(2)
-5531	Subroutine ptxdiag_out: prop is below 0.5*min(tminfluid) or 0.5*min(pminfluid) respectively
-5555	Subroutine SATPLOT: MIX: Phase envelope calculation failed
-5566	Subroutine SYSOFFEQS_PT: MIX: Internal error in pt-flash
-5660	Density maximum not implemented for mixtures or wrong input code (only TP valid)
-5661	Iteration of density maximum failed
-5662	Iteration of temperature failed
-5666	Function DSPIN_EOS: Spinodals: No valid input code, only TLIQ and TVAP possible
-5667	Function DSPIN_CALC: Spinodals: Change in curvature between minimum and phase boundary (unreasonable result)
-5668	Function DSPIN_EOS: Spinodales not implemented for mixtures
-5669	Function DSPIN_EOS: Error when calculating the density of the spinodal
-5700	Function PROP_EOS: Valid input combination for PNUMER_EOS is "TD" only
-5777	Costald EOS: Different EOS types cannot be combined here

-5778	Function PROP_EOS: Costald EOS: No valid input code, only TLIQ or TP possible or wrong property (only density possible)
-5888	Function VSATTAIT: Costald EOS: Temperature out of valid temperature range
-5997	Function PROP_EOS: RKM EOS: No valid input code, only TLIQ possible or wrong property (only density possible)
-5998	Function PROP_EOS: ERKM EOS: No valid input code, only TLIQ or TP possible or wrong property (only density possible)
-5999	Function v_RKM: Revised Klosek-McKinley EOS: Temperature and or pressure out of valid range
-6000	Subroutine REF_CALC: No reference state set
-6001	Acentric factor for generalized negative => calculation not possible
-6600	No strict equation boundaries available
-6666	Property in two-phase region undefined
-6667	Property in homogeneous region undefined
-7000	UNCERTAINTIES: Estimation of uncertainties only possible for pure fluids
-7001	UNCERTAINTIES: Uncty File not found
-7002	UNCERTAINTIES: Estimation of uncertainties only possible for Helmholtz EOS (see uncty file)
-7003	UNCERTAINTIES: estimation in 2phase region not yet implemented
-7777	MIX: Calculation of vapor fugacities failed
-7778	MIX: Calculation of liquid fugacities failed
-7779	MIX: Calculation of solid fugacities failed
-7877	DLL could not be opened in Excel
-7878	SETUP: Fluid name or path wrong
-7879	SETUP Error: Opening fluid file, does not exist in CAS list
-7880	SETUP Error: End of fluid-file is reached during read
-7881	SETUP Error: Opening .MIX file
-7882	SETUP Error: End of .MIX-file is reached during read
-7883	SETUP Error: Opening atcoeff file
-7884	SETUP Error: CAS list was not found
-7885	SETUP Error: Opening SRK file
-7886	SETUP Error: Opening PR file
-7887	SETUP Error: Opening LKP file
-7888	SETUP Error: Opening BIN SRK or PR file
-7889	SETUP Error: Opening BIN LKP file
-7890	SETUP Error: CAS-ID not found
-7891	SETUP Error: Opening COSTALD file
-7892	SETUP Error: Only Helmholtz EOS, PR, SRK, LKP and the corresponding mixing rules are hardcoded at the moment
-7893	SETUP Error: Opening RKM files
-7894	SETUP Error: Read error in srkfluids.fld
-7895	SETUP Error: Read error in bin_srk.mix or bin_pr.mix
-7896	SETUP Error: Read error in rk_qk.par
-7897	SETUP Error: Read error in Interac.par
-7898	SETUP Error: COSMO-SAC
-7899	COSMO-SAC_CALC Error
-7999	Wrong equation format (e.g. ECS)
-8000	Internal error Helmholtz_reader (sub_part found twice)

-8001	Internal error: Read error in Costald.fld
-8002	RM: Fluid components do not match the 8 possible components of the RKM
-8877	PURE: Density iteration failed
-8878	Fluid not found
-8879	gE-Model: Fluid or file not found
-8880	Costald fluid not found
-8881	Costald parameter file not found
-8888	Density iteration failed
-8889	find_crit_tpd: iteration of critical point failed
-9000	SETUP Error: Parameter file for generalized EOS not found
-9876	NAN in FNRDERIVSMIX - fugcoef_pure, SRK, dlog(<0)
-9901	Calculation not possible for pure fluids
-9902	Calculation not possible for mixtures
-9903	Calculation not possible for pure substances or binary mixtures
-9904	Calculation not possible for solid phase of chosen substance
-9907	Pressure <= lower pressure limit of the corresponding equation
-9908	Pressure >= lower pressure limit of the corresponding equation
-9909	Temperature <= lower temperature limit of the corresponding equation
-9910	Temperature >= upper temperature limit of the corresponding equation
-9911	Temperature input <= 0
-9912	Temperature <= Tminfluid
-9913	Temperature >= Tmaxfluid
-9914	Density >= Rhomaxfluid
-9915	p >= pmelt --> solid phase
-9916	Input parameters out of range (viscosity of water)
-9917	ALLPROP_HOM: phase_ind out of range (phase_ind is an input parameter that specifies the phase which is tried)
-9918	Temperature <= Tmin of transport equations
-9919	Temperature >= Tmax of transport equations
-9920	Density >= rhomax of transport equations
-9922	Density input <= 0
-9932	Pressure input >= Pmaxfluid
-9933	Pressure input <= 0
-9935	Property not available
-9936	Input Property out of range (seawater or brines); see manual for range of validity
-9942	Entropy input out of range
-9941	Enthalpy input out of range
-9943	T rho flash, density cannot be found in the given range of pmin to pmax
-9950	Error in composition convertion
-9951	One mole fraction exceeds 0 < x < 1
-9952	Sum of the mole fractions is not 1
-9953	Number of fluids =/ number of mole fractions =/ number of eqtypes
-9954	Error in composition entry
-9955	Wrong Input (combination)
-9956	AGA8: Wrong Input, only TD is valid
-9957	EOS_Indicator does not exist or wrong mixtype
-9958	Cubic EOS cannot be mixed with Helmholtz EOS

-9959	Error in EOS_Indicator entry, wrong format
-9960	Error in fluid entry (e.g. fluidname contains blanks)
-9961	Option only valid for Helmholtz, PR, SRK, and LKP
-9971	Negative radical in calculation of speed of sound
-9981	Call of Flash_pure with Temp <= ttp or Temp >= tc
-9982	Call of Flash_pure with press <= ptp or press >= pc
-9994	AGA8: Only valid in gas phase
-9995	AGA8: A fnr-function is needed for the calculation, which is not provided by the AGA8
-9996	AGA8: Fluid components do not match the 21 possible components of the AGA8
-9997	AGA8: Density out of range (valid only up to 50% of critical density of mixture)
-9998	AGA8: Temperature out of range (valid between 143.15K and 453.15K)
-9999	AGA8: Pressure out of range (valid up to 280MPa)
-12800	Property not implemented for seawater or brines
-12900	Property not provided / implemented for solid equation
-12901	Input combination not implemented for solids
-12902	No solid model available for chosen substances
-12910	Input combination not implemented for seawater or brines
-14444	Wrong value in solidtype(1). Either internal error, or the solid former does not exist
-15566	Internal error in PhaseDet_sol
-15567	Internal error in PhaseDet_ph_ps_sol
-15570	Internal error in Flash_PhaseBoundary_sol
-15571	Internal error in ptflash_sol_NC_4P
-15572	Internal error in ptflash_sol_NC_2P
-18867	Pressure iteration for solid failed
-19900	Prediction of solids only possible in combination with Helmholtz EOS
-19912	Temperature <= tmin of solid equation
-19914	Density >= rhomax for solid
-19915	p >= pmelt -->
-19932	Pressure >= pmax for solid equation
-19941	Enthalpy or entropy input out of range
-44444	PURE: Density iteration failed (rho_calc)
-101010	Internal error in Phasedet_sol for mixtures
-111111	Solid function not activated
-121212	Error while generating start values for VLE pure, press or Temp <= 0
-121213	Invalid iFlash entry in VLE pure
-123456	Error in molar specific handling (only "molar", "specific", or "reduced" allowed)
-123457	Prop_unit subroutine: Invalid Property
-898964	Flash_Pure_PhaseBoundary_calc: Density iteration failed
-898965	Flash_Pure_PhaseBoundary_calc did not converge in specified number of iterations
-898966	Flash_Pure_PhaseBoundary_calc: safety caution for numerical effects (see oil, Pvap is 1.d-10 --> very small steps)
-898967	Flash_Pure_PhaseBoundary_calc: wrong solution (wrong slope)
-898968	Flash_Pure_PhaseBoundary_calc: pure fluid in two phase region, density cannot be determined