



Progas

Calculator for Caloric and Dynamic Properties of Mixtures of Real Natural Gases

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1 Features

- Composition of components in mole %, volume %, weight % normative and ultimate weight % for C-H-N-O-S-He-Ar
- Molar mass & gas constant according to DIN 1871-1999, ISO 6976-1995, ASTM D3588-98 (2003)
- Low heat value, high heat value, lower wobbe index, upper wobbe index according to DIN 51850-1980, ISO 6976-1995 (0°C 15°C 20°C 25°C), ASTM-D3588-98 (2003)
- Caloric properties according to AGA8-DC92 (ISO 12213-2) and ISO 20765-1-2005 (Helmholtz free energy approach):
 - Density
 - Compression factor
 - Internal energy
 - Enthalpy
 - Entropy
 - Isobaric heat capacity
 - Isochoric heat capacity
 - Isentropic exponent
 - Joule Thomson coefficient
 - Speed of sound
- Transport Properties according to Schley VDI Reihe 7 No. 418-2001
 - Dynamic viscosity
 - Heat circuit capacity
- Optional flow Calculation all devices in ISO 5167-2003
 - Orifice with Corner Tapping
 - Orifice with Flange Tapping
 - Orifice with D and D/2 Tapping
 - ISA 1932 Nozzle
 - Long Radius Nozzle
 - Venturi Nozzle
 - Classical Venturi Tube with »as cast« convergent section
 - Classical Venturi Tube with machined convergent section
 - Classical Venturi Tube with rough-welded sheet-iron convergent section
 - Optional calibrated discharge coefficient
 - Optional diameter correction for temperature



2 About the software

Fuel consumption and fuel heat input belong to the most sensitive parameters in today's gas turbine operation. For large consumers and power plants 0.1% difference in heat rate can have hundreds of thousands of dollars impact on fuel costs within just one year, which is also why penalties to manufacturers are extraordinary high when not meeting the heat rate guarantees. Gas turbine operators are well advised to have their own calculation tool, being able to crosscheck thermal performance, but also monthly bills coming from gas suppliers.

Of course there are enough other reasons for engineers to stay up to date with natural gas properties.

I have developed this application to have a light-weight, easy to use and fast calculation for real gas properties. The calculator works on Command Prompt level and therefore on any on Windows NT-based operating system including Windows 2000, XP, Vista, 7 (32-Bit and 64-Bit). There is no installation required, but to unlock the full version a license key has to be entered into the registry. The application runs out of the box. Input and Output files are ASCII Text. Other applications could easily call the tool and further process the produced results.

For handling the input file a fast and light-weight text editor with »overwrite« option is recommended e.g. [Notepad2](#).

2.1 Real gas density vs. ideal gas density

The effect of compression factor tells that the real gas density is higher than the ideal gas density, typically by 1...5%. Ideal gas density neglects the compression factor.

$$\rho = \frac{M}{R} \cdot \frac{p}{z \cdot T} = \frac{p}{R_s \cdot z \cdot T} \quad (2.1)$$

ρ	real gas density [kg/m ³]
p	absolute gas pressure [Pa = N/m ²]
T	absolute temperature [K]
z	compression factor: typical values 0.95...0.99, in ideal gas $z = 1.0$
M	molar mass [kg/mol]
R	universal gas constant: 8.31451 J/(mol·K) = 8.31451 (N·m)/(mol·K)
R_s	specific gas constant [J/(kg·K)]



2.2 Real gas enthalpy vs. ideal gas enthalpy

Real gas enthalpy being part of the overall heat input is smaller than ideal gas enthalpy. Example with the gas from chapter 5 (input) and chapter 6 (results) with 0°C and 0.101325 MPa as reference conditions:

$$HI = m \cdot (LHV + \Delta h)$$

$$\frac{HI}{m} = 39729 \frac{\text{kJ}}{\text{kg}} + [54.101 - (-51.494)] \frac{\text{kJ}}{\text{kg}} = 39835 \frac{\text{kJ}}{\text{kg}} \quad (2.2)$$

HI total real heat input [kW = kJ/s]

m fuel gas mass flow [kg/s]

LHV Low heat value combustion at 0 °C [kJ/kg]

Δh real gas enthalpy difference between metering pressure and temperature and reference conditions [kJ/kg]

When using the simplified method with ideal gas enthalpy the heat input would be calculated just with the temperature difference and a typical heat capacity of 2.3 kJ/(kg·K):

$$HI = m \cdot (LHV + c_p \Delta T)$$

$$\frac{HI}{m} = 39729 \frac{\text{kJ}}{\text{kg}} + 2.3 \frac{\text{kJ}}{\text{kg} \cdot \text{K}} \cdot (76.85 - 0) \text{K} = 39906 \frac{\text{kJ}}{\text{kg}} \quad (2.3)$$

HI heat input [kW = kJ/s]

m fuel gas mass flow [kg/s]

LHV Low heat value combustion at 0 °C [kJ/kg]

c_p heat capacity for the ideal gas (depending only on temperature) [kJ/(kg·K)]

ΔT difference between metering temperature and reference temperature [K]

The real heat input in this example is 0.18% lower.

3 Prepare the first run

After reception of payment a license file »progas.reg« and a download link for the software are sent to the email address which has been used for the order.

The download link is a zipped folder (appr. 380 kB), which has to be saved on the computer and unzipped. The license file has to be temporary saved on the computer and must be executed once to unlock the full version. This stores the license information into the registry. The software is unlocked with the next start. The license file is no longer needed on this computer and can be deleted; however a safety backup of the license file should be made on a CD or other external storage device and kept it in a safe place. A license file cannot be replaced if it got lost.

The following files are in the unzipped folder:

- [pginput.txt](#)
- progas.exe
- progas.bat



4 Run the program

Adjust progas.bat if necessary to point to the editor of your choice and then start the batch file.

[PROGAS.BAT](#)

```
..\notepad2\notepad2.exe pginput.txt
progas.exe
Pause
..\notepad2\notepad2.exe pgsresult.txt
```

The self-explaining input file pginput.txt is opened. Choose the overwrite option of your editor before updating any requested value. Lines must not be deleted nor shall be changed positions of any comment information. Otherwise the program will not run correct or will not run at all. In case of damaging the input file – download the sample input file from the website [pginput.txt](#) and try again. Save the input file before leaving the editor.

The program will start automatically. Comments like out of range for given conditions are shown on the screen and written into the output file. In the example below pressure, temperature and various components are outside of the recommended range.

[VIEW FROM DOS SHELL](#)

```
D:\Progs\Progas>..\notepad2\notepad2.exe pginput.txt

D:\Progs\Progas>progas.exe
p out of range for ISO 20765-1 and transport properties: p = 350.000 bar > 300 bar
T out of range for ISO 20765-1: T = 175.300 C > 76.85 C
CH4 out of range for ISO 20765-1: CH4 = 65.337 Mol% < 70 Mol%
H2 out of range for ISO 20765-1: H2 = 14.019 Mol% > 10 Mol%
Trace components out of range: Sum = 3.855 Mol% > 0.05 Mol%
D:\Progs\Progas>Pause
Press any key to continue . . .

D:\Progs\Progas>..\notepad2\notepad2.exe pgsresult.txt
```

The pause command will give sufficient time to read the comments and confirm for proceeding to the final step.

The results are written into the output file pgsresult.txt, which is displayed at the end of the batch-procedure.

Using the editor the output file could be renamed thereafter, e.g. result_gas1.docx for future reference and easy printing with fixed width font.



5 Input file pginput.txt

The sample input file uses the gas composition from example 4 (page 39 of ISO 20765).

PGINPUT.TXT

```
GAS 4 ISO 20765-1 2005(E)
100.0      ,'= gas pressure.....[bar absolute]'
76.85     ,'= gas temperature.....[deg C]'
0.432     ,'= pressure drop across flow element.....0 no flow calculation.[bar]'
0.2025    ,'= pipe diameter.....[m]'
22.3      ,'= pipe diameter reference temperature.....[deg C]'
11        ,'= pipe material      10NOcorr 11steel1 12steel2 13steel3 14steel4 15steel5.[-]'
0.1229    ,'= flow element diameter orifice/nozzle/venturi nozzle/venturi tube.....[m]'
8.33      ,'= flow element diameter reference temperature.....[deg C]'
15        ,'= flow element material 16steel6 17SnBz4 18E-Cu 19Rg9 20Ms63 21Ni 22HaC.[-]'
0.6002    ,'= discharge coefficient 1 from calibration.....0 no calibration.[-]'
0.6004    ,'= discharge coefficient 2 from calibration.....[-]'
0.61305D5 ,'= reynoldsnumber 1 from calibration with pipe diameter.....[-]'
0.68345D7 ,'= reynoldsnumber 2 from calibration with pipe diameter.....[-]'
ISO00.DTA ,'= data filename for heat values & molar masses.....[-]'
0         ,'= gas composition given in.....0[mol%] 1[vol%] 2[wght%]'
3        ,'= flow element 1ORcor 2ORfla 3ORdd2 4NOisa 5NOLra 6VEnoz 7VTasc 8VTmac 9VTrw'
9.5       ,'= (1)      ,%,H2.....hydrogen      |
0.02      ,'= (2)      ,%,He.....helium          |
0.01      ,'= (3)      ,%,H2O.....water vapor      |
1.0       ,'= (4)      ,%,CO.....carbon monoxide   |
10.       ,'= (5)      ,%,N2.....nitrogen          |
0.01      ,'= (6)      ,%,O2.....oxygen            |
0.01      ,'= (7)      ,%,H2S.....hydrogen sulfide |
0.01      ,'= (8)      ,%,Ar.....argon            |
1.6       ,'= (9)      ,%,CO2.....carbon dioxide   |
73.50     ,'= (10)     ,%,CH4.....methane          |
3.3       ,'= (11)     ,%,C2H6.....ethane          |
0.74      ,'= (12)     ,%,C3H8.....propane         |
0.08      ,'= (13)     ,%,i-C4H10.....iso-butane   |
0.08      ,'= (14)     ,%,n-C4H10.....n-butane     |
0.        ,'= (15)     ,%,neo-C5H12....neo-pentane |
0.04      ,'= (16)     ,%,i-C5H12.....iso-pentane  |
0.04      ,'= (17)     ,%,n-C5H12.....n-pentane    |
0.02      ,'= (18)     ,%,n-C6H14.....n-hexane     |
0.01      ,'= (19)     ,%,n-C7H16.....n-heptane    |
0.01      ,'= (20)     ,%,n-C8H18.....n-octane     |
0.01      ,'= (21)     ,%,n-C9H20.....n-nonane     |
0.01      ,'= (22)     ,%,n-C10H22....n-decane     |
0.        ,'= (23)     ,%,SO2.....sulfur dioxide   |
0.        ,'= (24)     ,%,c-C5H10.....cyclopentane  |
0.        ,'= (25)     ,%,c-C6H12.....cyclohexane  |
0.        ,'= (26)     ,%,CH3-C5H9....methylcyclopentane |
0.        ,'= (27)     ,%,CH3-C6H11....methylcyclohexane |
0.        ,'= (28)     ,%,2,2-i-C6H14..2,2-dimethylbutane |
0.        ,'= (29)     ,%,2,3-i-C6H14..2,3-dimethylbutane |
0.        ,'= (30)     ,%,C6H6.....benzene        |
0.        ,'= (31)     ,%,C7H8.....toluene        |
0.        ,'= (32)     ,%,o-C8H10.....o-xylene     |
```



5.1 Disable flow calculation

To disable the flow calculation the pressure drop should be set to zero.

[PGINPUT.TXT](#)

```
0.0      ,'= pressure drop across flow element .....0 no flow calculation.[bar]'
```

5.2 Standard specification for heat values and molar masses

Higher and Lower heating value are calculated per weight and also per volume at different conditions.

String for molar masses and molar heat values according to different standards

[PGINPUT.TXT](#)

```
ISO00.DTA ,'= data filename for heat values & molar masses.....[-]'
```

ASTM.DTA	ASTM-D3588-1998, Calorific Values at 60F
DIN.DTA	DIN 1871-1999 and DIN 51850-1980, Calorific Values at 25degC
ISO25.DTA	ISO 6976-1995, Calorific Values at 25degC
ISO20.DTA	ISO 6976-1995, Calorific Values at 20degC
ISO15.DTA	ISO 6976-1995, Calorific Values at 15degC
ISO00.DTA	ISO 6976-1995, Calorific Values at 0degC
(any other string)	ISO 6976-1995, Calorific Values at 0degC

5.3 Flow elements

A standard ISO 5167-2003 flow rate calculation can be selected for the individual elements giving the details for the pipe and the flow element.

Control parameter for the flow element

[PGINPUT.TXT](#)

```
3      ,'= flow element 1ORcor 2ORfla 3ORdd2 4NOisa 5NOLra 6VEnoz 7VTasc 8VTmac 9VTrw'
```

1	Orifice with Corner Tapping
2	Orifice with Flange Tapping
3	Orifice with $d \& d/2$ Tapping
4	ISA 1932 Nozzle
5	Long Radius Nozzle
6	Venturi Nozzle
7	Classical Venturi Tube with "as cast" convergent section
8	Classical Venturi Tube with machined convergent section
9	Classical Venturi Tube with rough-welded sheet-iron convergent section

5.4 Calibrated or standard flow elements

If no calibration shall be considered (standard ISO 5167 calculation) the "discharge coefficient 1" has to be set to zero.

[PGINPUT.TXT](#)

```
0.      ,'= discharge coefficient 1 from calibration.....0 no calibration.[-]'
0.6255 ,'= discharge coefficient 2 from calibration.....[-]'
0.62345D5 ,'= reynoldsnumber 1 from calibration with pipe diameter.....[-]'
0.62345D7 ,'= reynoldsnumber 2 from calibration with pipe diameter.....[-]'
```



If calibration shall be considered a linear interpolation will be made between the given discharge coefficients. The output will include a remark with the deviation of the calibrated flow to standard ISO 5167 calculation. In the example below the calculated mass flow using the calibration data is 0.83 % lower than the mass flow using just the standard formulae. The mass flow using standard formulae would be $17.817 * (1 + 0.0083) = 17.965$ kg/s.

[PGRESULT.TXT](#)

```
ISO 5167-2003 for Flow Calculation

Flow Element Diameter 123.05 mm (122.90 mm at 8.33 degC Steel 5)
Pipe Diameter          202.64 mm (202.50 mm at 22.30 degC Steel 1)
Diameter Ratio         0.6072
Pressure Difference    0.4320 bar = 6.2656 psi
Calibrated Discharge Coefficient
Calibration differs from ISO standard formulae by -0.83 %
Orifice with D and D/2 Tapping
Mass Flow              = 17.817 kg/s
Kinematic Viscosity    = 0.24551E-06 m2/s
Reynolds Number (dPipe) = 0.73032E+07 [-]
Discharge Coefficient  = 0.60041 [-]
Flow Coefficient       = 0.64592 [-]
Expansion Factor       = 0.99877 [-]
Mach number            = 0.05046 [-]
```

5.5 Temperature correction for flow elements

[PGINPUT.TXT](#)

```
11      ,'= pipe material 10NOcorr 11steel1 12steel2 13steel3 14steel4 15steel5....[-]'
...
15      ,'= flow element material 16steel6 17SnBz4 18E-Cu 19Rg9 20Ms63 21Ni 22HaC..[-]'
```



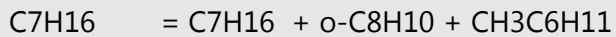
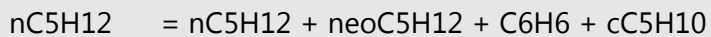
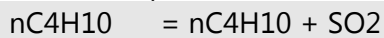
10 No Correction		take diameter as actual					
		Material-No.	DIN-term	Material-No.	DIN-term		
11	Steel I	1.0037	St 37 - 2	14	Steel IV	1.3355	S 18-0-1
		1.0038	R ST 37 - 2			1.3922	X 7 Cr 14
		1.0254	St 37.0			1.4001	X 6 Cr Al 13
		1.0305	St 35.8			1.4002	X 10 Cr 17
		1.0308	St 35			1.4006	X 10 Cr 13
		1.0309	St 35.4			1.4016	X 8 Cr 17
		1.0345	H I			1.4021	X 20 Cr 13
		1.0356	TT St 35			1.4034	X 46 Cr 13
		1.0402	C 22			1.4104	X 12 Cr Mo S 17
		1.0405	St 45.8			1.4120	X 12 Cr Mo 13
		1.0425	H II			1.4510	X 8 Cr Ti 17
		1.0435	H III			1.4713	X 10 Cr Al 7
		1.0445	H IV			1.4717	Cr Al 8 5
		1.0460	C 22.8			1.4724	X 10 Cr Al 18
		1.0486	St E 285			1.4742	X 10 Cr Al 24
		1.0505	St E 315			1.4762	Cr Al 25 5
		1.1151	Ck 22			1.4765	X 20 Cr Mo V 12 1
		1.1191	Ck 45			1.4922	12 Cr Mo V 12 1
		1.5415	15 Mo 3			1.7362	12 Cr Mo 19 5
		1.5423	16 Mo 5			1.7386	X 12 Cr Mo 9 1
1.6918	15 Mn Ni Mo V 5 3						
1.6919	11 Ni Mn Cr Mo 5 5						
1.7335	13 Cr Mo 4 4						
1.8900	St E 380						
1.8902	St E 420						
1.8905	St E 460						
12	Steel II	1.0437	19 Mn 6	15	Steel V	1.4301	X 5 Cr Ni 18 10
		1.0485	21 Mn 6			1.4401	X 5 Cr Ni Mo 17 12 2
		1.0562	St E 355			1.4541	X 6 Cr Ni Ti 18 10
		1.1169	20 Mn 6			1.4550	X 6 Cr Ni Nb 18 19
		1.5141	53 Mn Si 4			1.4571	X 6 Cr Ni Mo Ti 17 12 2
		1.5403	17 Mn Mo V 6 4			1.4580	X 6 Cr Ni Mo Nb 17 12 2
		1.6210	15 Mn Ni 6 3			1.4910	X 3 Cr Ni Mo N 17 13
		1.6310	20 Mn Mo Ni 5 5			1.4919	X 6 Cr Ni Mo N 7 13
		1.6311	20 Mn Mo Ni 4 5			1.4948	X 6 Cr Ni 18 11
		1.6368	15 Ni Cu Mo Nb 5			1.4949	X 3 Cr Ni N 18 11
		1.6751	22 Ni Mo Cr 3 7			1.4961	X 8 Cr Ni Nb 16 13
		1.7715	14 Mo V 6 3			1.4981	X 8 Cr Ni Mo Nb 16 16
		1.8812	15 Mn Mo V 5 2			1.4988	X 8 Cr Ni Mo V Nb 16 13
		1.8815	15 Mn Mo V 6 3			1.6903	X 10 Cr Ni Ti 18 10
1.8817	17 Mn Mo V 6 4	1.5152	X 40 Mn Cr 22				
13	Steel III	1.0481	17 Mn 4	16	Steel VI	1.5152	X 40 Mn Cr 22
		1.0482	19 Mn 5				
		1.5662	X 8 Ni 9				
		1.7033	34 Cr 4				
		1.7220	34 Cr Mo 4				
		1.7380	10 Cr Mo 9 10				
		1.7779	20 Cr Mo V 13 5				
		1.8075	10 Cr Si Mo V 7				
		17	Bronze	SnBz4			
		18	Copper	E-Cu			
		19	Copper	Rg9			
		20	Brass	Ms63			
		21	Nickel				
		22	Hastelloy C				



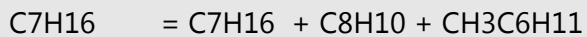
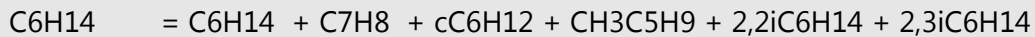
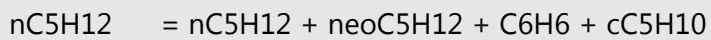
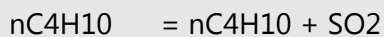
5.6 Assigning components

The codes do not cover all components found in gas analysis. Progas follows the assignment below.

Caloric Properties in accordance with ISO 20765-1 Annex E



Transport Properties



The density is calculated with the compression factor found by the reduced number of components, however with the true gas constant from all components.



5.7 Range of Application

ISO 20765-1 is applicable for the range given below.

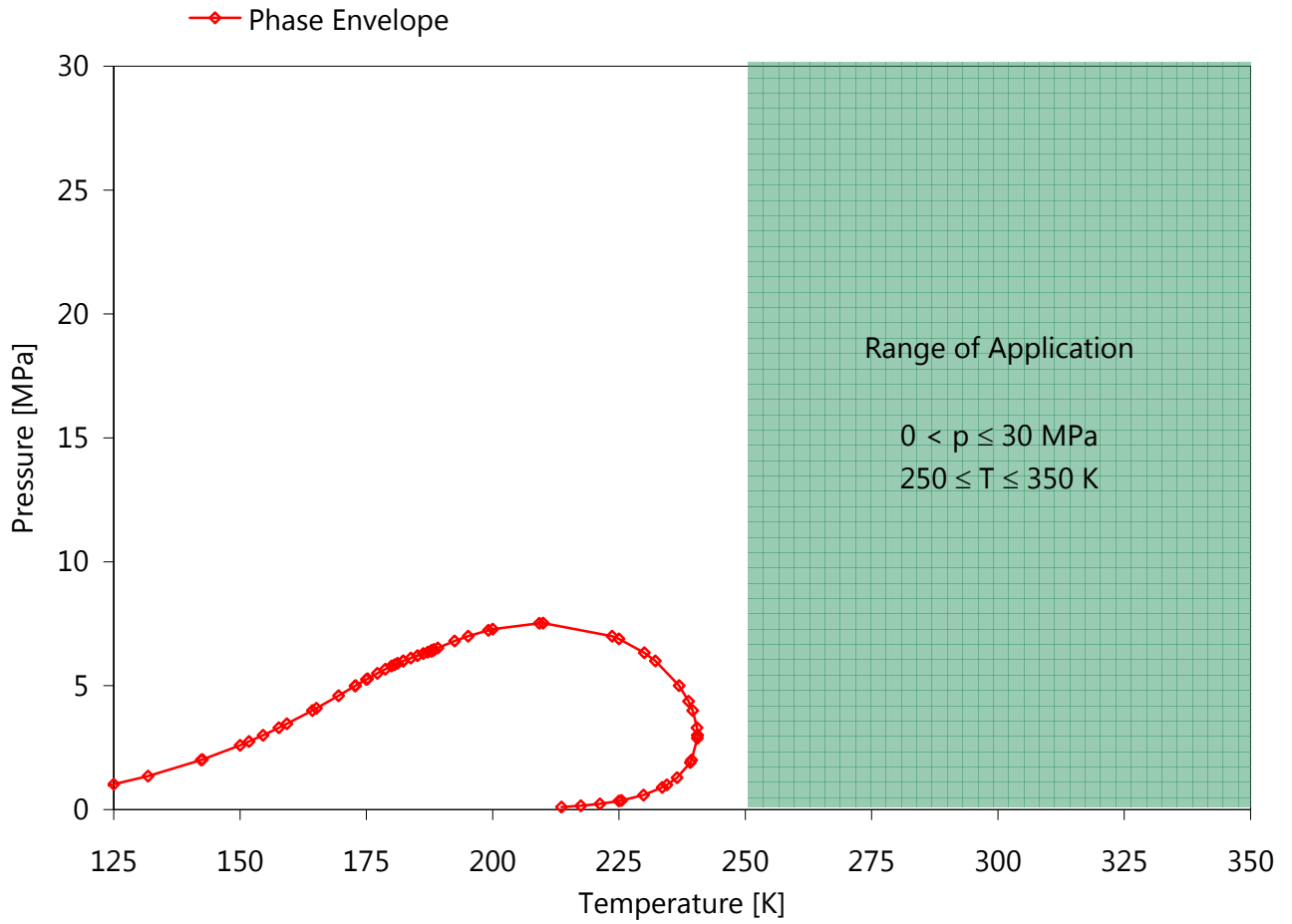
Pressure	0 MPa (0 bar) ... 30 MPa (300 bar)
Temperature	250 K (-23 °C) ... 350 K (77 °C)

Components	Mole %
Methane	Min 70
Carbon dioxide	Max 20
Nitrogen	Max 20
Ethane	Max 10
Propane	Max 3.5
Butanes	Max 1.5
Pentanes	Max 0.5
Hexanes	Max 0.1
Heptane	Max 0.05
Octane + Nonane + Decane	Max 0.05
Helium	Max 0.5
Hydrogen	Max 10
Carbon monoxide	Max 3
Argon	Max 0.02
Oxygen	Max 0.02
Water	Max 0.015
Hydrogen Sulfide	Max 0.02

A notification will be displayed should the user provide data out of range. Most probably the program will run through and set a remark in the output file. Results should still be suitable especially for low pressures with sufficient distance to the condensation line.

[PGRESULT.TXT](#)

```
p out of range for ISO 20765-1 and transport properties: p = 350.000 bar > 300 bar
T out of range for ISO 20765-1: T = 175.300 C > 76.85 C
CH4 out of range for ISO 20765-1: CH4 = 65.337 Mol% < 70 Mol%
H2 out of range for ISO 20765-1: H2 = 14.019 Mol% > 10 Mol%
Trace components out of range: Sum = 3.855 Mol% > 0.05 Mol%
```





Density	kg/m3	0.7741	0.7336	0.7088	0.7338	62.4360
Density	lb/ft3	0.0483	0.0458	0.0443	0.0458	3.8979
Relative Density	[-]	0.5987	0.5986	0.5985	0.5986	
Compression Factor	[-]	0.99803	0.99839	0.99859	0.99840	0.95309
Internal Energy	kJ/kg	-182.385	-159.342	-143.749	-158.483	-106.063
Enthalpy	kJ/kg	-51.494	-21.214	-0.799	-20.087	54.101
Entropy	kJ/(kg*K)	0.2860	0.3939	0.4636	0.3967	-1.5311
Heat Capacity cp	kJ/(kg*K)	2.0058	2.0321	2.0512	2.0331	2.5087
Heat Capacity cv	kJ/(kg*K)	1.5206	1.5475	1.5671	1.5486	1.7374
Isentropic Exponent	[-]	1.3165	1.3110	1.3071	1.3108	1.4123
Joule Thomson Coeff.	K/bar	0.4627	0.4137	0.3845	0.4120	0.1996
Speed of Sound	m/s	415.105	425.537	432.263	425.915	475.610
Dynamic Viscosity	Pa*s*E-6	10.954	11.477	11.821	11.496	15.329
HeatCircuitCapacityW	/(m*K)	0.0286	0.0306	0.0320	0.0307	0.0462

ISO 6976-1995 for Molar Mass and Calorific Values at 0degC
 ISO 20765-1 2005 for Thermodynamic Properties
 ISO 5167-2003 for Flow Calculation

Flow Element Diameter 123.05 mm (122.90 mm at 8.33 degC Steel 5)
 Pipe Diameter 202.64 mm (202.50 mm at 22.30 degC Steel 1)
 Diameter Ratio 0.6072
 Pressure Difference 0.4320 bar = 6.2656 psi
 Calibrated Discharge Coefficient
 Calibration differs from ISO standard formulae by -0.83 %
 Orifice with D and D/2 Tapping
 Mass Flow = 17.817 kg/s
 Kinematic Viscosity = 0.24551E-06 m2/s
 Reynolds Number (dPipe) = 0.73032E+07 [-]
 Discharge Coefficient = 0.60041 [-]
 Flow Coefficient = 0.64592 [-]
 Expansion Factor = 0.99877 [-]
 Mach number = 0.05046 [-]

<http://progas.axelebert.org>

6.1 Ultimate analysis

The ultimate analysis given in weight % is suitable for manual mixture calculations.

PGRESULT.TXT

Ultimate Analysis in Weight%						
C=59.9415	H=19.9273	O= 3.9081	N=16.1769	S= 0.0185	HE= 0.0046	AR= 0.0231
C+H+O+N+S+HE+AR = 100.0001						



6.2 Enthalpy and entropy in heat balance calculations

Enthalpy and entropy are always differences to certain reference conditions. PROGAS calculates in reference to 1.01325bar and 25°C of ideal gas, and enthalpy and entropy would then have the value of zero. Results in the output file are always for the real gas mixture. The output file contains the values for the actual conditions as well as for the most common reference conditions, so the needed differences can be easily determined.

For example in a gas turbine heat balance calculation the reference conditions of air, exhaust gas and heat value are usually 0°C & 1.01325bar. In this case the fuel gas enthalpy and entropy to be considered is the difference between the actual conditions and 0°C & 1.01325bar, in the example below:

fuel gas enthalpy: 54.101 kJ/kg - (-51.494 kJ/kg) = 105.595 kJ/kg

fuel gas entropy: -1.5311 kJ/ (kg*K) - 0.2860 kJ/ (kg*K)) = -1.8171 kJ/ (kg*K)

PGRESULT.TXT

	1.013bar	1.013bar	1.013bar	14.73psi	Actual	
Pressure						
Temperature	0. degC	15. degC	25. degC	60. degF	Actual	
=====+=====+=====+=====+=====+						
Density	kg/m3	0.7741	0.7336	0.7088	0.7338	62.4360
Compression Factor		0.99803	0.99839	0.99859	0.99840	0.95309
Inner Energy	kJ/kg	-182.385	-159.342	-143.749	-158.483	-106.063
Enthalpy	kJ/kg	-51.494	-21.214	-0.799	-20.087	54.101
Entropy	kJ/ (kg*K)	0.2860	0.3939	0.4636	0.3967	-1.5311

To calculate the relevant heat value at 0°C before/ after combustion the relevant data file has to be selected in pginput.txt, see 5.2.

6.3 Validation

ISO 20765 is state of the art calculation for real natural gas mixtures and requires a large amount of processing. A manual check of the results is hardly possible. The tool can be validated versus the published example calculations provided in Annex G of ISO 20765-1:2005

The example above meets the therein published numbers for Gas 4 at 10 MPa and 350 K. I have chosen this gas because it contains all 21 components used in the code.

Heat values and flow calculations have been validated and can be checked with published sample calculations or little manual effort. For transport properties there are no sample calculations published, but the results have been checked with another proprietary tool (GASCALC).



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9 Additional Information

9.1 Flow calculation from pressure differential devices

When installation requirements and flow conditions from ISO 5167 are met, standardized flow devices can provide flow rate results with good accuracy.

The diameter ratio is defined

$$\beta = \frac{d}{D} \quad (9.1)$$

- D upstream internal pipe diameter under working conditions [mm]
- d diameter of the flow device (orifice or throat) under working conditions [mm]
- β diameter ratio [-]

The Reynolds number, expressing the ratio between the inertia and viscous forces in the upstream pipe is

$$Re_D = \frac{m}{\frac{\pi}{4} \cdot \mu_1 \cdot D} \quad (9.2)$$

- D upstream internal pipe diameter under working conditions [mm]
- Re_D Reynolds number with respect to D [mm]
- m mass flow [kg/s]
- μ_1 dynamic viscosity upstream of the flow device [Pa·s]

The expansion factor takes into account the compressibility of the fluid

Orifice plates

$$\varepsilon = 1 - (0.351 + 0.256\beta^4 + 0.93\beta^8) \left[1 - \left(\frac{p_2}{p_1} \right)^{\frac{1}{\kappa}} \right] \quad (9.3)$$

Nozzles
Venturi nozzles
Venturi tubes

$$\varepsilon = \sqrt{\left(\frac{\kappa \left(\frac{p_2}{p_1} \right)^{\frac{2}{\kappa}}}{\kappa - 1} \right) \left(\frac{1 - \beta^4}{1 - \beta^4 \left(\frac{p_2}{p_1} \right)^{\frac{2}{\kappa}}} \right) \left(\frac{1 - \left(\frac{p_2}{p_1} \right)^{\frac{\kappa-1}{\kappa}}}{1 - \left(\frac{p_2}{p_1} \right)} \right)} \quad (9.4)$$

- p_1 absolute static pressure upstream of flow device [Pa]
- p_2 absolute static pressure at flow device [Pa]; required is $p_2/p_1 \geq 0.75$
- β diameter ratio [-]
- ε expansion factor [-]
- κ isentropic exponent [-]



The discharge coefficient is defined for an incompressible fluid flow and relates actual vs. theoretical flowrate.

$$\begin{aligned}
 C = & 0.5961 + 0.0261\beta^2 - 0.216\beta^8 + 0.000521 \cdot \left(\frac{10^6\beta}{Re_D}\right)^{0.7} \\
 & + \left[0.0188 + 0.0063 \cdot \left(\frac{19000 \cdot \beta}{Re_D}\right)^{0.8} \right] \cdot \beta^{3.5} \cdot \left(\frac{10^6}{Re_D}\right)^{0.3} \\
 \text{Orifice plates} \quad & + \left(0.043 + 0.080e^{-10L_1} - 0.123e^{-7L_1} \right) \cdot \left[1 - 0.11 \left(\frac{19000 \cdot \beta}{Re_D}\right)^{0.8} \right] \frac{\beta^4}{1 - \beta^4} \\
 & - 0.031 \left[\frac{2L'_2}{1 - \beta} - 0.8 \left(\frac{2L'_2}{1 - \beta}\right)^{1.1} \right] \cdot \beta^{1.3} \\
 & + \left\{ 0.011(0.75 - \beta) \cdot \left(2.8 - \frac{D}{25.4} \right) \right\} \Big|_{\text{add } \{ \} \text{ only for } D < 71.12\text{mm}}
 \end{aligned} \tag{9.5}$$

$$\begin{aligned}
 \text{ISA 1932} \\
 \text{Nozzles} \quad C = & 0.9900 - 0.2262\beta^{4.1} - \left(0.00175\beta^2 - 0.0033\beta^{4.15} \right) \cdot \left(\frac{10^6}{Re_D}\right)^{1.15}
 \end{aligned} \tag{9.6}$$

$$\begin{aligned}
 \text{Long radius} \\
 \text{nozzles} \quad C = & 0.9965 - 0.00653 \sqrt{\frac{10^6\beta}{Re_D}}
 \end{aligned} \tag{9.7}$$

$$\begin{aligned}
 \text{Venturi} \\
 \text{nozzles} \quad C = & 0.9858 - 0.196\beta^{4.5}
 \end{aligned} \tag{9.8}$$

$$\begin{aligned}
 \text{Classical} \\
 \text{venturi tubes} \quad C = & 0.984 \text{ with an "as cast" convergent section}
 \end{aligned} \tag{9.9}$$

$$\begin{aligned}
 \text{Classical} \\
 \text{venturi tubes} \quad C = & 0.995 \text{ with a machined convergent section}
 \end{aligned} \tag{9.10}$$

$$\begin{aligned}
 \text{Classical} \\
 \text{venturi tubes} \quad C = & 0.985 \text{ with a rough-welded sheet-iron convergent section}
 \end{aligned} \tag{9.11}$$

- C discharge coefficient [-]
- D upstream internal pipe diameter under working conditions [mm]
- L'₂ quotient for downstream tapping distance [-]
- L₁ quotient for upstream tapping distance [-]
- Re_D Reynolds number with respect to D [mm]
- β diameter ratio [-]

Corner tappings: L₁ = L'₂ = 0

Flange tappings: L₁ = L'₂ = 25.4/D with D [mm]

D and D/2 tappings: L₁ = 1; L'₂ = 0.47



Discharge coefficient and flow coefficient are related

$$\alpha = \frac{C}{\sqrt{1-\beta^4}} \quad (9.12)$$

- C discharge coefficient [-]
- β diameter ratio [-]
- α flow coefficient [-]

Where the discharge coefficient depends on the Reynolds number the mass flow can only be found by iteration.

$$m = \frac{C}{\sqrt{1-\beta^4}} \cdot \varepsilon \cdot \frac{\pi}{4} d^2 \cdot \sqrt{2 \cdot \Delta p \cdot \rho_1} = \frac{\pi}{4} \cdot \mu_1 \cdot D \cdot Re_D \quad (9.13)$$

- C discharge coefficient [-]
- D upstream internal pipe diameter under working conditions [mm]
- Re_D Reynolds number with respect to D [mm]
- d diameter of the flow device (orifice or throat) under working conditions [mm]
- m mass flow [kg/s]
- p_1 absolute static pressure upstream of flow device [Pa]
- β diameter ratio [-]
- μ_1 dynamic viscosity upstream of the flow device [Pa·s]
- ε expansion factor [-]
- ρ_1 density upstream of the flow device [kg/m³]
- Δp pressure difference across the flow device [Pa]

9.2 Heat values

The higher heating value (HHV) (or gross energy or upper heating value or gross calorific value (GCV) or higher calorific value (HCV)) is determined by bringing all the products of combustion back to the original pre-combustion temperature, and in particular condensing any vapor produced. The higher heating value takes into account the latent heat of vaporization of water in the combustion products, and is useful in calculating heating values for fuels where condensation of the reaction products is practical, HHV assumes all the water component is in liquid state at the end of combustion (in product of combustion).

The lower heating value (LHV) (net calorific value (NCV) or lower calorific value (LCV)) is determined by subtracting the heat of vaporization of the water vapor from the higher heating value. This treats any H₂O formed as a vapor. The energy required to vaporize the water therefore is not realized as heat. The LHV assumes that the latent heat of vaporization of water in the fuel and the reaction products is not recovered. It is useful in comparing fuels where condensation of the combustion products is impractical, or heat at a temperature below 150 °C cannot be put to use, for example in gas turbines.



9.3 Caloric properties using Helmholtz free energy approach

The Helmholtz free energy is a thermodynamic potential that measures the »useful« work obtainable from a closed thermodynamic system at a constant temperature and volume.

c_p°	molar ideal gas specific isobaric heat capacity [kJ/(kmol·K)]
c_p	molar isobaric heat capacity [kJ/(kmol·K)]
c_v	molar isochoric heat capacity [kJ/(kmol·K)]
f°	ideal gas contribution to the molar Helmholtz energy [kJ/kmol]
f	molar Helmholtz free energy [kJ/kmol]
f^r	residual part contribution to the molar Helmholtz energy [kJ/kmol]
h°	molar ideal gas enthalpy [kJ/kmol]
h_0°	ideal gas integration constant for zero enthalpy at the reference state of 298.15 K and 0.101325 MPa [kJ/kmol]
M	molar mass [kg/kmol]
R	molar gas constant 8.31451 kJ/(kmol·K)
s°	molar ideal gas entropy [kJ/(kmol·K)]
s_0°	ideal gas integration constant for zero entropy at the reference state of 298.15 K and 0.101325 MPa [kJ/(kmol·K)]
s	molar entropy [kJ/(kmol·K)]
T	absolute temperature [K]
u	molar internal energy [kJ/kmol]
w	speed of sound [m/s]
x_i	mole fraction of component i [-]
δ°	molar density at the reference state of 298.15 K and 0.101325 MPa [-]
δ	reduced density $\delta = K^3 \cdot \rho$ [-], where K is a mixture size parameter using the constants from annex D of ISO 20765-1
κ	isentropic exponent [-]
μ	Joule-Thomson coefficient [K/MPa]
Φ°	ideal gas contribution to the reduced Helmholtz energy [-]
Φ	reduced Helmholtz energy $f/(RT)$ [-]
Φ^r	residual part contribution to the reduced Helmholtz energy [-]
ρ	molar density [kmol/m ³]
τ	inverse reduced temperature (T_r/T) [-], where $T_r = 1K$

The Helmholtz energy is defined as

$$f \equiv u - T \cdot s \quad (9.14)$$

All single-phase thermodynamic properties can be calculated as derivatives of the Helmholtz energy, as a function of temperature and density.

$$f(\rho, T) = f^0(\rho, T) + f^r(\rho, T) \quad (9.15)$$

The dimensionless Helmholtz energy Φ uses independent variables of dimensionless density and temperature.

$$\Phi(\delta, \tau) = \Phi^0(\delta, \tau) + \Phi^r(\delta, \tau) \quad (9.16)$$



For a certain composition of a mixture the ideal Helmholtz energy is

$$f^0 = h^0 - RT - Ts^0 = \int_{T_0}^T c_p^0 dT + h_0^0 - RT - T \left[\int_{T_0}^T \frac{c_p^0}{T} dT - R \ln \left(\frac{\rho}{\rho_0} \right) - R \ln \left(\frac{T}{T_0} \right) + s_0^0 - R \sum_{i=1}^n x_i \cdot \ln x_i \right] \quad (9.17)$$

$$\Phi^0 = -\tau \int_{\tau_0}^{\tau} \frac{c_p^0}{R \cdot \tau^2} d\tau + \frac{h_0^0}{R} \tau - 1 + \int_{\tau_0}^{\tau} \frac{c_p^0}{R \cdot \tau} d\tau + \ln \frac{\delta}{\delta_0} + \ln \frac{\tau_0}{\tau} - \frac{s_0^0}{R} + \sum_{i=1}^n x_i \cdot \ln x_i$$

The ideal gas part as well as the real fluid behavior is often described using empirical models.

The functions for calculating compressibility factor, internal energy, enthalpy, entropy, heat capacity, speed of sound and other caloric properties are all related to the Helmholtz free energy and its derivatives.

Compression Factor $z = \delta \Phi_{\delta}$ (9.18)

Internal Energy $\frac{u}{R \cdot T} = \tau \Phi_{\tau}$ (9.19)

Enthalpy $\frac{h}{R \cdot T} = \tau \Phi_{\tau} + \delta \Phi_{\delta} = \frac{u}{R \cdot T} + z$ (9.20)

Entropy $\frac{s}{R} = \tau \Phi_{\tau} - \Phi = \frac{u}{R \cdot T} - \Phi$ (9.21)

Isochoric Heat Capacity $\frac{c_v}{R} = -\tau^2 \Phi_{\tau\tau}$ (9.22)

Isobaric Heat Capacity $\frac{c_p}{R} = -\tau^2 \Phi_{\tau\tau} + \frac{\Phi_2^2}{\Phi_1}$ (9.23)

Joule Thomson Coefficient $\mu \cdot R \cdot \rho = \frac{\Phi_2 - \Phi_1}{\Phi_2^2 - \tau^2 \Phi_{\tau\tau} \Phi_1} = \frac{R}{c_p} \left(\frac{\Phi_2}{\Phi_1} - 1 \right)$ (9.24)

Isentropic Exponent $\kappa = \frac{\Phi_1 - \frac{\Phi_2^2}{\tau^2 \Phi_{\tau\tau}}}{\delta \Phi_{\delta}}$ (9.25)

Speed of Sound $\frac{w^2 \cdot M}{R \cdot T} = \Phi_1 - \frac{\Phi_2^2}{\tau^2 \Phi_{\tau\tau}} = z \cdot \kappa$ (9.26)

with $\Phi_1 = \left(\delta^2 \Phi_{\delta} \right)_{\delta} = 2\delta \Phi_{\delta} + \delta^2 \Phi_{\delta\delta}$ (9.27)

and $\Phi_2 = -\tau^2 \left(\frac{\delta \Phi_{\delta}}{\tau} \right)_{\tau} = \delta \Phi_{\delta} - \tau \delta \Phi_{\tau\delta}$ (9.28)



The common functional forms of the fundamental equations are

$$\Phi = \Phi^0 + \frac{B}{K^3} \delta - \delta \sum_{n=13}^{18} C_n^* \cdot \tau^{u_n} + \sum_{n=13}^{58} C_n^* \cdot \tau^{u_n} \cdot \delta^{b_n} \cdot \exp(-c_n \cdot \delta^{k_n}) \quad (9.29)$$

$$\begin{aligned} \tau \Phi_\tau = \tau \left(\frac{\partial \Phi}{\partial \tau} \right)_{\delta x} &= \tau \cdot \Phi_\tau^0 + \frac{\delta}{K^3} \cdot \sum_{n=1}^{18} u_n \cdot \tau^{u_n} \cdot B_n^* - \delta \sum_{n=13}^{18} u_n \cdot \tau^{u_n} \cdot C_n^* \\ &+ \sum_{n=13}^{58} u_n \cdot \tau^{u_n} \cdot C_n^* \cdot \delta^{b_n} \cdot \exp(-c_n \cdot \delta^{k_n}) \end{aligned} \quad (9.30)$$

$$\begin{aligned} \tau^2 \Phi_{\tau\tau} = \tau^2 \left(\frac{\partial^2 \Phi}{\partial \tau^2} \right)_{\delta x} &= \tau^2 \cdot \Phi_{\tau\tau}^0 + \frac{\delta}{K^3} \cdot \sum_{n=1}^{18} (u_n^2 - u_n) \cdot \tau^{u_n} \cdot B_n^* - \delta \sum_{n=13}^{18} (u_n^2 - u_n) \cdot \tau^{u_n} \cdot C_n^* \\ &+ \sum_{n=13}^{58} (u_n^2 - u_n) \cdot \tau^{u_n} \cdot C_n^* \cdot \delta^{b_n} \cdot \exp(-c_n \cdot \delta^{k_n}) \end{aligned} \quad (9.31)$$

$$\begin{aligned} \delta \Phi_\delta = \delta \left(\frac{\partial \Phi}{\partial \delta} \right)_{\tau x} &= 1 + \frac{B}{K^3} \delta - \delta \sum_{n=13}^{18} C_n^* \cdot \tau^{u_n} \\ &+ \sum_{n=13}^{58} C_n^* \cdot \tau^{u_n} \cdot \delta^{b_n} \cdot (b_n - c_n \cdot k_n \cdot \delta^{k_n}) \cdot \exp(-c_n \cdot \delta^{k_n}) \end{aligned} \quad (9.32)$$

$$\begin{aligned} \Phi_1 = \left(\delta^2 \Phi_\delta \right)_\delta &= \left(\frac{\partial (\delta^2 \cdot \Phi_\delta)}{\partial \delta} \right)_{\tau x} = 1 + 2 \frac{B}{K^3} \delta - 2 \cdot \delta \sum_{n=13}^{18} C_n^* \cdot \tau^{u_n} \\ &+ \sum_{n=13}^{58} C_n^* \cdot \tau^{u_n} \cdot \delta^{b_n} \cdot \left(b_n - (1 + k_n) \cdot c_n \cdot k_n \cdot \delta^{k_n} + (b_n - c_n \cdot k_n \cdot \delta^{k_n})^2 \right) \cdot \exp(-c_n \cdot \delta^{k_n}) \end{aligned} \quad (9.33)$$

$$\begin{aligned} \Phi_2 = -\tau^2 \left(\frac{\delta \Phi_\delta}{\tau} \right)_\tau &= -\tau^2 \left(\frac{\partial \left(\frac{\delta \Phi_\delta}{\tau} \right)}{\partial \tau} \right)_{\delta x} = 1 + \frac{\delta}{K^3} \sum_{n=1}^{18} B_n^* \cdot (1 - u_n) \cdot \tau^{u_n} - \delta \sum_{n=13}^{18} C_n^* \cdot (1 - u_n) \cdot \tau^{u_n} \\ &+ \sum_{n=13}^{58} C_n^* \cdot \tau^{u_n} \cdot \delta^{b_n} \cdot (1 - u_n) \cdot (b_n - c_n \cdot k_n \cdot \delta^{k_n}) \cdot \exp(-c_n \cdot \delta^{k_n}) \end{aligned} \quad (9.34)$$

The various constants are given in the detailed documentation for the equation of state in annex D of ISO 20765-1.