Combustion of Gaseous Fuels

Air and flue gas per Nm³ and per kg of fuel gas, flue gas composition, molar mass and GCV/NCV from the volumetric analysis and excess air.

Method: ASME PTC 4-2013 (air composition); NIST Chemistry WebBook (standard enthalpies of combustion at 25 °C); ...

Input parameters

Unit system: SI

Parameter	Value	Unit
Methane (CH4)	95.000	%
Ethane (C2H6)	2.5000	%
Propane (C3H8)	0.20000	%
Butane (C4H10)	0	%
Pentane (C5H12)	0	%
Ethylene (C2H4)	0	%
Propylene (C3H6)	0	%
Benzene (C6H6)	0	%
Hydrogen (H2)	0	%
Carbon monoxide (CO)	0	%
Hydrogen sulphide (H2S)	0	%
Water vapour (H2O)	0	%
Carbon dioxide (CO2)	0.60000	%
Nitrogen (N2)	1.7000	%
Oxygen (O2)	0	%
Sulphur dioxide (SO2)	0	%
Excess air	10.000	%
Air humidity (kg water per kg dry air)	0.013000	kg/kg

Calculated results

Parameter	Value	Unit
Molar mass of the fuel gas	16.821	kg/kmol
Fuel gas density (normal)	0.75047	kg/m³
Gross calorific value per Nm³	39,686	kJ/Nm³
Net calorific value per Nm³	35,795	kJ/Nm³
Gross calorific value per kg	52,882	kJ/kg
Net calorific value per kg	47,696	kJ/kg
Stoichiometric oxygen	1.9975	Nm³/Nm³
Theoretical dry air	9.5346	Nm³/Nm³
Actual wet air	10.707	Nm³/Nm³
Wet flue gas	11.722	Nm³/Nm³
Dry flue gas	9.5196	Nm³/Nm³
Actual wet air	18.295	kg/kg

Parameter	Value	Unit
Wet flue gas	19.295	kg/kg
Dry flue gas	16.937	kg/kg
CO_2 in wet flue gas	8.6693	%
H_2O in wet flue gas	18.787	%
N_2 in wet flue gas	70.007	%
Ar in wet flue gas	0.83212	%
O_2 in wet flue gas	1.7041	%
SO_2 in wet flue gas	0	%
O_2 in dry flue gas (analyser reading)	2.0983	%

Formula and method

$$V_{O_2} = \sum_i y_i \left(c_i + \frac{h_i}{4} + s_i - \frac{o_i}{2} \right) - y_{O_2,f} \qquad V_{a,th} = \frac{V_{O_2}}{0.2095} \qquad V_a = V_{a,th}(1+EA) \qquad V_{a,wet} = V_a + \omega V_a \frac{M_{air}}{M_{H_2O}}$$

$$V_{CO_2} = \sum_i y_i c_i + y_{CO_2,f} + 0.0004\,V_a \qquad V_{H_2O} = \sum_i y_i \frac{h_i}{2} + y_{H_2O,f} + \omega V_a \frac{M_{air}}{M_{H_2O}} \qquad V_{SO_2} = \sum_i y_i s_i + y_{SO_2,f} \qquad V_{N_2+Ar} = y_{N_2,f} + 0.7901\,V_a \qquad V_{O_2,x} = 0.2095\,V_a - V_{O_2}$$

$$V_{g,wet} = V_{CO_2} + V_{H_2O} + V_{SO_2} + V_{N_2+Ar} + V_{O_2,x} \qquad V_{g,dry} = V_{g,wet} - V_{H_2O} \qquad m_j = \frac{V_j\, M_j}{M_f}$$

$$M_f = \sum_i y_i M_i \qquad \rho_f = \frac{M_f}{V_m} \qquad GCV_v = \frac{\sum_i y_i\, \Delta H_{c,i}}{V_m} \qquad NCV_v = GCV_v - \frac{\sum_{i\,\in\,\text{combustibles}} y_i \frac{h_i}{2}\, h_{fg,25}\, M_{H_2O}}{V_m} \qquad GCV = \frac{GCV_v}{\rho_f}$$

Variables

$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}\$, \$y_{i}$	combustible species, volume fractions of the fuel gas	–
$y_{H_2O}\$, \$y_{CO_2}\$, \$y_{N_2}\$, \$y_{O_2}\$, \$y_{SO_2}$	inert and oxygen species of the fuel gas (as inputs)	–
$c_i\$, \$h_i\$, \$s_i\$, \$o_i$	atoms of C, H, S, O in species *i*	–
EA	excess air fraction	–
ω	humidity of combustion air, kg water per kg dry air	kg/kg
M_f	molar mass of the fuel gas	kg/kmol
ρ_f	fuel gas density at 0 °C and 101.325 kPa	kg/Nm³
$GCV_v\$, \$NCV_v$	gross and net calorific value per normal cubic metre	J/Nm³
$GCV\$, \$NCV$	gross and net calorific value per kilogram	J/kg
V_{O_2}	stoichiometric oxygen per Nm³ fuel	Nm³/Nm³
$V_{a,th}\$, \$V_{a,wet}$	theoretical dry air and actual wet air per Nm³ fuel	Nm³/Nm³
$V_{g,wet}\$, \$V_{g,dry}$	wet and dry flue gas per Nm³ fuel	Nm³/Nm³
$m_{a,wet}\$, \$m_{g,wet}\$, \$m_{g,dry}$	the same per kg of fuel	kg/kg
$y_{CO_2}\$, \$y_{H_2O}\$, \$y_{N_2}\$, \$y_{Ar}\$, \$y_{O_2}\$, \$y_{SO_2}$	wet flue gas composition by volume (as outputs)	–
$y_{O_2,dry}$	oxygen in dry flue gas, as an analyser reads it	–
V_m	molar volume at normal conditions, 22.41397	Nm³/kmol
$h_{fg,25}$	latent heat of water at 25 °C (IF97)	J/kg

Method and standards

Volumetric stoichiometry at normal conditions with PTC 4 air (20.95 % O_2, 79.05 % atmospheric nitrogen, carried as N_2 + Ar + CO_2). Heating values are built from the standard molar enthalpies of combustion of each species at 25 °C (NIST Chemistry WebBook) divided by the ideal-gas molar volume, so the GCV of methane is 890.6 kJ/mol ÷ 22.414 L/mol = 39.73 MJ/Nm³. The net value subtracts the IF97 latent heat of the water formed. Mass-basis results divide by the fuel gas molar mass.

Assumptions and limits

- Ideal gas: volume fraction equals mole fraction; real-gas corrections (about 1–2 % for propane and butane at normal conditions) are not applied.
- Complete combustion; H_2S goes entirely to SO_2.
- Air is 78.08 % N_2, 0.93 % Ar and 0.04 % CO_2 besides its oxygen: the air's CO_2 is counted in y_{CO_2} and the N_2 + Ar in V_{N_2+Ar}. The water vapour already in the fuel gas is not deducted from the NCV.
- An analysis that does not sum to 100 % is normalised with a warning; check it before relying on the result.
- Volumes per Nm^3 are at 0 °C and 101.325 kPa; values shown per scf are converted to the US standard cubic foot (60 °F, 14.696 psia).
- Benzene is taken as vapour; hydrocarbons heavier than pentane are not listed and should be lumped into pentane by carbon content.

References

- ASME PTC 4-2013 (air composition)
- NIST Chemistry WebBook (standard enthalpies of combustion at 25 °C)
- ideal gas at 0 °C and 101.325 kPa

Report details

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Release checks	5 reference cases of this calculator, computed independently, are checked on every release

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