KCE

ThermoFluidProperties

Property Library for Ideal Gas Mixtures in Energy-Technological Process Modelling

LibIdGasMix

Prof. Hans-Joachim Kretzschmar
Dr. Sebastian Herrmann
Prof. Matthias Kunick
Ines Jaehne
K. Knobloch
B. Nowak

Property Functions of LibIdGasMix

1. Gases of the library

Table 1. Gases and algorithms for the calculation of thermodynamic properties.

Gas no.	Gas / component		Algorithm, bibliographic reference
1	Ar	Argon	VDI 4670 [21]
2	Ne	Neon	VDI 4670 [21]
3	N_2	Nitrogen	VDI 4670 [21]
4	O_2	Oxygen	VDI 4670 [21]
5	CO	Carbon monoxide	VDI 4670 [21]
6	CO_2	Carbon dioxide	VDI 4670 [21]
7	H_2O	Steam	VDI 4670 [21]
8	SO_2	Sulfur dioxide	VDI 4670 [21]
9	AIR	Air (dry)	Mixture, VDI 4670 [1] [21]
10	AIR-N_2	Air nitrogen	Mixture, VDI 4670 [2] [21]
11	NO	Nitrogen oxide	NASA [40]
12	H_2S	Sulfur hydrogen	Span, Lemmon [41]
13	OH	Hydroxyl	NASA [40]
14	CH_3OH	Methanol	IUPAC [26]
15	CH_4	Methane	IUPAC [27]
16	C_2H_4	Ethylene	IUPAC [35]
17	C_2H_6	Ethane	Buecker [29]
18	C_3H_6	Propylene	Overhoff [42]
19	C_3H_8	Propane	Lemmon [43]
20	n-C_4H_{10}	n-Butane	Buecker [29]
21	Iso-C_4H_{10}	Iso-Butane	Buecker [29]
22	C_6H_6	Benzene	Polt [44]
23	H_2	Hydrogen	Leachman [45]
24	He	Helium	GERG [46]
25	NH_3	Ammonia	Tillner-Roth [38]/ NASA [40] [3]
26	free [4]		
27	free [4]		
28	free [4]		
29	free [4]		
30	F_2	Fluorine [5]	IUPAC [28]

[1] Composition of dry air

Mole fractions	78.1109 % N_2	20.9548 % O_2	0.9343 % Ar
Mass fractions	75.5577 % N_2	23.1535 % O_2	1.2888 % Ar

[2] Composition of air nitrogen

Mole fractions	98.8180 % N_2	1.1820 % Ar
Mass fractions	98.3229 % N_2	1.6771 % Ar

[3] Thermodynamic properties of ammonia are calculated on the algorithms corresponding to *Tillner-Roth* [38] to a temperature of 1273.15 °C. Equations of NASA [40] are applied when calculating with temperatures which are higher than 1273.15 °C. Data are smoothed between temperatures ranging from 1273.15 °C to 2273.15 °C.

[4] The gas numbers 26 to 29 are currently not defined.

[5] Due to its chemical properties, fluorine can not be calculated as a mixture gas but as a single gas.

Table 2. Gases and algorithms for the calculation of transport properties.

Gas no.	Mixture gas		Algorithm, bibliographic reference
1	Ar	Argon	Brandt [15]
2	Ne	Neon	Brandt [15]
3	N_2	Nitrogen	Brandt [15]
4	O_2	Oxygen	Brandt [15]
5	CO	Carbon monoxide	Brandt [15]
6	CO_2	Carbon dioxide	Brandt [15]
7	H_2O	Steam	Brandt [15]
8	SO_2	Sulfur dioxide	Brandt [15]
9	AIR	Air (dry)	Brandt [15]
10	AIR-N_2	Air nitrogen	Brandt [15]
11	NO	Nitrogen oxide	Brandt [15]
12	H_2S	Sulfur hydrogen	Brandt [15]
13	OH	Hydroxyl	- [6)]
14	CH_3OH	Methanol	VB [33]
15	CH_4	Methane	Brandt [15]
16	C_2H_4	Ethylene	VB [33]
17	C_2H_6	Ethane	Brandt [15]
18	C_3H_6	Propylene	VB [33]
19	C_3H_8	Propane	Brandt [15]
20	C_4H_{10}	n-Butane	VB [33]
21	C_4H_{10}	Iso-Butane	VB [33]
22	C_6H_6	Benzene	VB [33]
23	H_2	Hydrogen	Brandt [15]
24	He	Helium	Brandt [15]
25	NH_3	Ammonia	Brandt [15]
26 to 29	free		
30	F_2	Fluorine	VB [33]

6) Regarding hydroxyl OH, there are no algorithms for the transport properties. The following details are valid for mixtures with the gas hydroxyl:

Mass fraction up to 10% OH	→	when calculating transport properties the fraction of OH is not considered
Mass fraction from 10% up to 100%	→	Error message -130666

2. Property Functions for Ideal Gas Mixtures (igmix-Functions)

Property function	Function Name	Call from Fortran	Property or function	Unit of the value calculated	Details
a = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	a_pt_igmix	A_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ A_PT_IGMIX (A_P,T,TYPE,COMP(0:30))	Thermal diffusivity of the mixture	m^2/s	3/1
c_p = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	cp_pt_igmix	CP_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ CP_PT_IGMIX (CP_P,T,TYPE,COMP(0:30))	Isobaric heat capacity of the mixture	kJ/(kg K)	3/2
c_v = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	cv_pt_igmix	CV_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ CV_PT_IGMIX(CV_P,T,TYPE,COMP(0:30))	Isochoric heat capacity of the mixture	kJ/(kg K)	3/3
η = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	eta_pt_igmix	ETA_T_IGMIX(P,T,TYPE,COMP(0:30)) C_ ETA_T_IGMIX(ETA,P,T,TYPE,COMP(0:30))	Dynamic viscosity of the mixture	Pa s = kg/(m s)	3/4
h = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	h_pt_igmix	H_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ H_PT_IGMIX(P,T,TYPE,COMP(0:30))	Enthalpy of the mixture	kJ/kg	3/5
κ = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	kappa_pt_igmix	KAPPA_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ KAPPA_PT_IGMIX(KAPPA,P,T,TYPE,COMP(0:30))	Isentropic exponent of the mixture		3/6
λ = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	lambda_pt_igmix	LAMBDA_T_IGMIX(P,T,TYPE,COMP(0:30)) C_ LAMBDA_T_IGMIX(LAMBDA,P,T,TYPE,COMP(0:30))	Thermal conductivity of the mixture	W/(m K)	3/7
M = f(type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	M_igmix	M_IGMIX(TYPE,COMP(0:30)) C_ M_IGMIX(M,TYPE,COMP(0:30))	Molar mass of the mixture	kg/kmol	3/8
ν = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	ny_pt_igmix	NY_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_NY_PT_IGMIX(NY,P,T,TYPE,COMP(0:30))	Kinematic viscosity of the mixture	m^2/s	3/9
p = f(t,s,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	p_ts_igmix	P_TS_IGMIX(T,S,TYPE,COMP(0:30)) C_ P_TS_IGMIX(P,T,S,TYPE,COMP(0:30))	Backward function: Mixture pressure from temperature and entropy	bar	3/10

Property function	Function Name	Call from Fortran	Property or function	Unit of the value calculated	Details
p = f(t,v,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	p_tv_igmix	P_TV_IGMIX(T,V,TYPE,COMP(0:30)) C_ P_TV_IGMIX(P,T,V,TYPE,COMP(0:30))	Backward function: Mixture pressure from temperature and specific volume	bar	3/11
Pr = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	Pr_pt_igmix	PR_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ PR_PT_IGMIX(PR,P,T,TYPE,COMP(0:30))	Prandtl number of the mixture		3/12
ψ_i = f(igas,$\xi_1 \ldots \xi_{30}$)	psi_igas_xsi_igmix	PSI_IGAS_XSI_IGMIX(IGAS,XSI(0:30)) C_ PSI_IGAS_XSI_IGMIX(PSI,IGAS,XSI(0:30))	Mole fraction of the gas igas from the mass fractions of all components	kmol/kmol	3/13
R = f(type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	R_igmix	R_IGMIX(TYPE,COMP(0:30)) C_ R_IGMIX(R,TYPE,COMP(0:30))	Specific gas constant of the mixture	kJ/(kg K)	3/14
ρ = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	rho_pt_igmix	RHO_PT_IGMIX(P,T,COMP(0:30)) C_ RHO_PT_IGMIX(RHO,P,T,COMP(0:30))	Density of the mixture	kg/m^3	3/15
s = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	s_pt_igmix	S_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ S_PT_IGMIX(S,P,T,TYPE,COMP(0:30))	Entropy of the mixture	kJ/(kg K)	3/16
t = f(p,h,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	t_ph_igmix	T_PH_IGMIX(P,H,TYPE,COMP(0:30)) C_ T_PH_IGMIX(T,P,H,TYPE,COMP(0:30))	Backward function: Temperature from mixture pressure and enthalpy	°C	3/17
t = f(p,s,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	t_ps_igmix	T_PS_IGMIX(P,S,TYPE,COMP(0:30)) C_ T_PS_IGMIX(T,P,S,TYPE,COMP(0:30))	Backward function: Temperature from mixture pressure and entropy	°C	3/18
t = f(p,v,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	t_pv_igmix	T_PV_IGMIX(P,V, IGAS) C_ T_PV_IGMIX(T,P,V, IGAS)	Backward function: Temperature from mixture pressure and specific volume	°C	3/19

Property function	Function Name	Call from Fortran	Property or function	Unit of the value calculated	Details
u = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	u_pt_igmix	U_PT_IGMIX(P,T, IGAS) C_ U_PT_IGMIX(U,P,T, IGAS)	Internal energy of the mixture	kJ/kg	3/20
v = f(p,t,ttype,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	v_pt_igmix	V_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ V_PT_IGMIX(V,P,T,TYPE,COMP(0:30))	Specific volume of the mixture	m^3/kg	3/21
w = f(p,t,type,$\xi_1 \ldots \xi_{30}$ or $\psi_1 \ldots \psi_{30}$)	w_pt_igmix	W_PT_IGMIX(P,T,TYPE,COMP(0:30)) C_ W_PT_IGMIX(W,P,T,TYPE,COMP(0:30))	Isentropic speed of sound of the mixture	m/s	3/22
ξ_i = f(igas,$\psi_1 \ldots \psi_{30}$)	xsi_igas_psi_igmix	XSI_IGAS_PSI_IGMIX(IGAS,PSI(0:30)) C_ XSI_IGAS_PSI_IGMIX(XSI,IGAS,PSI(0:30))	Mass fraction of the gas igas from the mole fractions of all components	kg/kg	3/23

Units

Symbol	Name	Unit
T	Temperature	°C
p	Total pressure	bar
ξ_1 ... ξ_{30}	Mass fractions of the mixture gases	kg/kg
ψ_1... ψ_{30}	Mole fractions/volume fractions of the mixture gases	kmol/kmol
type	Input parameter: type = 1 for the composition as mass fractions ξ_1, ... ξ_{30} type = 0 for the composition as mole fractions ψ_1, ... ψ_{30}	
comp(0:30) for type =1	Composition as mass fractions ξ_1, ... ξ_{30}	kg/kg
comp(0:30) for type =0	Composition as mole fractions ψ_1, ... ψ_{30}	kmol/kmol

Reference states:

Property	Gases (except steam)	Steam
Pressure	1.01325 bar	0.006112127 bar
Temperature	0 °C	0 °C
Enthalpy	0 kJ/kg	2500.9342 kJ/kg
Entropy	0 kJ/(kg K)	9.15591 kJ/(kg K)

Types of variables for the function call from the LibIdGasMix DLL:

All functions	Real*8
Variable p, T, v, h, s	Real*8
Variable comp(1..30)	Real*8
Variable type, i	Integer*4

3. Property Functions for Single Ideal Gases (igas-Functions)

Property function	Function Name	Call from Fortran	Property or function	Unit of the value calculated	Details
a = f(p,t,igas)	a_pt_igas	A_PT_IGAS(P,T,IGAS) C_ A_PT_IGAS(A,P,T, IGAS)	Thermal diffusivity of the gas igas	m^2/s	4/1
c_p = f(p,t,igas)	cp_pt_igas	CP_PT_IGAS(P,T, IGAS) C_ CP_PT_IGAS(CP,P,T, IGAS)	Isobaric heat capacity of the gas igas	kJ/(kg K)	4/2
c_v = f(p,t,igas)	cv_pt_igas	CV_PT_IGAS(P,T, IGAS) C_ CV_PT_IGAS(CV,P,T, IGAS)	Isochoric heat capacity of the gas igas	kJ/(kg K)	4/3
η = f(p,t,igas)	eta_pt_igas	ETA_T_IGAS(P,T, IGAS) C_ ETA_T_IGAS(ETA,P,T,IGAS)	Dynamic viscosity of the gas igas	Pa s = kg/(m s)	4/4
h = f(p,t,igas)	h_pt_igas	H_PT_IGAS(P,T, IGAS) C_ H_PT_IGAS(P,T, IGAS)	Enthalpy of the gas igas	kJ/kg	4/5
κ = f(p,t,igas)	kappa_pt_igas	KAPPA_PT_IGAS(P,T IGAS) C_ KAPPA_PT_IGAS(KAPPA,P,T IGAS)	Isentropic exponent of the gas igas		4/6
λ = f(p,t,igas)	lambda_pt_igas	LAMBDA_T_IGAS(P,T, IGAS) C_ LAMBDA_T_IGAS(LAMBDA,P,T, IGAS)	Thermal conductivity of the gas igas	W/(m K)	4/7
M = f(igas)	M_igas	M_IGAS(IGAS) C_ M_IGAS(M,IGAS)	Molar mass of the gas igas	kg/kmol	4/8
ν = f(p,t,igas)	ny_pt_igas	NY_PT_IGAS(P,T, IGAS) C_ NY_PT_IGAS(NY,P,T, IGAS)	Kinematic viscosity of the gas igas	m^2/s	4/9
p = f(t,s,igas)	p_ts_igas	P_TS_IGAS(T,S, IGAS) C_ P_TS_IGAS(P,T,S, IGAS)	Backward function: Pressure from temperature and entropy of the gas igas	bar	4/10
p = f(t,v,igas)	p_tv_igas	P_TV_IGAS(T,V, IGAS) C_ P_TV_IGAS(P,T,V, IGAS)	Backward function: Pressure from temperature and specific volume of the gas igas	bar	4/11

Property function	**Function Name**	**Call from Fortran**	**Property or function**	**Unit of the value calculated**	**Details**
Pr = f(*p*,*t*,igas)	Pr_pt_igas	PR_PT_IGAS(P,T, IGAS) C_ PR_PT_IGAS(PR,P,T, IGAS)	Prandtl number of the gas igas		4/12
R = f(igas)	R_igas	R_IGAS(IGAS) C_ R_IGAS(R,IGAS)	Specific gas constant of the gas igas	kJ/(kg K)	4/13
ρ = f(*p*,*t*,igas)	rho_pt_igas	RHO_PT_IGAS(P,T, IGAS) C_ RHO_PT_IGAS(RHO,P,T IGAS)	Density of the gas igas	kg/m^3	4/14
s = f(*p*,*t*,igas)	s_pt_igas	S_PT_IGAS(P,T, IGAS) C_ S_PT_IGAS(S,P,T, IGAS)	Entropy of the gas igas	kJ/(kg K)	4/15
t = f(*p*,*h*,igas)	t_ph_igas	T_PH_IGAS(P,H, IGAS) C_ T_PH_IGAS(T,P,H IGAS)	Backward function: Temperature from pressure and enthalpy of the gas igas	°C	4/16
t = f(*p*,*s*,igas)	t_ps_igas	T_PS_IGAS(P,S, IGAS) C_ T_PS_IGAS(T,P,S, IGAS)	Backward function: Temperature from pressure and entropy of the gas igas	°C	4/17
t = f(*p*,*v*,igas)	t_pv_igas	T_PV_IGAS(P,V, IGAS) C_ T_PV_IGAS(T,P,V, IGAS)	Backward function: Temperature from pressure and specific volume of the gas igas	°C	4/18
u = f(*p*,*t*,igas)	u_pt_igas	U_PT_IGAS(P,T, IGAS) C_ U_PT_IGAS(U,P,T, IGAS)	Specific internal energy of the gas igas	kJ/kg	4/19
v = f(*p*,*t*,igas)	v_pt_igas	V_PT_IGAS(P,T, IGAS) C_ V_PT_IGAS(V,P,T, IGAS)	Specific volume of the gas igas	m^3/kg	4/20
w = f(*p*,*t*,igas)	w_pt_igas	W_PT_IGAS_SI(P,T IGAS) C_ W_PT_IGAS(W,P,T, IGAS)	Isentropic speed of sound of the gas igas	m/s	4/21

Units:

Symbol	Name	Unit
t	Temperature	°C
p	Mixture pressure	bar
igas	Number of the gas	

Reference states:

Property	Gases (except steam)	Steam
Pressure	1.01325 bar	0.006112127 bar
Temperature	0 °C	0 °C
Enthalpy	0 kJ/kg	2500.9342 kJ/kg
Entropy	0 kJ/(kg K)	9.15591 kJ/(kg K)

Types of variables for the function call from the LibIdGasMix DLL:

All functions	Real*8
Variable p, t, v, h, s	Real*8
Variable igas	Integer*4

1.4 Range of Validity

Table 1 contains a list of gases which can be calculated in the LibIdGasMix property library either as a component of a gas mixture or as a single gas. The calculation of thermodynamic properties is carried out by the algorithms stated in Table 1. The algorithms for the transport properties are listed in Table 2.

The calculation programs are valid in a temperature range

from t = -73.15 °C to 3026.85 °C.

Exceptions are:

Fluorine from -73.15 °C to 976.85 °C.

The pressure range is limited to the region where the mixture gases or single gases can be considered as ideal gases and, thus, ranges

from above 0.01 bar to 10 (30) bar, maximum 50 bar.

For temperatures above 1000 °C and mole fractions of oxygen of more than 1 % ($\psi_{O_2} \geq 0.01$) the dissociation based on the VDI 4670 for the gases nitrogen, oxygen, carbon dioxide, steam, and sulfur dioxide are considered. The dissociation of other gases is not considered. For programming reasons, the calculation of the correction for the dissociation is already carried out from 500 °C.

Note:
A calculated value of -9999 indicates that the input values have been entered outside the range of validity and/or the sum of the values $\xi_1, \ldots \xi_{30}$ *or* $\psi_1, \ldots \psi_{30}$ *entered does not result in 1.*

Additional Information

For further information, please see Table 3 which provides data of critical points (c) and triple states (t) of the gas *i* which is determined as follows:

$t_{t,i} > t_{min}$

and/or

$t_{c,i} > t_{min}$.

This means the triple state and/or the critical point of the gas *i* is located in the LibIdGasMix range of validity. In the LibIdGasMix program, corresponding to Figure 1, for every gas i = igas is examined whether it is actually existent in the gaseous state at the given temperature *t* and its present partial pressure p_i.

If the given temperature *t* is lower than the triple temperature $t_{t,i}$ of the gas *i*, $p_i \le p_{sub,i}(t)$ has to be fulfilled with $p_{sub,i}(t)$ as the sublimation pressure of the gas number *i*; see Figure 1. If not, the result is - xx999, for which xx is the number of the gas corresponding to Table 1. This test is carried out for H_2O and CO_2.

If the given temperature *t* has a value between the triple temperature and the critical temperature the relation $p_i \le p_{s,i}(t)$ has to be valid for the partial pressure p_i, where $p_{s,i}(t)$ is the saturation pressure of the gas *i*; see Figure 1. If not, the result will again be - xx999. The gases to be tested are listed in Table 3. This table also contains values of the critical and tripel states.

The calculation is carried out in any case at temperatures above the critical temperature.

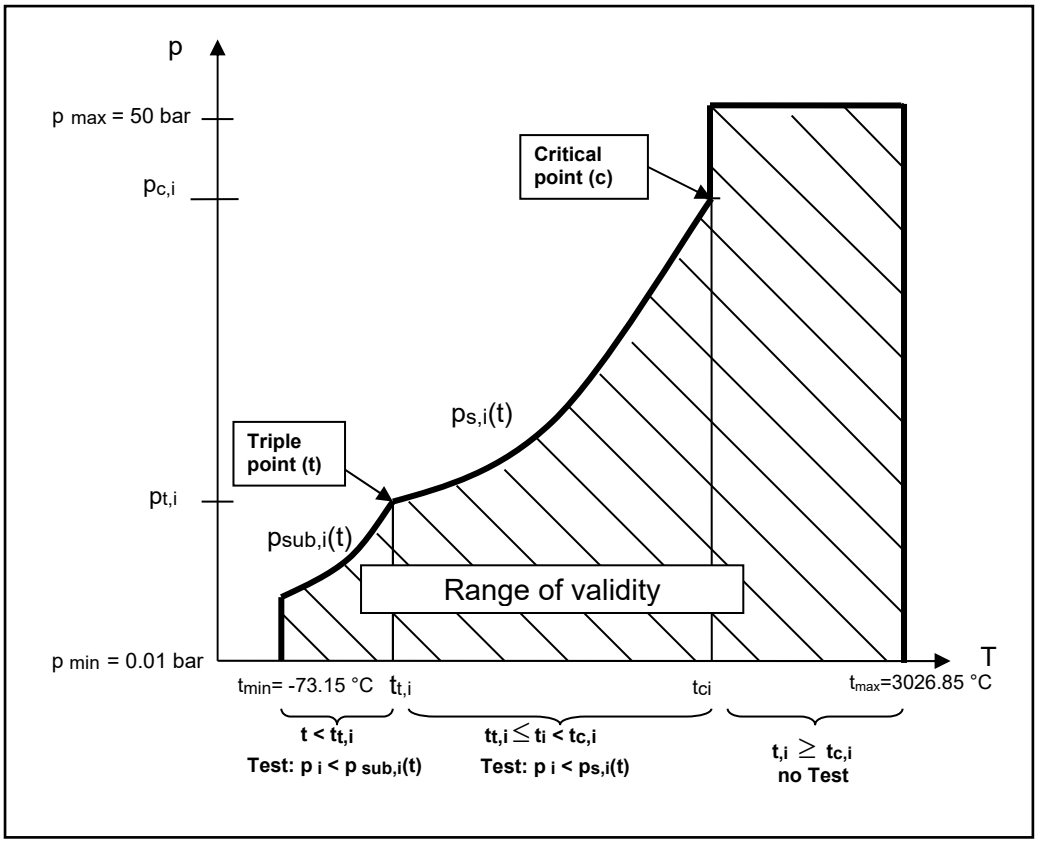

Figure 1. p-t diagram with the range of validity of a gas i = igas of the LibIdGasMix property library.

Table 3. Data of triple states (t) and critical points (c).

			Critical point			Triple state		
Gas No. i	**Mixture gas**		**$p_{c\,i}$ in bar[Source]**	**$t_{c\,i}$ in °C[Source]**	**$p_s(t)$**	**$p_{t\,i}$ in bar[Source]**	**$t_{t\,i}$ in °C [Source]**	**$p_{sub}(t)$[Source]**
1	Ar	Argon						
2	Ne	Neon						
3	N_2	Nitrogen						
4	O_2	Oxygen						
5	CO	Carbon monoxide						
6	CO_2	Carbon dioxide	73.773 [36]	30.9782 [36]	[36]	5.1795 [36]	- 56.558 [36]	[36]
7	H_2O	Steam	220.69 [39]	373.946 [39]	[39]	0.00611657 [39]	0.01 [39]	[39]
8	SO_2	Sulfur dioxide	78.8 [20]	157.45 [20]	[20]			
9	AIR	Air (dry)						
10	AIR-N_2	Air nitrogen						
11	NO	Nitrogen oxide						
12	H_2S	Sulfur hydrogen		99.95 [41]	[41]			
13	OH	Hydroxyl						
14	CH_3OH	Methanol	81.035 [26]	239.45 [26]	[26]			
15	CH_4	Methane						
16	C_2H_4	Ethylene	50.418 [35]	9.2 [35]	[35]			
17	C_2H_6	Ethane	48.722 [26]	32.172 [26]	[29]			
18	C_3H_6	Propylene	46.646 [42]	92.42 [42]	[42]			
19	C_3H_8	Propane	42.4766 [43]	96.675 [43]	[43]			
20	n-C_4H_{10}	n-Butane	37.96 [26]	151.975 [26]	[26]			
21	Iso-C_4H_{10}	Iso-Butane	36.29 [26]	134.66 [26]	[26]			
22	C_6H_6	Benzene	48.9794 [44]	289.01 [44]	[44]			
23	H_2	Hydrogen						
24	He	Helium						
25	NH_3	Ammonia	113.3926 [38],[40]	132.36 [38],[40]	[38],[40]			
26 to 29	free		-	-		-	-	
30	F_2	Fluorine[2)]						