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Abstract

Fuelsim - Average is a relatively simple, but useful, mass, volume and energy balance spreadsheet for continuous combustion applications, but can also be used for other thermal conversion processes where solid fuel is converted to a fuel gas mixture of O_2, CO, NO, NO_2, UHC (unburned hydrocarbons), SO_2, N_2O, H_2, NH_3, HCN, Tar, CO_2, N_2, Ar and H_2O. The fuel can either be a solid fuel, a liquid fuel or a fuel gas, and the oxidant can either be ISO 2533 Standard air, with a user defined relative humidity, or a gas mixture of O_2 (the only oxidant), N_2, CO_2, Ar and H_2O.

Fuelsim - Average calculates emissions in various denominations based on the user input. However, also a separate emission conversion section is included, where emission values in various denominations can be inserted and converted between the various denominations. The corresponding emission levels in volume fractions can be inserted into the Fuelsim - Average main calculations and additional useful information are then calculated.

	Indexing terms: English	Indexing Terms: Norwegian
Group 1	Combustion	Forbrenning
Group 2	Fuels	Brensler
Selected by author	Mass, volume and energy balances	Masse-, volum- og energibalanser
	Emissions	Utslipp
	Emission conversion	Utslippskonvertering

Fuelsim - Average v1.1:

A mass, volume and energy balance spreadsheet for continuous combustion applications

Øyvind Skreiberg

August 2002

Preface to version 1.1

Version 1.1 is an update to version 1.0 with respect to several aspects. Version 1.0 contained a couple of errors and needs for clarification, which was corrected in a revision 1 (Fuelsim - Average_v1.0-r1.xls, of April 9, 2002). See the revision history included in the spreadsheet for further details. However, this report was not updated in the revision. In version 1.1 several additional updates have been included, mainly concerning implementation of water injection, further examples, printout appearance, inclusion of high temperature thermodynamic coefficients in the Gas conversion sheet and addition of the ISO 11042-1 sheet, comparing the ISO 11042-1 [1] standard and Fuelsim - Average. This report has therefore been updated to take into account all relevant changes up to now. Again, see the revision history included in the spreadsheet for further details.

Preface to version 1.0

This PostDoc has been carried out as a part of a Norwegian industry project, Research and development of user- and environmentally friendly wood stoves and fireplaces, financially supported by the Research Council of Norway. SINTEF Energy Research has been the research partner in the project, and the PostDoc has been concerned with one of three main subjects of research in the industry project. The PostDoc has been carried out as a 50% position over a three-year period.

The goal has been to study the potential of staged air combustion for NOx reduction in wood stoves and fireplaces, and to develop modelling tools for design of wood stoves and fireplaces. Initially, significant focus was put on use of CFD, using CFX from AEA Technology. However, due to the complexity of fuel NOx chemical kinetics, the usefulness of using global, or even reduced, chemical kinetics for studies of NOx reduction by staged air combustion is highly questionable. Therefore, the modelling work has mainly been concerned with detailed studies of detailed chemical kinetics and modelling of staged air combustion in ideal reactors, plug flow reactors and perfectly stirred reactors, representing two extremities of mixing conditions. Three different detailed chemical kinetics mechanisms have been used, compared and analysed in the modelling work.

Two relatively simple, but useful, modelling tools have been developed as tools for design of wood stoves and fireplaces. Fuelsim - Average is a general mass, volume and energy balance spreadsheet for continuous combustion applications, for adiabatic conditions. This spreadsheet has been made publicly available at the Internet homepage of IEA Task 32 - Biomass Combustion and Co-firing. Fuelsim - Transient is a transient version of Fuelsim - Average, designed for batch combustion of wood in wood stoves and fireplaces. It includes a number of transient models and also heat transfer calculations.

The author would like to thank our industry partner, Nord-Interiør AS, and the Research Council of Norway for financial support. Project leader and Research Scientist Edvard Karlsvik at SINTEF Energy Research and Professor Johan E. Hustad are acknowledged for their support through these three years. Dr. Pia Kilpinen, Vesna Barisic and Edgardo Coda Zabetta at Åbo Akademi in Finland are acknowledged for their contribution to the NOx part of this work trough collaboration, as is Dr. Peter Glarborg at the Technical University of Denmark. Finally, the Nordic Energy Research Program is acknowledged for their indirect support through the Nordic Senior Research Scientist position of the author.

[1] ISO 11042-1. Gas turbines - Exhaust gas emission - Part 1: Measurement and evaluation, 1996.

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1. Summary

Fuelsim - Average is a relatively simple, but useful, mass, volume and energy balance spreadsheet for continuous combustion applications, but can also be used for other thermal conversion processes where solid fuel is converted to a fuel gas mixture of O_2, CO, NO, NO_2, UHC (unburned hydrocarbons), SO_2, N_2O, H_2, NH_3, HCN, Tar, CO_2, N_2, Ar and H_2O. The fuel can either be a solid fuel, a liquid fuel or a fuel gas, and the oxidant can either be ISO 2533 [2] Standard air, with a user defined relative humidity, or a gas mixture of O_2 (the only oxidant), N_2, CO_2, Ar and H_2O.

Fuelsim - Average calculates emissions in various denominations based on the user input. However, also a separate emission conversion section is included, where emission values in various denominations can be inserted and converted between the various denominations. The corresponding emission levels in volume fractions can be inserted into the Fuelsim - Average main calculations and additional useful information are then calculated.

Sammendrag (Summary in Norwegian)

Fuelsim - Average er et relativt enkelt masse-, volum- og energibalanse regneark for kontinuerlige forbrenningsprosesser, men kan også brukes for andre termiske konverteringsprosesser hvor faste brensler konverteres til en brenselgass av O_2, CO, NO, NO_2, UHC (uforbrente hydrokarboner), SO_2, N_2O, H_2, NH_3, HCN, Tjære, CO_2, N_2, Ar og H_2O. Brenselet kan enten være et fast brensel, et flytende brensel eller en brenselgass, og oksidanten kan enten være ISO 2533 [2] Standard luft, med en brukerdefinert relativ luftfuktighet, eller en blanding av O_2 (eneste oksidant), N_2, CO_2, Ar og H_2O.

Fuelsim - Average beregner utslipp i ulike benevninger basert på brukerens input. Også en separat utslippskonverteringsdel er inkludert, hvor utslipp i flere forskjellige benevninger kan settes inn og konverteres til andre benevninger. De korresponderende utslippene i volumfraksjoner kan settes inn i Fuelsim - Average og ytterligere informasjon vil bli beregnet.

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[2] ISO 2533. Standard Atmosphere, 1975.

2. Introduction

Mass, volume and energy balances form the basis for any thermal conversion process where a fuel (solid, liquid or gas) is converted to products. Combustion processes are highly complex conversion processes where a large number of elementary reactions influence the conversion of the fuel to products, in addition to a number of operational parameters. To be able to adequately model the conversion process and the formation of emissions such as NOx, detailed chemical kinetics should be applied in combination with Computational Fluid Dynamics (CFD). Today, this is possible but very time consuming, and still the degree of uncertainty in for example NOx emission prediction is considerable. However, to design combustion applications such as wood stoves and fireplaces a global combustion reaction is quite sufficient as a first engineering approach. From a global combustion equation, the necessary information regarding global mass, volume and energy flows can be derived relatively easily, as well as the concentration of major species. To study transient effects in batch combustion applications, transient models may be used in combinations with the formulas shown in Appendix 1. Transient modelling of batch combustion processes is the subject of Part 3 of this PostDoc work.

If information regarding minor species emissions is available, the global combustion equation can easily be extended to include also these species. This makes it possible to carry out a number of calculations for the minor species, including emission conversion to various denomination, conversion factors for each species, etc.

Conversion of emissions to other denominations is in principle very simple. However, in practise it is not always that simple. Formulas and procedures for emission conversion between the most common denominations are shown in Appendix 1. These formulas and procedures are based directly on the combustion equation used in Fuelsim - Average and do not include the simplifications usually applied in many other formulas for emission conversion. These formulas and procedures are applied in the separate emission conversion section in Fuelsim - Average. The accuracy of the emission conversion process is limited by the amount of information stated in addition to the specific emission level in some denomination.

Appendix 2 gives a short introduction to Fuelsim - Average while Appendix 3 includes description and documentation of the spreadsheet, in addition to the formulas included in Appendix 1. Examples of use are included in Appendix 4, while an exercise is included in Appendix 5. Finally, Appendix 6 compares Fuelsim - Average versus ISO 11042-1.

3. Description of Fuelsim - Average

3.1 Introduction

Fuelsim - Average is a relatively simple, but useful, mass, volume and energy balance spreadsheet for continuous combustion applications, but can also be used for other thermal conversion processes where solid fuel is converted to a fuel gas mixture of O_2, CO, NO, NO_2, UHC (unburned hydrocarbons), SO_2, N_2O, H_2, NH_3, HCN, Tar, CO_2, N_2, Ar and H_2O.

The fuel can either be a solid fuel, a liquid fuel or a fuel gas, and the oxidant can either be ISO 2533 Standard air, with a user defined relative humidity, or a gas mixture of O_2 (the only oxidant), N_2, CO_2, Ar and H_2O.

Preheating, relative to an ambient temperature, of solid or liquid fuel (including moisture content), fuel gas, water for water injection and oxidant (separated into primary and secondary air) is possible. The temperature of the products is calculated assuming adiabatic conditions (no heat loss).

Fuelsim - Average uses thermodynamic data on CHEMKIN [3] format for all gas species and also liquid water, while the specific heat capacity of a solid or liquid fuel is user defined. The heating value of a fuel gas is calculated directly from the thermodynamic data, while the heating value of a solid fuel is estimated from the elemental composition using an empirical expression. However, the heating value may also be inserted manually. The heating value of a liquid fuel should be inserted manually.

The user may add new fuel gas species, including accompanying thermodynamic data on CHEMKIN format.

Thermal efficiency (using a user defined chimney inlet temperature), combustion efficiency and total efficiency are calculated, together with further useful mass, volume and energy balance output.

Fuelsim - Average calculates emissions in various denominations based on the user input. However, also a separate emission conversion section is included, where emission values in various denominations can be inserted and converted between the various denominations. The corresponding emission levels in volume fractions can be inserted into the Fuelsim - Average main calculations and additional useful information are then calculated.

The emission conversion procedure is based directly on the combustion equation, no simplified expressions are applied. When converting emission levels between different oxygen concentrations, the defined oxidant is added to, or removed from, the given flue gas composition until the calculated oxygen concentration equals the reference oxygen concentration.

Fuelsim - Average is an Excel spreadsheet and uses programmed functions and procedures in addition to formulas inserted directly in the spreadsheet cells. The user interface consists of input cells (marked with the colour white) various push-buttons (marked with the colour grey), input forms (revealed when pushing a push-button), option-buttons (black: option is selected, white: option is not selected) and pull-down menus. Cells marked with the colour green are not user changeable.

The spreadsheet is protected to prevent accidental deletion of cell contents or objects. Formulas (only in the Average sheet), functions and procedures can not be seen by the user. However, all cells are selectable when using for example the Goal Seek command in Excel and other spreadsheets/sheets can refer to cells in the Average sheet. Also, additional sheets can be inserted into the Fuelsim - Average spreadsheet.

The main purpose of Fuelsim - Average is to provide the user with information regarding mass, volume and energy flows in continuous combustion applications, depending on a number of inputs described in more detail in the appendixes. The goal here is only to give a brief introduction to Fuelsim - Average and the reader is referred to the appendixes for further details.

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[3] CHE-036-1, CHEMKIN Collection Release 3.6, A Software Package for the Analysis of Gas-Phase Chemical and Plasma Kinetics, September 2000

3.2 Methods

The global combustion equation used in Fuelsim - Average (F-A) is shown in Equation 1. By balancing this equation mass and volume flow calculations can be carried out. By also introducing thermodynamic data for the reactants and products, energy calculations can be carried out in addition. Additionally, solid or liquid fuels may contain water in F-A. Further formulas are given in Appendix 1.

$$a \cdot \left(Y_C + Y_H + Y_O + Y_N + Y_S\right)_{Fuel} + \frac{z}{Y_{O_2}} \cdot \left(Y_{O_2} + Y_{N_2} + Y_{Ar} + Y_{CO_2} + Y_{H_2O}\right)_{Air}$$
$$\Rightarrow \quad b_{CO_2} + c_{H_2O} + d_{O_2} + e_{N_2} + f_{CO} + g_{NO} + h_{NO_2} + i_{C_xH_y}$$
$$+ j_{SO_2} + k_{N_2O} + l_{H_2} + m_{NH_3} + n_{HCN} + o_{C_{xt}H_{yt}} + p_{Ar} + q_{CO_{2,Air}} + r_{H_2O_{Air}}$$

Equation 1

3.3 Areas of use

Figure 1, Figure 2 and Figure 3 shows schematically the main areas of use for F-A.

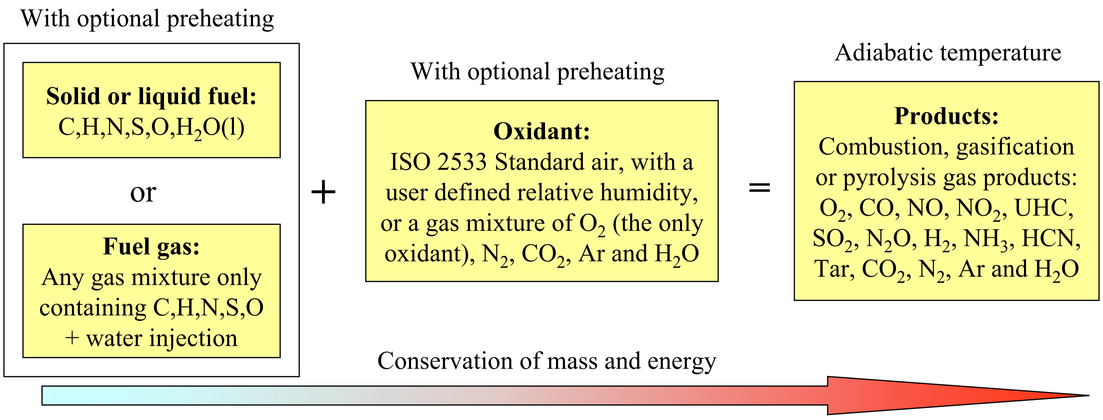

Figure 1 Conservation of mass and energy - schematic overview.

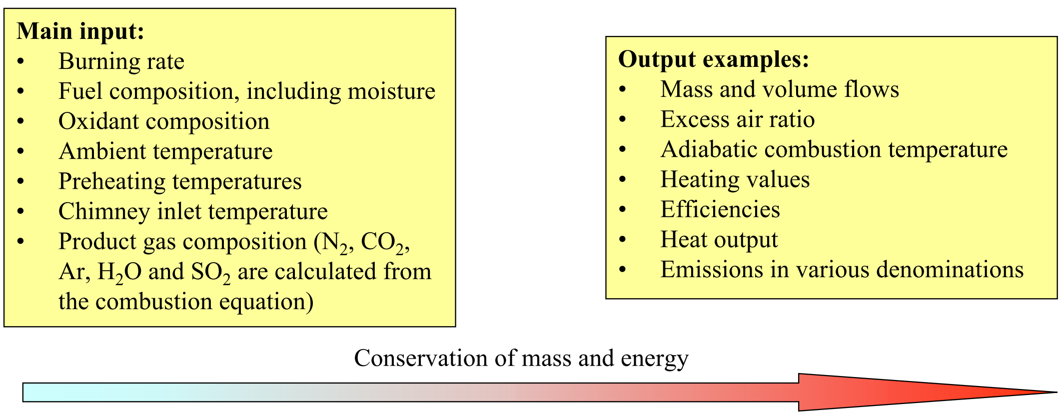

Figure 2 Main input, and output examples.

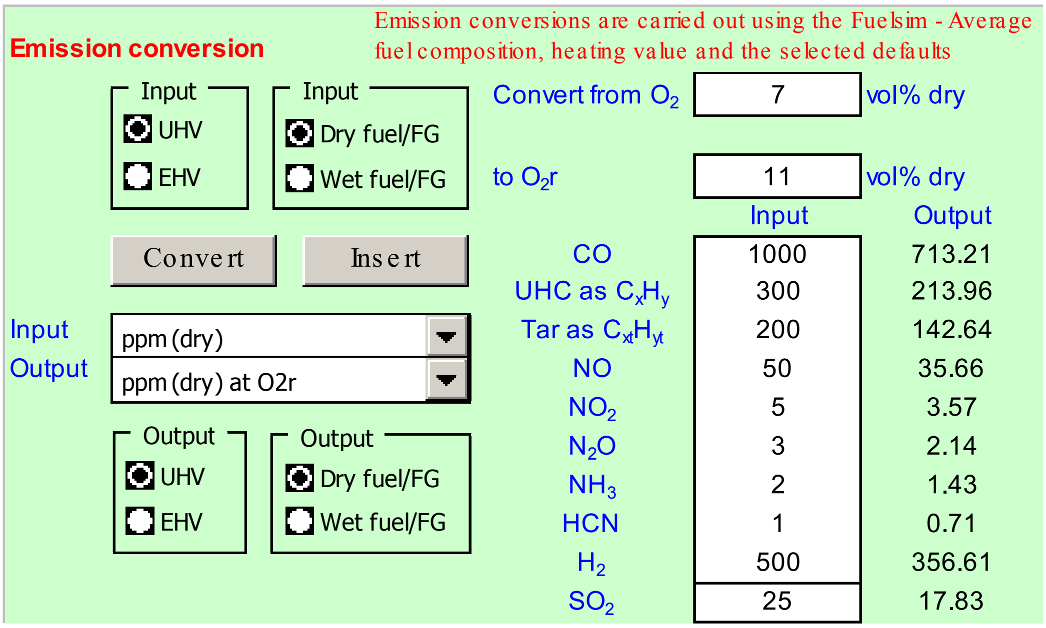

Figure 3 Emission conversion with separate emission conversion module.

3.4 ISO 2533 Standard dry air composition

The oxidant in F-A can be either ISO Standard dry air together with a user-defined relative humidity or a mixture of O_2 (the only oxidant), N_2, H_2O, Ar and CO_2. In the latter case H_2O is user input directly. Figure 4 shows the ISO 2533 Standard dry air composition. F-A uses the ISO 2533 concentration of O_2, N_2 and CO_2, and regards the difference as Ar.

Gas			Content of volume %
Nitrogen	N2		78.084
Oxygen	O2		20.9476
Argon	Ar		0.934
Carbon dioxide	CO2 *		0.0314
Neon	Ne		1.818E-03
Helium	He		5.24E-04
Krypton	Kr		1.14E-04
Xenon	Xe		8.70E-06
Hydrogen	H2		5.00E-05
Nitrogen monoxide	N2O *		5.00E-05
Methane	CH4		2.00E-04
Ozone	O3 summer *	up to	7.00E-06
	O3 winter *	up to	2.00E-06
Sulphur dioxide	SO2 *	up to	1.00E-04
Nitrogen dioxide	NO2 *	up to	2.00E-06
Iodine	I2 *	up to	1.00E-06
Air			**100**

* The content of the gas may undergo significant variations from time to time or from place to place

Figure 4 ISO 2533 Standard air composition - Dry clean air composition near sea level.

3.5 Relative air humidity

Relative air humidity is user input in F-A if ISO Standard air has been selected as oxidant. The relative air humidity is the ratio between the air H_2O concentration at real and saturated conditions. The saturation partial pressure of H_2O in a gas mixture depends only on temperature at a given total pressure. The expression shown in Equation 2 is used, assuming a (atmospheric) total pressure of 1 atm (101325 Pa). It is a curvefit to tabular data provided in Mørstedt and Hellsten [4]. This expression is visualised in Figure 5. As the saturation partial pressure of H_2O increases exponentially with increasing temperature the user should take care to insert the best possible value for the ambient temperature in addition to the relative air humidity. Knowing the relationship between H_2O saturation partial pressure and temperature makes it easy to find the dew point temperature of the flue gas for a specific H_2O partial pressure in the flue gas.

$$p_{H_2O,sat} = e^{\left(\frac{a+c\cdot T_{Amb}}{1+b\cdot T_{Amb}+d\cdot T_{Amb}^2}\right)}, T_{Amb} \text{ in } ^\circ\text{C}$$

$$a = -5.0994261$$

$$b = 0.0042323322$$

$$c = 0.051182703$$

$$d = 0.00000090148628$$

Equation 2

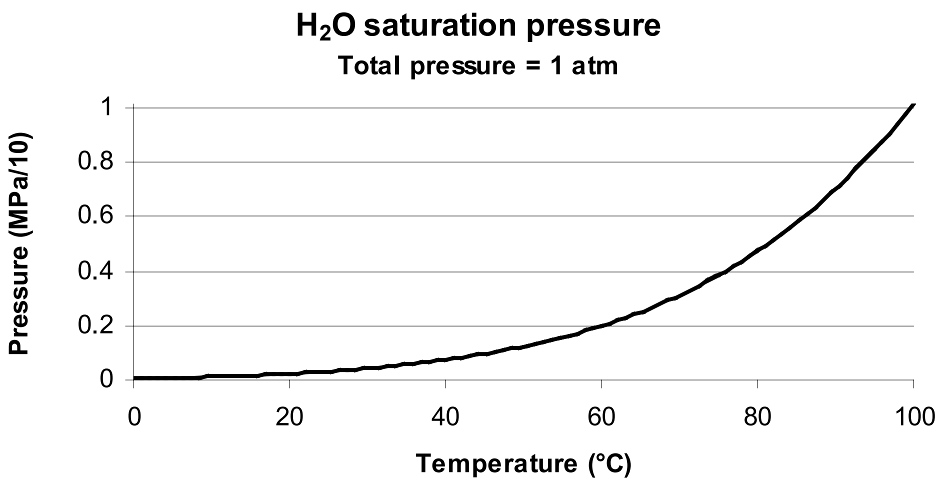

Figure 5 H_2O saturation partial pressure as a function of temperature at a total pressure of 1 atm.

[4] Mørstedt, S.-E. and Hellsten, G. Data och Diagram: Energi- och Kemitekniska Tabeller, Norstedts Tryckeri, Stockholm, 1983.

Appendix 1

Mass, volume and energy balance equations and emission calculations

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Mass, volume and energy balance equations and emission calculations

INPUT VALUES:

X_C - Mass fraction of carbon in dry ash free fuel
X_H - Mass fraction of hydrogen in dry ash free fuel
X_{Ash} - Mass fraction of ash in dry fuel
$X_{H_2O,w}$ - Mass fraction of H_2O in wet ash free fuel
Y_C - Volume fraction of carbon in dry ash free fuel
Y_H - Volume fraction of hydrogen in dry ash free fuel
Y_N - Volume fraction of nitrogen in dry ash free fuel
Y_S - Volume fraction of sulphur in dry ash free fuel
d_{O_2} - O_2 in dry flue gas (vol%)
f_{CO} - CO in dry flue gas (vol%)
g_{NO} - NO in dry flue gas (vol%)
h_{NO_2} - NO_2 in dry flue gas (vol%)
$i_{C_xH_y}$ - UHC (C_xH_y) in dry flue gas (vol%)
k_{N_2O} - N_2O in dry flue gas (vol%)
l_{H_2} - H_2 in dry flue gas (vol%)
m_{NH_3} - NH_3 in dry flue gas (vol%)
n_{HCN} - HCN in dry flue gas (vol%)
$o_{C_{xt}H_{yt}}$ - Tar ($C_{xt}H_{yt}$) in dry flue gas (vol%)
$Y_{O_2,Air}$ - Volume fraction of O_2 in air
$Y_{N_2,Air}$ - Volume fraction of N_2 in air
$Y_{H_2O,Air}$ - Volume fraction of H_2O in air
$Y_{Ar,Air}$ - Volume fraction of Ar in air
$Y_{CO_2,Air}$ - Volume fraction of CO_2 in air
$m_{F,w}$ - Burning rate (kg wet ash free fuel/h)
$m_{H_2O,i}$ - Water injection rate (kg/h)
V_{Mole} - Mole volume (Nm^3/kmole)
T_{Amb} - Ambient temperature (K)
$T_{Air,P}$ - Inlet primary air temperature (K)
$T_{Air,S}$ - Inlet secondary air temperature (K)
T_{Fuel} - Inlet fuel (and moisture) or fuel gas temperature (K)

$T_{H_2O,i}$ - Water for water injection temperature (K)
T_{Ch} - Chimney inlet temperature (K)
Cp_{Fuel} - Specific heat capacity of inlet fuel (kJ/kgK)
P_{Air} - Weight fraction primary air of total air

CONSTANTS:

M_C - Mole weight of carbon (kg/kmole)
M_H - Mole weight of hydrogen (kg/kmole)
M_N - Mole weight of nitrogen (kg/kmole)
M_S - Mole weight of sulphur (kg/kmole)
M_O - Mole weight of oxygen (kg/kmole)
M_{Ar} - Mole weight of argon (kg/kmole)

Mole weights of flue gas species are calculated from the elementary mole weights

Mass, volume and energy balance equations and emission calculations

Combustion equation:

$$a\cdot\left(Y_C+Y_H+Y_O+Y_N+Y_S\right)_{Fuel}+\frac{z}{Y_{O_2}}\cdot\left(Y_{O_2}+Y_{N_2}+Y_{Ar}+Y_{CO_2}+Y_{H_2O}\right)_{Air}$$
$$\Rightarrow\quad b_{CO_2}+c_{H_2O}+d_{O_2}+e_{N_2}+f_{CO}+g_{NO}+h_{NO_2}+i_{C_xH_y}$$
$$+j_{SO_2}+k_{N_2O}+l_{H_2}+m_{NH_3}+n_{HCN}+o_{C_{xt}H_{yt}}+p_{Ar}+q_{CO_{2,Air}}+r_{H_2O_{Air}} \qquad \text{Eq. 1}$$

Elemental balances:

$$z=\frac{100-ceX1+ceX4+\dfrac{ceX6}{2}-\dfrac{ceX9}{ceX8}\cdot\left(Y_C+\dfrac{Y_N}{2}+Y_S\right)}{\dfrac{Y_{N_2,Air}}{Y_{O_2,Air}}+\dfrac{Y_N+2\cdot Y_C+2\cdot Y_S}{ceX8}+ceX2} \qquad \text{Eq. 2}$$

$$a=\frac{2\cdot z+ceX9}{ceX8} \qquad \text{Eq. 3}$$

$$b=a\cdot Y_C-ceX4 \qquad \text{Eq. 4}$$

$$c=\frac{a\cdot Y_H-ceX5}{2} \qquad \text{Eq. 5}$$

$$j=a\cdot Y_S \qquad \text{Eq. 6}$$

$$p=z\cdot\frac{Y_{Ar,Air}}{Y_{O_2,Air}} \qquad \text{Eq. 7}$$

$$q=z\cdot\frac{Y_{CO_2,Air}}{Y_{O_2,Air}} \qquad \text{Eq. 8}$$

$$r=z\cdot\frac{Y_{H_2O,Air}}{Y_{O_2,Air}} \qquad \text{Eq. 9}$$

Dry flue gas balance:

$$e=100-ceX1-b-z\cdot ceX2-j \qquad \text{Eq. 10}$$

where:

$$ceX1=d+f+g+h+i+k+l+m+n+o \qquad \text{Eq. 11}$$

$$ceX2=\frac{\mathrm{Y_{Ar,Air}}+\mathrm{Y_{CO_2,Air}}}{\mathrm{Y_{O_2,Air}}} \qquad \text{Eq. 12}$$

$$ceX4 = f + i \cdot x + n + o \cdot xt \quad \text{Eq. 13}$$

$$ceX5 = i \cdot y + 2 \cdot l + 3 \cdot m + n + o \cdot yt \quad \text{Eq. 14}$$

$$ceX6 = g + h + 2 \cdot k + m + n \quad \text{Eq. 15}$$

$$ceX7 = 2 \cdot d + f + g + 2 \cdot h + k \quad \text{Eq. 16}$$

$$ceX8 = 2 \cdot Y_C + \frac{Y_H}{2} + 2 \cdot Y_S - Y_O \quad \text{Eq. 17}$$

$$ceX9 = 2 \cdot ceX4 + \frac{ceX5}{2} - ceX7 \quad \text{Eq. 18}$$

Combustion equation at stoichiometric conditions:

$$a \cdot \left(Y_C + Y_H + Y_O + Y_N + Y_S\right)_{Fuel} + \frac{z}{Y_{O_2}} \cdot \left(Y_{O_2} + Y_{N_2} + Y_{Ar} + Y_{CO_2} + Y_{H_2O}\right)_{Air}$$
$$\Rightarrow \quad b_{CO_2} + c_{H_2O} + e_{N_2} + j_{SO_2} + p_{Ar} + q_{CO_{2,Air}} + r_{H_2O_{Air}} \quad \text{Eq. 19}$$

Elemental balances:

$$z_S = \frac{100}{\dfrac{Y_{N_2,Air}}{Y_{O_2,Air}} + \dfrac{Y_N + 2 \cdot Y_C + 2 \cdot Y_S}{ceX8} + ceX2} \quad \text{Eq. 20}$$

$$a_S = \frac{2 \cdot \mathrm{z_S}}{\mathrm{ceX8}} \quad \text{Eq. 21}$$

$$b_S = a_S \cdot Y_C \quad \text{Eq. 22}$$

$$c_S = \frac{a_S \cdot Y_H}{2} \quad \text{Eq. 23}$$

$$j_S = a_S \cdot Y_S \quad \text{Eq. 24}$$

$$p_S = z_S \cdot \frac{Y_{Ar,Air}}{Y_{O_2,Air}} \quad \text{Eq. 25}$$

Mass, volume and energy balance equations and emission calculations

$$q_S = z_S \cdot \frac{Y_{CO_2,Air}}{Y_{O_2,Air}} \qquad \text{Eq. 26}$$

$$r_S = z_S \cdot \frac{Y_{H_2O,Air}}{Y_{O_2,Air}} \qquad \text{Eq. 27}$$

Dry flue gas balance:

$$e = 100 - b_S - z_S \cdot ceX2 - j_S \qquad \text{Eq. 28}$$

where:

$ceX2$ and $ceX8$ are given in Eq. 12 and Eq. 17.

MASS AND VOLUME CALCULATIONS:

Volume fraction of oxygen in dry ash free fuel:

$$Y_O = 1 - Y_C - Y_H - Y_N - Y_S \qquad \text{Eq. 29}$$

CO_2 in dry flue gas (vol%):

$$b_{CO_2} = b + q \qquad \text{Eq. 30}$$

N_2 in dry flue gas (vol%):

$$e_{N_2} = e \qquad \text{Eq. 31}$$

SO_2 in dry flue gas (vol%):

$$j_{SO_2} = j \qquad \text{Eq. 32}$$

Stoichiometric CO_2 in dry flue gas (vol%):

$$CO_{2,Max} = b_S + q_s \qquad \text{Eq. 33}$$

Volume dry flue gas produced (Nm^3/h):

$$\text{If } X_C > 0 : V_{FG} = \frac{X_C \cdot V_{Mole}}{M_C \cdot \frac{b + ceX4}{100}} \cdot m_{F,w} \cdot (1 - X_{H_2O,w})$$
$$\text{If } X_C = 0 : V_{FG} = \frac{X_H \cdot V_{Mole}}{M_H \cdot \frac{2 \cdot c + ceX5}{100}} \cdot m_{F,w} \cdot (1 - X_{H_2O,w}) \qquad \text{Eq. 34}$$

Volume dry flue gas produced at stoichiometric conditions (Nm^3/h):

$$\text{If } X_C > 0 : V_{FG,S} = \frac{X_C \cdot V_{Mole}}{M_C \cdot \frac{b_S}{100}} \cdot m_{F,w} \cdot (1 - X_{H_2O,w})$$
$$\text{If } X_C = 0 : V_{FG,S} = \frac{X_H \cdot V_{Mole}}{M_H \cdot \frac{2 \cdot c_S}{100}} \cdot m_{F,w} \cdot (1 - X_{H_2O,w}) \qquad \text{Eq. 35}$$

Volume air added (Nm^3/h):

$$V_{Air} = V_{FG} \cdot \frac{z}{Y_{O_2,Air} \cdot 100} \qquad \text{Eq. 36}$$

Volume air added at stoichiometric conditions (Nm^3/h):

$$V_{Air,S} = V_{FG,S} \cdot \frac{z_S}{Y_{O_2,Air} \cdot 100} \qquad \text{Eq. 37}$$

Excess air ratio:

$$\lambda = \frac{V_{Air}}{V_{Air,S}} \qquad \text{Eq. 38}$$

Volume of water from hydrogen in fuel (Nm^3/h):

$$V_{H_2O,H} = \frac{X_H \cdot V_{Mole}}{2 \cdot M_H} \cdot \left(1 - \frac{ceX5}{a \cdot Y_H}\right) \cdot m_{F,w} \cdot (1 - X_{H_2O,w}) \qquad \text{Eq. 39}$$

Volume of water from water in fuel (Nm^3/h):

$$V_{H_2O,E} = \frac{V_{Mole}}{M_{H_2O}} \cdot m_{F,w} \cdot X_{H_2O,w} \qquad \text{Eq. 40}$$

Volume of water from water vapour in air (Nm^3/h):

$$V_{H_2O,Air} = V_{FG} \cdot \frac{r}{100} \qquad \text{Eq. 41}$$

Volume of water from water injection (Nm^3/h):

$$V_{H_2O,i} = \frac{V_{Mole}}{M_{H_2O}} \cdot m_{H_2O,i} \qquad \text{Eq. 42}$$

Total flue gas volume (Nm^3/h):

$$V_{FG,w} = V_{FG} + V_{H_2O,H} + V_{H_2O,E} + V_{H_2O,Air} + V_{H_2O,i} \qquad \text{Eq. 43}$$

Weight of air added (kg/h):

$$m_{Air} = V_{Air} \cdot \frac{M_{Air}}{V_{Mole}} \qquad \text{Eq. 44}$$

Weight of total flue gas produced (kg/h):

$$m_{FG,w} = m_{Air} + m_{F,w} + m_{H_2O,i} \qquad \text{Eq. 45}$$

Weight of H_2O produced (kg/h):

Mass, volume and energy balance equations and emission calculations

$$m_{H_2O,H} = V_{H_2O,H} \cdot \frac{M_{H_2O}}{V_{Mole}} \qquad \text{Eq. 46}$$

Weight of evaporated water (kg/h):

$$m_{H_2O,E} = m_{F,w} \cdot X_{H_2O,w} \qquad \text{Eq. 47}$$

Volume of single species (Nm^3/h):

$$V_i = V_{FG} \cdot \frac{i}{100} \qquad \text{Eq. 48}$$

$$\text{except: } V_{H_2O} = V_{H_2O,H} + V_{H_2O,E} + V_{H_2O,Air} + V_{H_2O,i}$$

Weight of single species (kg/h):

$$m_i = V_i \cdot \frac{M_i}{V_{Mole}} \qquad \text{Eq. 49}$$

Emissions of NO_X as NO_2 equivalents (mg/kg dry ash free fuel):

$$E_{NO_X} = \frac{m_{NO} \cdot \frac{M_{NO_2}}{M_{NO}} + m_{NO_2}}{m_{F,w} \cdot (1 - X_{H_2O,w})} \cdot 10^6 \qquad \text{Eq. 50}$$

Emissions of UHC (C_xH_y) as CH_4 equivalents (mg/kg dry ash free fuel):

$$E_{C_xH_y} = \frac{m_{C_xH_y} \cdot \frac{x \cdot M_{CH_4}}{M_{C_xH_y}}}{m_{F,w} \cdot (1 - X_{H_2O,w})} \cdot 10^6 \qquad \text{Eq. 51}$$

Emissions of Tar ($C_{xt}H_{yt}$) as CH_4 equivalents (mg/kg dry ash free fuel):

$$E_{C_{xt}H_{yt}} = \frac{m_{C_{xt}H_{yt}} \cdot \frac{xt \cdot M_{CH_4}}{M_{C_{xt}H_{yt}}}}{m_{F,w} \cdot (1 - X_{H_2O,w})} \cdot 10^6 \qquad \text{Eq. 52}$$

Emissions of other single species (mg/kg dry ash free fuel):

$$E_i = \frac{m_i}{m_{F,w} \cdot (1 - X_{H_2O,w})} \cdot 10^6 \qquad \text{Eq. 53}$$

Emissions of NO_X as NO_2 equivalents (mg/Nm^3 dry flue gas):

$$E_{NO_X} = \frac{m_{NO} \cdot \frac{M_{NO_2}}{M_{NO}} + m_{NO_2}}{V_{FG}} \cdot 10^6 \qquad \text{Eq. 54}$$

Emissions of UHC (C_xH_y) as CH_4 equivalents (mg/Nm^3 dry flue gas):

$$E_{C_xH_y} = \frac{m_{C_xH_y} \cdot \frac{x \cdot M_{CH_4}}{M_{C_xH_y}}}{V_{FG}} \cdot 10^6 \qquad \text{Eq. 55}$$

Emissions of Tar ($C_{xt}H_{yt}$) as CH_4 equivalents (mg/Nm^3 dry flue gas):

$$E_{C_{xt}H_{yt}} = \frac{m_{C_{xt}H_{yt}} \cdot \frac{xt \cdot M_{CH_4}}{M_{C_{xt}H_{yt}}}}{V_{FG}} \cdot 10^6 \qquad \text{Eq. 56}$$

Emissions of other single species (mg/Nm^3 dry flue gas):

$$E_i = \frac{m_i}{V_{FG}} \cdot 10^6 \qquad \text{Eq. 57}$$

Conversion factor for fuel-N to NO:

$$\frac{NO}{Fuel-N} = \frac{m_{NO} \cdot M_N}{M_{NO} \cdot X_N \cdot m_{F,w} \cdot (1 - X_{H_2O,w})} \qquad \text{Eq. 58}$$

Conversion factor for fuel-N to NO_2:

$$\frac{NO_2}{Fuel-N} = \frac{m_{NO_2} \cdot M_N}{M_{NO_2} \cdot X_N \cdot m_{F,w} \cdot (1 - X_{H_2O,w})} \qquad \text{Eq. 59}$$

Conversion factor for fuel-N to N_2O:

$$\frac{N_2O}{Fuel-N} = \frac{m_{N_2O} \cdot 2 \cdot M_N}{M_{N_2O} \cdot X_N \cdot m_{F,w} \cdot (1 - X_{H_2O,w})} \qquad \text{Eq. 60}$$

Conversion factor for fuel-N to NO_X:

$$\frac{NO_X}{Fuel-N} = \frac{NO}{Fuel-N} + \frac{NO_2}{Fuel-N} \qquad \text{Eq. 61}$$

EMISSION CONVERSION:

Various denominations are used when reporting emission levels from combustion applications, which makes it difficult to compare emission levels directly. Typical denominations are mg/Nm^3 flue gas at a given vol% O_2 on dry basis (d.b.), ppm in flue gas at a given vol% O_2 (d.b.), mg/kg dry fuel and mg/MJ (based on UHV, or EHV). However, it is possible to convert the reported emission levels to the other denominations by applying the following formulas and procedures for each species:

To: **From:**	A mg/Nm^3 at O_2	B mg/Nm^3 at O_2r	C ppm at O_2	D mg/kg	E mg/MJ
A mg/Nm^3 at O_2	A	$A \cdot X$	$A \cdot \frac{V_{Mole}}{M_i}$	$A \cdot V_{FG}$	$A \cdot \frac{V_{FG}}{UHV}$
B mg/Nm^3 at O_2r	$\frac{B}{X}$	B	$\frac{B}{X} \cdot \frac{V_{Mole}}{M_i}$	$B \cdot V_{FGr}$	$B \cdot \frac{V_{FGr}}{UHV}$
C ppm at O_2	$C \cdot \frac{M_i}{V_{Mole}}$	$C \cdot \frac{M_i}{V_{Mole}} \cdot X$	C	$C \cdot \frac{M_i}{V_{Mole}} \cdot V_{FG}$	$C \cdot \frac{M_i}{V_{Mole}} \cdot \frac{V_{FG}}{UHV}$
D mg/kg	$\frac{D}{V_{FG}}$	$\frac{D}{V_{FGr}}$	$\frac{D}{V_{FG}} \cdot \frac{V_{Mole}}{M_i}$	D	$\frac{D}{UHV}$
E mg/MJ	$E \cdot \frac{UHV}{V_{FG}}$	$E \cdot \frac{UHV}{V_{FGr}}$	$E \cdot \frac{V_{Mole}}{M_i} \cdot \frac{UHV}{V_{FG}}$	$E \cdot UHV$	E

where:

$$X = \frac{V_{FG}}{V_{FGr}} = \frac{100 \cdot Y_{O_2,Air} - O_2 r}{100 \cdot Y_{O_2,Air} - O_2} \qquad \text{Eq. 62}$$

O_2 - vol% O_2 at operating condition

$O_2 r$ - Reference vol% O_2

V_{FG} - Nm^3 dry flue gas pr. kg dry fuel at O_2

V_{FGr} - Nm^3 dry flue gas pr. kg dry fuel at O_2r

V_{Mole} - Mole volume at normal condition [Nm^3/kmole]

M_i - Mole weight of species i [kg/kmole]

UHV - Upper Heating Value [MJ/kg, d.b.], or alternatively EHV - Effective Heating Value

1) Emission conversion: mg/Nm^3 ⇔ ppm, mg/kg ⇔ mg/MJ

The conversion between mg/Nm^3 and ppm, and between mg/kg and mg/MJ, is straightforward.

2) Emission conversion: mg/Nm^3, ppm ⇒ mg/kg, mg/MJ

For conversion between volumetric- and mass units the flue gas volume produced pr. kg dry fuel is needed. The flue gas volume produced pr. kg dry fuel, assuming that carbon is converted to CO_2, CO, UHC (C_xH_y), Tar ($C_{xt}H_{yt}$) and HCN, is given by:

$$V_{FG} = \frac{X_C \cdot V_{Mole}}{M_C \cdot \left(\frac{CO_2 + CO + x \cdot C_x H_y + xt \cdot C_{xt} H_{yt} + HCN}{100} \right)}, \text{ at } O_2 \qquad \text{Eq. 63}$$

where:

X_C - mass fraction of carbon in dry ash free fuel

CO_2, CO, C_xH_y, $C_{xt}H_{yt}$ and HCN - vol% in dry flue gas at O_2

Since the emission level of CO and/or H_2, UHC, Tar, NO, NO_2, N_2O, NH_3, HCN are given in volumetric units at O_2, CO_2 is the only remaining species that needs to be calculated, using Eq. 2, Eq. 3 and Eq. 4. A representative dry fuel composition must be assumed if the fuel composition is not stated. If the fuel do not contain carbon, hydrogen can be used as basis instead, similar to Eq. 34.

3) Emission conversion: mg/Nm^3 at O_2 ⇒ mg/Nm^3 at O_2r

For conversion from mg/Nm^3 at a given vol% O_2 to another reference vol% O_2 (O_2r) we need to calculate the flue gas volume produced pr. kg dry fuel at O_2r. This can be done by considering the conversion as a dilution process where air is added or removed until O_2 equals O_2r. The following can be derived:

$$V_{FGr} = \frac{X_C \cdot V_{Mole}}{M_C \cdot \left(\frac{CO_2 r + COr + x \cdot C_x H_y r + xt \cdot C_{xt} H_{yt} r + HCNr}{100} \right)}, \text{ at } O_2 r \qquad \text{Eq. 64}$$

where:

$CO_2 r$, COr, $C_x H_y r$, $C_{xt} H_{yt} r$ and $HCNr$ - vol% in dry flue gas at O_2r

$$CO_2 r = CO_2 \cdot \frac{100}{\alpha}, \quad COr = CO \cdot \frac{100}{\alpha}, \quad C_x H_y r = C_x H_y \cdot \frac{100}{\alpha}$$

$$C_{xt} H_{yt} r = C_{xt} H_{yt} \cdot \frac{100}{\alpha}, \quad HCNr = HCN \cdot \frac{100}{\alpha}$$

where:

$$\alpha = 100 + dil \cdot \frac{z}{Y_{O_2,Air}} \cdot (1 - Y_{H_2O,Air}) = \frac{100}{X}$$

X is calculated from Eq. 62

$$dil = \frac{O_2 - O_2 r}{\frac{O_2 r}{100} \cdot z \cdot \left(\frac{Y_{CO_2,Air} + Y_{Ar,Air} + Y_{N_2,Air}}{Y_{O_2,Air}} + 1 \right) - z}$$

z is calculated from Eq. 2

However, while the coefficient *z,* and subsequently *dil*, changes with degree of burnout and fuel composition, the coefficient α does not. Hence, the ratio between the flue gas flow at O_2 and O_2r, X, is only dependent on these O_2 levels according to Eq. 62. This relationship can be derived from the combustion equation, as the ratio between the flue gas flow at O_2 and O_2r. In emission conversion cases where only V_{FG} or V_{FGr} are needed, Eq. 63 and Eq. 64 must be used, respectively. However, V_{FGr} can be calculated from Eq. 62 if V_{FG} is known.

4) Emission conversion: mg/kg, mg/MJ ⇒ mg/Nm^3, ppm

For conversion from mg/kg or mg/MJ to mg/Nm^3 or ppm at O_2 we need to calculate the flue gas volume produced pr. kg dry fuel at O_2. However, this is not straightforward and must be solved by an iteration procedure:

Step 1: Calculate CO_2 at O_2, not including CO, H_2, UHC, Tar, NO, NO_2, N_2O, NH_3 and HCN, hereafter called minor species
Step 2: Calculate V_{FG} at O_2
Step 3: Calculate mg/Nm^3 or ppm of minor species
Step 4: Calculate CO_2 at O_2, including minor species
Step 5: Calculate V_{FG} at O_2
Step 6: Calculate mg/kg or mg/MJ of minor species
Step 7: Go to Step 3 and repeat the iteration procedure until the emission levels calculated in Step 6 have converged to the reported emission levels in mg/kg or mg/MJ.

5) Emission conversion: SO_2, particles and trace compounds

As a significant fraction of the sulphur content in the fuel may be retained in the ashes, the dry flue gas flow should ideally be calculated using a dry fuel composition with a reduced sulphur content, equivalent to the sulphur content emitted as SO_2 (and other gaseous sulphur compounds). However, since the sulphur contents in most biomass fuels are low, this is usually not necessary.

Particle emission levels from biomass combustion applications can be quite high, especially from small-scale biomass combustion applications. Particle emissions can be divided into both emissions from complete- and incomplete combustion. As for SO_2, the amount of C, H,

O, N and S emitted as particles should ideally be corrected for in the dry fuel composition when calculating the dry flue gas flow. However, this is not necessary if the particle emission level is low.
Emissions of trace compounds can safely be neglected when calculating the dry flue gas flow, since these emission levels do not significantly influence the calculated dry flue gas flow.

ENERGY CALCULATIONS:

Upper Heating Value of solid fuel [1] (MJ/kg dry ash free fuel):

$$UHV = ((34.91 \cdot X_C + 117.83 \cdot X_H - 10.34 \cdot X_O + 10.05 \cdot X_S - 1.51 \cdot X_N) \cdot (1 - X_{Ash}) - 2.11 \cdot X_{Ash}) / (1 - X_{Ash}) \qquad \text{Eq. 65}$$

Upper Heating Value of gaseous fuel is calculated from its composition and enthalpy expressions for the involved species. Upper Heating Value of a liquid fuel should be inserted manually.

Upper Heating Value of fuel (MJ/kg wet fuel):

$$UHV,w = UHV \cdot (1 - X_{H_2O,w}) \qquad \text{Eq. 66}$$

Effective Heating Value of fuel (MJ/kg wet fuel):

$$EHV = UHV,w - \frac{H_{H_2O,g}^{T_{Amb}} - H_{H_2O,l}^{T_{Amb}}}{1000} \cdot \frac{m_{H_2O,H} + m_{H_2O,E}}{m_{F,w}} \qquad \text{Eq. 67}$$

where enthalpies for water vapour and water at ambient temperature are calculated from polynomial expressions.

Generated gross heat based on UHV and EHV (MJ/h):

$$Q_{UHV} = m_{F,w} \cdot UHV,w \qquad Q_{EHV} = m_{F,w} \cdot EHV \qquad \text{Eq. 68}$$

Total heat input based on UHV (MJ/h):

$$\begin{aligned} Q_{UHV,t} = Q_{UHV} + [&m_{H_2O,E} \cdot Cp_{H_2O,l} \cdot (T_{Fuel} - T_{Amb}) \\ &+ m_{H_2O,i} \cdot Cp_{H_2O,l,i} \cdot (T_{H_2O,i} - T_{Amb}) \\ &+ (m_{F,w} - m_{H_2O,E}) \cdot Cp_{Fuel} \cdot (T_{Fuel} - T_{Amb}) \\ &+ m_{Air} \cdot P_{Air} \cdot Cp_{Air,P} \cdot (T_{Air,P} - T_{Amb}) \\ &+ m_{Air} \cdot (1 - P_{Air}) \cdot Cp_{Air,S} \cdot (T_{Air,S} - T_{Amb})] / 1000 \end{aligned} \qquad \text{Eq. 69}$$

where specific heat capacities for water in inlet fuel, water for water injection, primary air, secondary air and fuel gas are calculated from polynomial expressions based on the given preheating temperatures and species compositions. Specific heat capacity of a solid or liquid fuel is an input value.

[1] GAUR, S. & REED, T.B. An Atlas of Thermal Data for Biomass and Other Fuels, NREL/TB-433-7965, UC Category:1310, DE95009212.

Thermal efficiency based on UHV:

$$\eta_{th,UHV} = \frac{Q_{UHV,t} - \frac{Cp_{FG} \cdot m_{FG,w} \cdot (T_{Ch} - T_{Amb})}{1000}}{Q_{UHV,t}} \qquad \text{Eq. 70}$$

Combustion efficiency based on UHV:

$$\eta_{c,UHV} = \frac{UHV,w - \frac{q_{loss}}{1000}}{UHV,w} \qquad \text{Eq. 71}$$

where q_{loss} (kJ/kg fuel) is calculated from the enthalpies and amount of unburned species.

Total efficiency based on UHV:

$$\eta_{t,UHV} = \frac{Q_{UHV,t} - \frac{Cp_{FG} \cdot m_{FG,w} \cdot (T_{Ch} - T_{Amb})}{1000} - \frac{q_{loss}}{1000} \cdot m_{F,w}}{Q_{UHV,t}} \qquad \text{Eq. 72}$$

where specific heat capacity for the flue gas is a weighted mean value between chimney inlet temperature and ambient temperature for the given flue gas composition.

Efficiencies based on EHV is found by replacing QUHV with QEHV and UHV,w with EHV.

Adiabatic combustion temperature is found by a iteration procedure, where energy in balances energy out.

Generated net heat based on UHV and EHV (MJ/h):

$$Q_{UHV,net} = Q_{UHV} \cdot \eta_{c,UHV} \qquad Q_{EHV,net} = Q_{EHV} \cdot \eta_{c,EHV} \qquad \text{Eq. 73}$$

Gross heat output based on UHV and EHV (kW):

$$P_{UHV} = \frac{Q_{UHV,net}}{3.6} \qquad P_{EHV} = \frac{Q_{EHV,net}}{3.6} \qquad \text{Eq. 74}$$

Net heat output based on UHV and EHV (kW):

$$P_{UHV,net} = P_{UHV} \cdot \eta_{th,UHV} \qquad P_{EHV,net} = P_{EHV} \cdot \eta_{th,EHV} \qquad \text{Eq. 75}$$

Appendix 2

Fuelsim - Average introduction

Øyvind Skreiberg

August 2002

Fuelsim - Average v1.1
introduction

by

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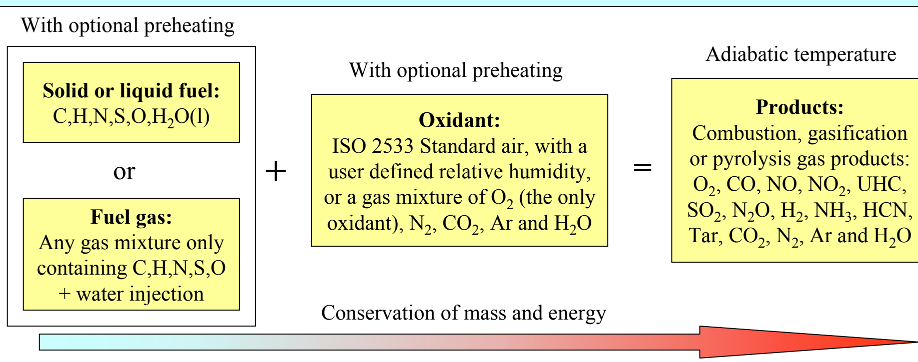
Documentation for v1.1 of Fuelsim - Average

Fuelsim - Average is a relatively simple, but useful, mass, volume and energy balance spreadsheet for continuous combustion applications, but can also be used for other thermal conversion processes where solid fuel is converted to a fuel gas mixture of O_2, CO, NO, NO_2, UHC (unburned hydrocarbons), SO_2, N_2O, H_2, NH_3, HCN, Tar, CO_2, N_2, Ar and H_2O.

The fuel can either be a solid fuel, a liquid fuel or a fuel gas, and the oxidant can either be ISO 2533 Standard air, with a user defined relative humidity, or a gas mixture of O_2 (the only oxidant), N_2, CO_2, Ar and H_2O.

Preheating, relative to an ambient temperature, of solid or liquid fuel (including moisture content), fuel gas, water for water injection and oxidant (separated into primary and secondary air) is possible. The temperature of the products is calculated assuming adiabatic conditions (no heat loss).



Fuelsim - Average uses thermodynamic data on CHEMKIN format for all gas species and also liquid water, while the specific heat capacity of a solid or liquid fuel is user defined. The heating value of a fuel gas is calculated directly from the thermodynamic data, while the heating value of a solid fuel is estimated from the elemental composition using an empirical expression. However, the heating value may also be inserted manually. The heating value of a liquid fuel should be inserted manually.

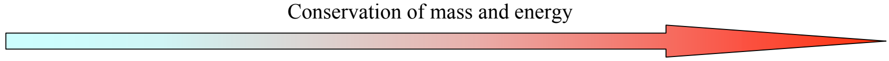
The user may add new fuel gas species, including accompanying thermodynamic data on CHEMKIN format.

Thermal efficiency (using a user defined chimney inlet temperature), combustion efficiency and total efficiency are calculated, together with further useful mass, volume and energy balance output.

Main input:
- Burning rate
- Fuel composition, including moisture
- Oxidant composition
- Ambient temperature
- Preheating temperatures
- Chimney inlet temperature
- Product gas composition (N_2, CO_2, Ar, H_2O and SO_2 are calculated from the combustion equation)

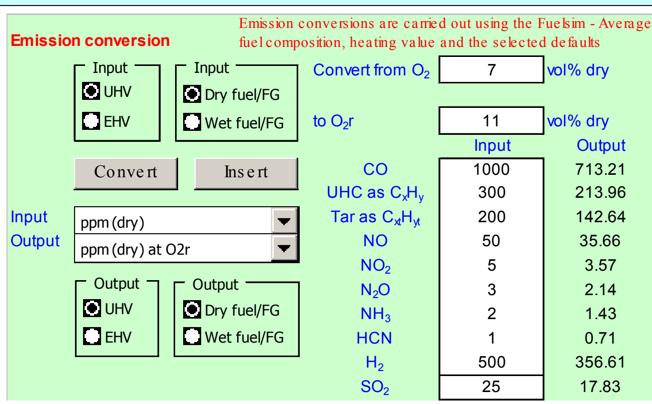
Output examples:
- Mass and volume flows
- Excess air ratio
- Adiabatic combustion temperature
- Heating values
- Efficiencies
- Heat output
- Emissions in various denominations

Conservation of mass and energy



Fuelsim - Average calculates emissions in various denominations based on the user input. However, also a separate emission conversion section is included, where emission values in various denominations can be inserted and converted between the various denominations. The corresponding emission levels in volume fractions can be inserted into the Fuelsim - Average main calculations and additional useful information is then calculated.

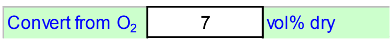
The emission conversion procedure is based directly on the combustion equation, no simplified expressions are applied. When converting emission levels between different oxygen concentrations, the defined oxidant is added to, or removed from, the given flue gas composition until the calculated oxygen concentration equals the reference oxygen concentration.



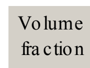
Fuelsim - Average is an Excel spreadsheet and uses programmed functions and procedures in addition to formulas inserted directly in the spreadsheet cells. The user interface consists of input cells (marked with the colour white) various push-buttons (marked with the colour grey), input forms (revealed when pushing a push-button), option-buttons (black: option is selected, white: option is not selected) and pull-down menus. Cells marked with the colour green are not user changeable.

The spreadsheet is protected to prevent accidental deletion of cell contents or objects. Formulas (only in the Average sheet), functions and procedures can not be seen by the user. However, all cells are selectable when using for example the Goal Seek command in Excel and other spreadsheets/sheets can refer to cells in the Average sheet. Also, additional sheets can be inserted into the Fuelsim - Average spreadsheet.

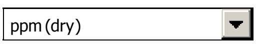
Input cell:



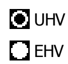
Push-button:



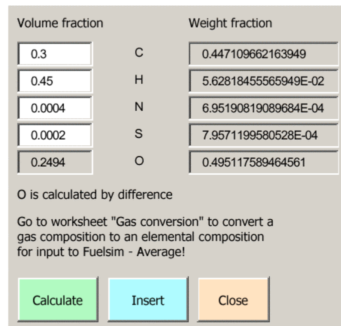
Pull-down menu:



Option-button:



Input box:



Further information can be found in the documentation (push the Documentation push-button) and illustrative examples can be found by pushing the Examples push-button.

Please direct questions, comments or proposals for improvements to Øyvind Skreiberg, The Norwegian University of Science and Technology, Institute of Thermal Energy and Hydropower, N-7491 Trondheim, Norway, e-mail: oesite@tev.ntnu.no

The Fuelsim - Average spreadsheet is an add-on to Chapter 2 - Basic principles of biomass combustion, in the "Handbook of Biomass Combustion and Co-Firing", which was compiled in a joint effort by the country representatives in the IEA Task 32 - Biomass Combustion and Cofiring. The handbook can be ordered at, and possible updates to the Fuelsim - Average spreadsheet can be downloaded from, the Task 32 www-site. Go to:

http://www.ieabioenergy-task32.com/

Appendix 3

Fuelsim - Average documentation

Øyvind Skreiberg

August 2002

NTNU **Institute of thermal energy and hydropower**

Fuelsim - Average v1.1
documentation

by

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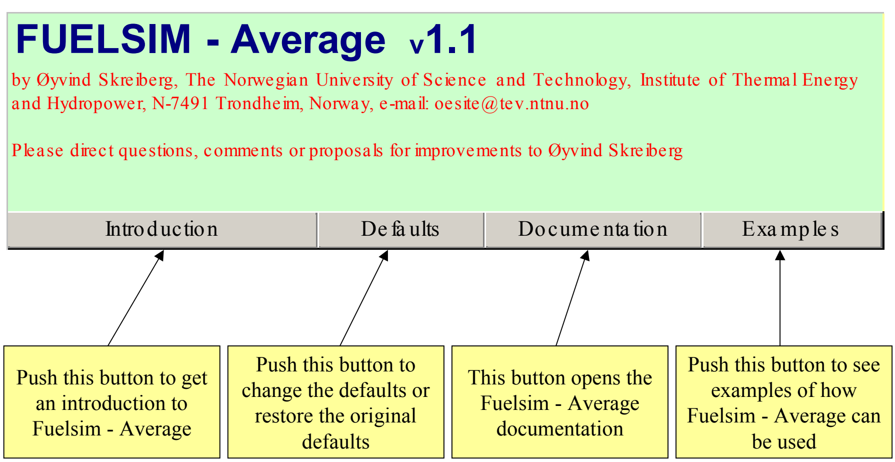
Documentation for v1.1 of Fuelsim - Average



Fuelsim - Average uses elementary weight fractions as fuel composition input. The elementary weight fractions are either inserted directly, calculated from elementary volume fractions or calculated from a fuel gas composition which can be inserted in the sheet “Gas conversion”.

Fuel and flue gas (FG) properties

Fuel composition (weight fraction, daf)
(Moisture: waf)

Volume fraction

C	H	O
0.5000	0.0600	0.4388
0.0007	0.1800	0.0005
N	H_2O	S

- C = Carbon (daf)
- H = Hydrogen (daf)
- O = Oxygen (daf)
- N = Nitrogen (daf)
- S = Sulphur (daf)
- H_2O = Moisture (waf)

daf = dry ash free
waf = wet ash free

Push this button to insert volume fractions instead

Weight fractions can be inserted directly in the cells marked with white colour

Oxygen is calculated by difference

Volume fraction		Weight fraction
0.3	C	0.447109662163949
0.45	H	5.62818455565949E-02
0.0004	N	6.95190819089684E-04
0.0002	S	7.9571199580528E-04
0.2494	O	0.495117589464561

O is calculated by difference

Go to worksheet "Gas conversion" to convert a gas composition to an elemental composition for input to Fuelsim - Average!

Calculate | Insert | Close

- Insert volume fractions in fields marked with white colour
- Push the “Calculate” button
- Push the “Insert” button to insert the calculated weight fractions into Fuelsim - Average
- Push the “Close button” to go back to Fuelsim - Average

Fuelsim - Average uses a “measured” dry flue gas composition as input. Hence, emissions are not estimated in any way. The flue gas composition is inserted on volume basis using ppm (parts per million), except for O_2, CO and H_2, where volume percent (vol%) is used.

Burning rate is always inserted as kg wet fuel per hour

Burning rate kg/h (dry / wet fuel) & kg/s (wet fuel)	1.640	2.000	5.556E-04
Water injection rate kg/h & kg/s		0.000	0.000E+00
O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0651	7.0000	70000
CO in wet / dry FG (vol%) & ppm (dry FG)	0.08664	0.10000	1000.0
NO in wet / dry FG (ppm)	43.322	50.000	Insert wet FG comp.
NO_2 in wet / dry FG (ppm)	4.332	5.000	
UHC as C_xH_y in wet / dry FG (ppm)	259.931	300.000	
SO_2 in wet / dry FG (ppm)	45.270	52.248	
N_2O in wet / dry FG (ppm)	2.599	3.000	
H_2 in wet / dry FG (vol%) & ppm (dry FG)	0.04332	0.05000	500.0
NH_3 in wet / dry FG (ppm)	1.733	2.000	
HCN in wet / dry FG (ppm)	0.866	1.000	
Tar as $C_{xt}H_{yt}$ in wet / dry FG (ppm)	173.288	200.000	

Unburned hydrocarbons (UHC) and Tar can be defined as any hydrocarbon species by changing the default values for x and y or xt and yt, respectively

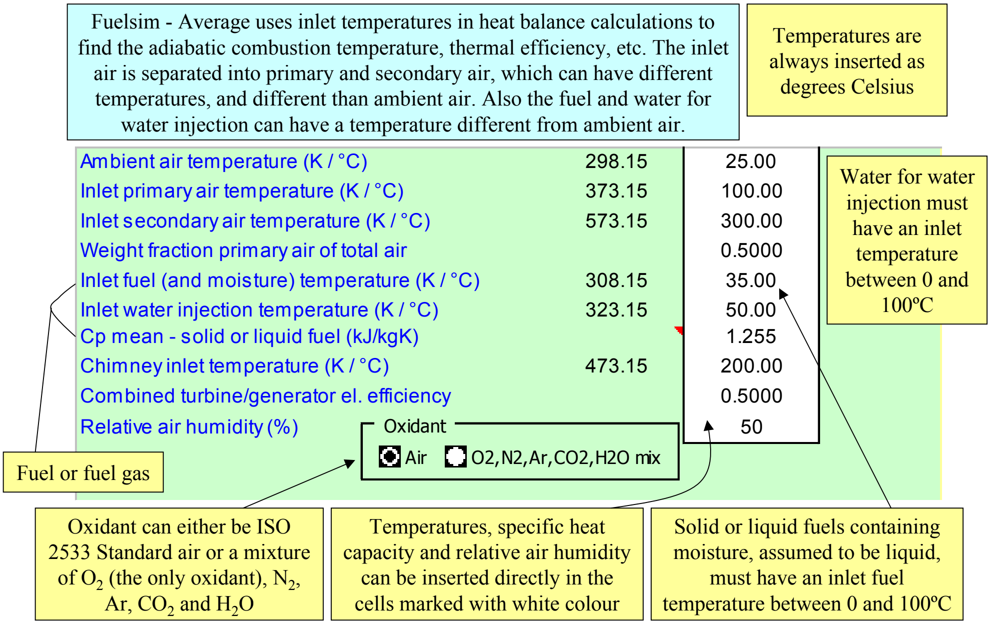
Dry flue gas composition on volume basis can be inserted directly in the cells marked with white colour

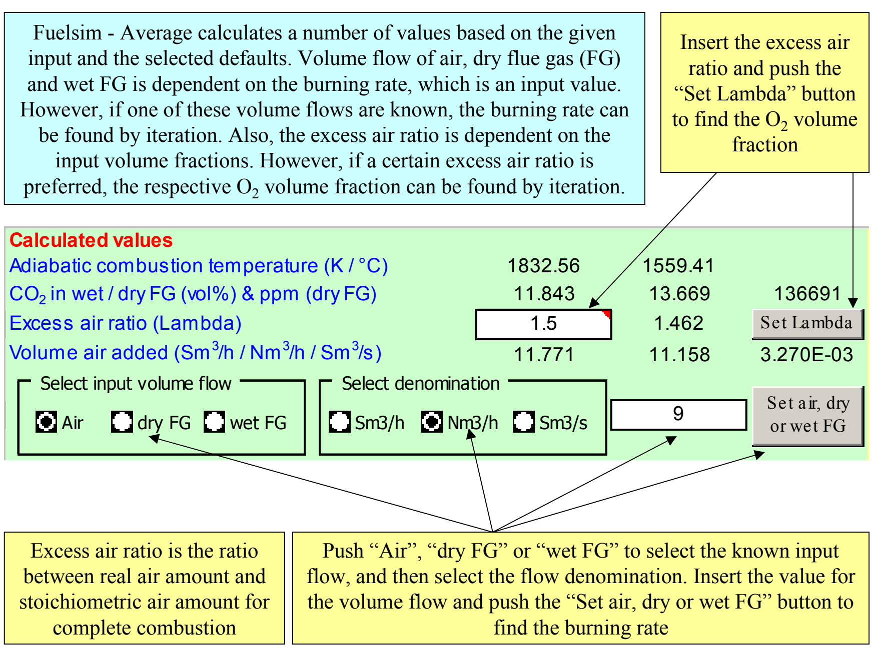
Push this button to insert a wet flue gas composition instead

Wet FG		Dry FG
7	O2 (vol%)	8.0095405104611
0.1	CO (vol%)	0.114422007292301
40	NO (ppm)	45.7688029169205
4	NO2 (ppm)	4.57688029169206
240	CxHy (ppm)	274.612817501523
2.5	N2O (ppm)	2.86055018230753
0.04	H2 (vol%)	4.57688029169205E-02
2	NH3 (ppm)	2.28844014584603
1	HCN (ppm)	1.14422007292301
160	Tar (ppm)	183.075211667682

Calculate Insert Close

- Insert wet flue gas composition
- Push the “Calculate” button
- Push the “Insert” button to insert the calculated dry flue gas composition into Fuelsim - Average
- Push the “Close button” to go back to Fuelsim - Average


Fuelsim - Average uses inlet temperatures in heat balance calculations to find the adiabatic combustion temperature, thermal efficiency, etc. The inlet air is separated into primary and secondary air, which can have different temperatures, and different than ambient air. Also the fuel and water for water injection can have a temperature different from ambient air.
Temperatures are always inserted as degrees Celsius
Ambient air temperature (K / °C) 298.15 25.00
Inlet primary air temperature (K / °C) 373.15 100.00
Inlet secondary air temperature (K / °C) 573.15 300.00
Weight fraction primary air of total air 0.5000
Inlet fuel (and moisture) temperature (K / °C) 308.15 35.00
Inlet water injection temperature (K / °C) 323.15 50.00
Cp mean - solid or liquid fuel (kJ/kgK) 1.255
Chimney inlet temperature (K / °C) 473.15 200.00
Combined turbine/generator el. efficiency 0.5000
Relative air humidity (%) 50
Oxidant
Air
O2,N2,Ar,CO2,H2O mix
Water for water injection must have an inlet temperature between 0 and 100ºC
Fuel or fuel gas
Oxidant can either be ISO 2533 Standard air or a mixture of O2 (the only oxidant), N2, Ar, CO2 and H2O
Temperatures, specific heat capacity and relative air humidity can be inserted directly in the cells marked with white colour
Solid or liquid fuels containing moisture, assumed to be liquid, must have an inlet fuel temperature between 0 and 100ºC


Fuelsim - Average calculates a number of values based on the given input and the selected defaults. Volume flow of air, dry flue gas (FG) and wet FG is dependent on the burning rate, which is an input value. However, if one of these volume flows are known, the burning rate can be found by iteration. Also, the excess air ratio is dependent on the input volume fractions. However, if a certain excess air ratio is preferred, the respective O2 volume fraction can be found by iteration.
Insert the excess air ratio and push the "Set Lambda" button to find the O2 volume fraction
Calculated values
Adiabatic combustion temperature (K / °C) 1832.56 1559.41
CO2 in wet / dry FG (vol%) & ppm (dry FG) 11.843 13.669 136691
Excess air ratio (Lambda) 1.5 1.462
Set Lambda
Volume air added (Sm3/h / Nm3/h / Sm3/s) 11.771 11.158 3.270E-03
Select input volume flow
Air
dry FG
wet FG
Select denomination
Sm3/h
Nm3/h
Sm3/s
9
Set air, dry or wet FG
Excess air ratio is the ratio between real air amount and stoichiometric air amount for complete combustion
Push "Air", "dry FG" or "wet FG" to select the known input flow, and then select the flow denomination. Insert the value for the volume flow and push the "Set air, dry or wet FG" button to find the burning rate

Fuelsim - Average calculates the volume of dry and wet flue gas produced. Also, if the fuel type is "Gas" then the volume of fuel gas is calculated from the fuel gas composition and mole weight.

Volume dry FG produced (Sm^3/h / Nm^3/h / Sm^3/s)	11.573	10.971	3.215E-03
+ Volume of water vapour from H (Nm^3/h)		1.069	
+ Volume of water vapour from H_2O in fuel (Nm^3/h)		0.448	
+ Volume of water vapour from H_2O in air (Nm^3/h)		0.174	
+ Volume of water vapour from water injection (Nm^3/h)		0.000	
= Total FG volume (Sm^3/h / Nm^3/h / Sm^3/s)	13.357	12.662	3.710E-03
Volume fuel gas (Sm^3/h / Nm^3/h / Sm^3/s)	NA	NA	NA
Mole weight of fuel gas (kg/kmole)		NA	

Fuel type: Solid or liquid / Gas

Push "Solid or liquid" or "Gas" to select the fuel type

"NA" means not applicable for solid or liquid fuels

Fuelsim - Average calculates the weight of dry and wet flue gas produced. Mass flow of air, dry flue gas (FG) and wet FG is dependent on the burning rate, which is an input value. However, if one of these mass flows are known, the burning rate can be found by iteration.

Weight of water vapour from H (kg/h)	0.859	
Weight of water vapour from H_2O (kg/h)	0.360	
Weight of air added (kg/h / kg/s)	14.334	3.982E-03
Weight of total FG produced (kg/h / kg/s)	16.334	4.537E-03
Weight of dry FG produced (kg/h / kg/s)	14.975	4.160E-03

Select input mass flow: Air / dry FG / wet FG

Select denomination: kg/h / kg/s

12

Set air, dry or wet FG

Push "Air", "dry FG" or "wet FG" to select the known input flow, and then select the flow denomination. Insert the value for the mass flow and push the "Set air, dry or wet FG" button to find the burning rate

Fuelsim - Average calculates the upper heating value of solid fuels based on an empirical expression, which includes ash, and for gas fuels based on thermodynamic data. Alternatively, the heating value can also be inserted manually. The heating value of a liquid fuel should be inserted manually. Also thermal efficiency, combustion efficiency and total efficiency is calculated.

Push "Empirical" to select the empirical expression for UHV

Weigth fraction of ash in dry fuel / total ash (g/h)	0.005	8.241
Upper Heating Value of fuel (MJ/kg, daf)	19.981	Empirical
Upper Heating Value of fuel (MJ/kg, waf)	16.384	
Effective Heating Value of fuel (MJ/kg, waf)	14.870	
Thermal efficiency, UHV / EHV	0.913	0.904
Combustion efficiency, UHV / EHV	0.975	0.972
Total efficiency, UHV / EHV	0.889	0.879

1 minus thermal efficiency is the ratio between heat loss to the surroundings through the chimney and total energy input to the combustion chamber

1 minus combustion efficiency is the ratio between heat loss due to incomplete combustion and the heating value of the fuel

UHV / EHV:
Upper or Effective Heating Value is used as the heating value of the fuel

Total efficiency is the total energy input minus chimney heat loss and loss due to incomplete combustion, divided by the total energy input

Fuelsim - Average calculates generated heat, and heat output OR power output.

UHV / EHV:
Upper or Effective Heating Value is used as the heating value of the fuel

Generated heat (MJ/h), UHV, Net / Gross	31.934	32.769
Generated heat (MJ/h), EHV, Net / Gross	28.906	29.740
Heat output (kW), UHV, Net / Gross	8.095	8.871
Heat output (kW), EHV, Net / Gross	7.261	8.029
Power output (kW) based on net EHV and el. efficiency	4.015	

Net / Gross - Generated heat:
Gross generated heat is the total generated heat based on UHV or EHV, assuming complete combustion
Net generated heat = Gross generated heat minus heat loss due to incomplete combustion

Net / Gross - Heat output:
Gross heat output is the total heat output based on UHV or EHV minus heat loss due to incomplete combustion
Net heat output = Gross heat output minus chimney heat loss

Power output is based on "Generated heat (MJ/h), EHV, Net" and "Combined turbine/generator el. efficiency"

Fuelsim - Average calculates conversion factors, the fraction of fuel elements that is converted to specific gas species.

Conversion factors		
Fuel-N to NO / NO2	0.299	0.030
Fuel-N to N_2O	0.036	
Fuel-N to NH_3 / HCN	0.012	0.006
Fuel-N to NO_X / TFN	0.328	0.382
Fuel-C to CO	0.00717	
Fuel-C to C_xH_y / $C_{xt}H_{yt}$	0.00645	0.00860
Fuel-H to H_2 / Fuel-S to SO_2	0.00501	1

NO_X = sum of NO and NO_2
TFN = Total Fixed nitrogen
= $NO_X + N_2O + NH_3$ + HCN

The conversion factor for sulphur (S) to SO_2 will always be unity since the SO_2 emission level is calculated directly from the fuel composition, assuming that all S is converted to SO_2

Fuelsim - Average calculates the mole volume and the respective density for air or oxidant mixture at the defined normal and standard condition.

Mole volume (Nm^3/kmole / Sm^3/kmole)	22.414	23.644
Air or oxidant mixture density (kg/Nm^3 / kg/Sm^3)	1.285	1.218

Fuelsim - Average calculates the flue gas energy balance to illustrate and analyse where the energy goes at both adiabatic combustion temperature and at chimney inlet temperature.

Where does the energy go?

at temperature: (●) Adiabatic ( ) Chimney inlet

Water in fuel:	MJ/kg wet fuel	
Heat of evaporation for H_2O in fuel	0.440	2.49 %
+ Heating of water vapour from H_2O in fuel	0.644	3.64 %
Heat of evaporation for H_2O from water injection	0.000	0.00 %
+ Heating of water vapour from H_2O from water injection	0.000	0.00 %
=	1.084	6.13 %

Dry fuel and (wet) air:

Heat of evaporation is heat needed for phase change from water to water vapour, and can only be recovered when the water vapour condenses

Heating of water vapour includes subsequent heating of water vapour originating from water in fuel or water injection

Where does the energy go? (continued).

Dry fuel and (wet) air:		
Heat of evaporation for water from H in fuel	1.050	5.93 %
+ Heating of water vapour from H in fuel and air	1.788	10.11 %
+ N_2	9.592	54.22 %
+ CO_2	2.722	15.39 %
+ O_2	0.906	5.12 %
+ CO	0.012	0.070 %
+ C_xH_y as CH_4	0.022	0.127 %
+ $C_{xt}H_{yt}$ as C_6H_6	0.015	0.086 %
+ NO	0.001	0.004 %
+ NO_2	0.000	0.001 %
+ N_2O	0.000	0.000 %
+ NH_3	0.000	0.000 %
+ HCN	0.000	0.000 %
+ H_2	0.006	0.033 %
+ SO_2	0.001	0.006 %
+ Ar	0.073	0.414 %
=	16.189	91.51 %

As for water in fuel, water vapour formed from hydrogen in the fuel demands phase change energy and energy for subsequent heating of the water vapour. Also heating of water vapour originating from the air is included here

All dry flue gas species conserves energy when heated, through their specific heat capacity

Where does the energy go? (continued).

Incomplete combustion	0.417	2.36 %
Total	17.691	100.00 %
of this accounts external preheating of primary air for	0.273	1.54 %
and external preheating of secondary air for	1.016	5.74 %
and external preheating of wet fuel for	0.018	0.10 %
and external preheating of water for water injection for	0.000	0.00 %

Fuel or fuel gas

Incomplete combustion means conservation of chemically bound energy in fuel gas species which have not been completely converted in the combustion process, and represents a heat loss

External preheating of primary and/or secondary air increase the total energy input to the combustion chamber, as do external preheating of the fuel or water for water injection

Fuelsim - Average calculates the mean specific heat capacity in a temperature interval, in this case between water at inlet fuel and water injection temperature respectively and ambient temperature, and between primary and secondary air at their respective inlet temperatures and ambient temperature. These values are used in the heat balance calculations.

Cp mean - Water, at inlet fuel / water injection temperature (kJ/kgK)	4.178	4.177
Cp mean - Inlet primary / secondary air (kJ/kgK)	1.016	1.030

Fuelsim - Average calculates the mean specific heat capacity in a temperature interval, in this case between the chimney inlet temperature and the ambient temperature, for all flue gas species as well as for the flue gas. The mean specific heat capacity times the temperature difference equals the enthalpy difference (h^0-$h^0_{,TAmb}$) for the two temperatures. For comparison, the specific heat capacity at the chimney inlet temperature is also included. Also the heat loss due to incomplete combustion (hr-hp) is calculated.

Cp and enthalpy	kJ/kgK	kJ/kg	kJ/kgK	kJ/kg
at chimney inlet temperature	Cp mean	h^0-$h^0_{,TAmb}$	Cp	(hr-hp)
CO_2	0.924	162	0.995	0
H_2O	1.898	332	1.939	0
O_2	0.938	164	0.963	0
N_2	1.046	183	1.054	0
CO	1.048	183	1.059	10102
NO	0.999	175	1.011	3041
NO_2	0.869	152	0.930	743
C_xH_y as CH_4	2.488	435	2.795	50024
SO_2	0.671	117	0.715	0
N_2O	0.956	167	1.025	1854
H_2	14.480	2534	14.539	119954
NH_3	2.246	393	2.412	18604
HCN	1.431	250	1.521	23874
$C_{xt}H_{yt}$ as C_6H_6	1.392	244	1.698	40573
Ar	0.520	91	0.520	0
Flue gas	1.082	189	1.107	417.47
				(wet fuel)

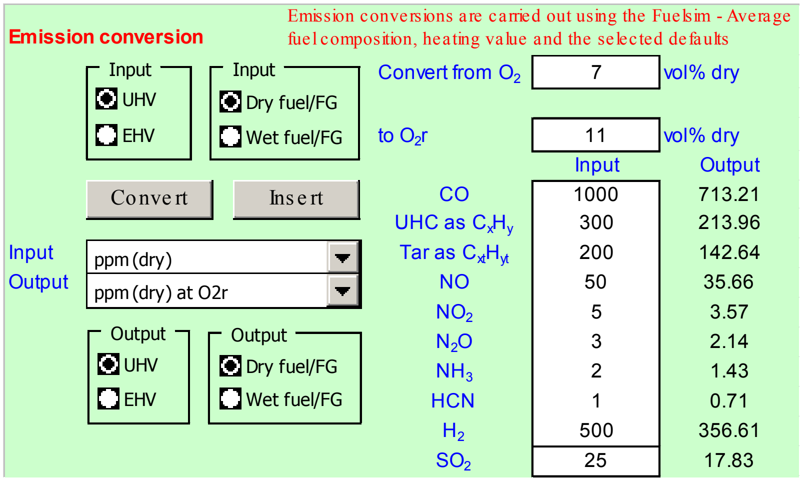
Fuelsim - Average calculates the residence time in the combustion chamber at a user defined combustion temperature given either the combustion chamber dimensions or the combustion chamber volume as input.

Combustion chamber dimensions	Temp. (°C):	1559.41	
Height / Width / Length (m)	0.400	0.300	0.500
Combustion chamber volume (m^3)		0.060	H/W/L
Comb. chamber residence time (s)		2.543	

Insert Height / Width / Length or combustion chamber volume

Push “H/W/L” to insert a formula which calculates the flue gas volume from the Height / Width / Length input

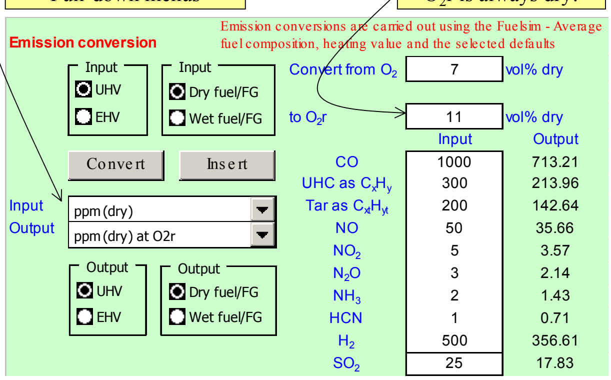
Fuelsim - Average can convert emissions given in various denominations to other denominations and reference O_2 levels. The Fuelsim - Average fuel composition, heating value and the selected defaults are used. Except for this, these calculations performs independently of the main calculations. However, the emission levels in volume fractions are always calculated and can be inserted as input to the main calculations. The main calculations should then give equal converted emission levels as this separate emission conversion section.



Emission conversion (continued).

Pull-down menus

O_2r is always dry!



Dependent on the input denomination, not all options influences the calculated results

SO_2 can be converted, but not inserted into Fuelsim - Average, where 100% conversion of fuel sulphur to SO_2 is always assumed

Complete procedure:

- Select UHV or EHV for input
- Select Dry fuel/FG or Wet fuel/FG for input
- Select input denomination
- Select output denomination
- Select UHV or EHV for output
- Select Dry fuel/FG or Wet fuel/FG for output
- Set dry or wet O_2 to convert from
- Set dry O_2 to convert to
- Insert emission levels
- Push the “Calculate” button
- If you want to, push the “Insert” button to insert the calculated dry flue gas composition into Fuelsim - Average

Emission conversion (continued).

Input
mg/Nm3 (dry)
ppm (dry)
mg/kg (dry)
mg/MJ (UHV)
mg/kWh (UHV)

Input
mg/Nm3 (wet)
ppm (wet)
mg/kg (wet)
mg/MJ (EHV)
mg/kWh (EHV)

Output
mg/Nm3 (dry) at O2r
ppm (dry) at O2r
mg/kg (dry), O2r = O2
mg/MJ (UHV), O2r = O2
mg/kWh (UHV), O2r = O2
ppm (dry) at O2r = O2

Output
mg/Nm3 (wet) at O2r
ppm (wet) at O2r
mg/kg (wet), O2r = O2
mg/MJ (EHV), O2r = O2
mg/kWh (EHV), O2r = O2
ppm (wet) at O2r = O2

Fuelsim - Average use the following combustion equation.

Combustion equation

$$a \cdot \left(Y_C + Y_H + Y_O + Y_N + Y_S\right)_{Fuel} + \frac{z}{Y_{O_2}} \cdot \left(Y_{O_2} + Y_{N_2} + Y_{Ar} + Y_{CO_2} + Y_{H_2O}\right)_{Air}$$

$$\Rightarrow \quad b_{CO_2} + c_{H_2O} + d_{O_2} + e_{N_2} + f_{CO} + g_{NO} + h_{NO_2} + i_{C_xH_y}$$

$$+ j_{SO_2} + k_{N_2O} + l_{H_2} + m_{NH_3} + n_{HCN} + o_{C_{xt}H_{yt}} + p_{Ar} + q_{CO_{2,Air}} + r_{H_2O_{Air}}$$

Fuelsim - Average calculates the fuel volume fractions from the input weight fractions. The volume fractions are used in the combustion equation. If you have the elemental fuel composition as volume fractions, push the “Volume fraction” button to convert these to elemental weight fractions.

Y_C - volume fraction C, daf / waf	0.3236	0.2956	H_2O
Y_H - volume fraction H, daf / waf	0.4627	0.4227	0.0865
Y_O - volume fraction O, daf / waf	0.2132	0.1947	
Y_N - volume fraction N, daf / waf	3.885E-04	3.549E-04	
Y_S - volume fraction S, daf / waf	1.212E-04	1.107E-04	

Fuelsim - Average calculates the coefficients in the combustion equation at both real, stoichiometric and reference O_2 level conditions.

	Real	Stoich.	Ref. O_2
a - Fuel	43.10	63.30	NA
z - Air	20.97	21.07	NA
b - CO_2	13.638	20.483	9.727
d - O_2	7.000	NA	11.000
e - N_2	78.18	78.54	78.15
f - CO	0.1000	NA	0.0713
g - NO	0.0050	NA	0.0036
h - NO_2	0.0005	NA	0.0004
i - C_xH_y	0.0300	NA	0.0214
j - SO_2	0.0052	0.0077	0.0037
k - N_2O	0.0003	NA	0.0002
l - H_2	0.0500	NA	0.0357
m - NH_3	0.0002	NA	0.0001
n - HCN	0.0001	NA	0.0001
o - $C_{xt}H_{yt}$	0.0200	NA	0.0143
p - Ar	0.9381	0.9423	0.9378
q - $CO_{2,Air}$	0.0314	0.0316	0.0314
sum - dry	100	100	100
c - H_2O from H in fuel	9.742	14.645	6.948
r - H_2O_{Air}	1.591	1.598	1.590
sum - wet FG, dry fuel basis	111.332	116.242	108.538
H_2O from water in fuel	4.083	5.995	2.912
H_2O from water injection	0.000	0.000	0.000
sum - wet FG, wet fuel basis	115.415	122.238	111.450

Fuelsim - Average calculates emission levels, based on the given flue gas composition, in various denominations.

Emissions				
NO_X as NO_2 eqv.	○ mg/kg fuel	◉ UHV	1.129E+02	
N_2O	○ mg/MJ	○ EHV	5.891E+00	
NH_3	○ mg/kWh		1.520E+00	
HCN	○ mg/kWhe	◉ Gross	1.206E+00	
CO	○ g/h	○ Net	1.250E+03	
UHC as C_xH_y / CH_4	○ ton/year	◉ Dry fuel/FG	5.902E+02	6.442E+02
SO_2	◉ mg/Nm3 FG	○ Wet fuel/FG	2.987E+02	
Tar as $C_{xt}H_{yt}$ / CH_4			6.970E+02	8.589E+02
Particles	mg/kg dry fuel	5000	7.474E+02	

Insert particle emission level here if it has been measured. Particles is not accounted for in the main calculations. However, tar is, and can be used as a substitute

Gross: No heat losses is taken into account
Net: Heat loss due to incomplete combustion and chimney heat loss is accounted for

Complete procedure:
- Select UHV or EHV for input
- Select Dry fuel/FG or Wet fuel/FG for input
- Select Gross or Net
- Insert particle emission level in g/kg dry fuel if wanted

Fuelsim - Average calculates emission levels at another vol% O_2, based on the given flue gas composition, in two denominations and on wet or dry FG basis. The dry and wet flue gas volume at the reference O_2 is needed in the emission conversion procedure.

Insert dry reference vol% O_2 here!

Dry / wet reference vol% O_2		11	9.870
CO_2 at dry / wet reference O_2 (vol%)		9.758	8.756
Dry / wet FG volume at dry reference O_2 (Nm^3/h)		15.382	17.143
at reference vol% O_2			
NO_X as NO_2 eqv.		39.23	
N_2O	◉ ppm	2.14	
NH_3	○ mg/Nm3 FG	1.43	
HCN		0.71	
CO		713.21	
UHC as C_xH_y / CH_4	◉ Dry FG	213.96	641.89
SO_2	○ Wet FG	37.26	
Tar as $C_{xt}H_{yt}$ / CH_4		142.64	855.85
Particles		NA	

Fuelsim - Average calculates the mean specific heat capacity in a temperature interval, in this case between the adiabatic combustion temperature and the ambient temperature, for all flue gas species as well as for the flue gas. The mean specific heat capacity times the temperature difference equals the enthalpy difference (h^0-$h^0_{,TAmb}$) for the two temperatures. For comparison, the specific heat capacity at the adiabatic combustion temperature is also included.

Cp and enthalpy	kJ/kgK	kJ/kg	kJ/kgK
at adiabatic combustion temperature	Cp mean	h^0-$h^0_{,TAmb}$	Cp
CO_2	1.205	1849	1.360
H_2O	2.333	3579	2.799
O_2	1.078	1653	1.169
N_2	1.166	1790	1.273
CO	1.179	1810	1.284
NO	1.123	1723	1.215
NO_2	1.120	1718	1.253
C_xH_y as CH_4	4.524	6941	6.084
SO_2	0.829	1272	0.904
N_2O	1.225	1880	1.378
H_2	15.277	23441	16.682
NH_3	3.307	5074	4.170
HCN	1.839	2822	2.126
$C_{xt}H_{yt}$ as C_6H_6	2.606	3998	3.302
Ar	0.520	798	0.520
Flue gas	1.260	1933	1.404

Fuelsim - Average calculates the volume flow of all flue gas species as well as for the flue gas.

Volumes	Nm^3/h	Nl/s	Nm^3/year
CO_2	1.496	0.416	13106
+ H_2O from H and H_2O in fuel	1.517	0.421	13286
+ O_2	0.768	0.213	6727
+ N_2	8.577	2.383	75135
+ CO	1.097E-02	3.047E-03	9.610E+01
+ NO	5.485E-04	1.524E-04	4.805E+00
+ NO_2	5.485E-05	1.524E-05	4.805E-01
+ C_xH_y	3.291E-03	9.142E-04	2.883E+01
+ SO_2	5.732E-04	1.592E-04	5.021E+00
+ N_2O	3.291E-05	9.142E-06	2.883E-01
+ H_2	5.485E-03	1.524E-03	4.805E+01
+ NH_3	2.194E-05	6.095E-06	1.922E-01
+ HCN	1.097E-05	3.047E-06	9.610E-02
+ $C_{xt}H_{yt}$	2.194E-03	6.095E-04	1.922E+01
+ Ar	1.029E-01	2.859E-02	9.016E+02
+ $CO_{2,Air}$	3.449E-03	9.580E-04	3.021E+01
+ H_2O_{Air}	0.174	0.048	1529
+ H_2O from water injection	0.000E+00	0.000E+00	0.000E+00
= Flue gas	12.662	3.517	110918

Fuelsim - Average calculates the mass flow of all flue gas species as well as for the flue gas. Finally, the flue gas dew point temperature is calculated, as well as vol% H_2O and N_2 in wet flue gas (FG), and wet and dry flue gas mole weight and density.

Weights	kg/h	g/s	ton/year
CO_2	2.938	0.816	25.735
+ H_2O from H and H_2O in fuel	1.219	0.339	10.679
+ O_2	1.096	0.305	9.604
+ N_2	10.720	2.978	93.907
+ CO	1.371E-02	3.808E-03	1.201E-01
+ NO	7.344E-04	2.040E-04	6.433E-03
+ NO_2	1.126E-04	3.128E-05	9.863E-04
+ C_xH_y	6.475E-03	1.799E-03	5.672E-02
+ SO_2	1.638E-03	4.551E-04	1.435E-02
+ N_2O	6.463E-05	1.795E-05	5.661E-04
+ H_2	4.934E-04	1.370E-04	4.322E-03
+ NH_3	1.667E-05	4.631E-06	1.460E-04
+ HCN	1.323E-05	3.675E-06	1.159E-04
+ $C_{xt}H_{yt}$	7.647E-03	2.124E-03	6.699E-02
+ Ar	1.834E-01	5.095E-02	1.607E+00
+ $CO_{2,Air}$	0.007	0.002	0.059
+ H_2O_{Air}	1.403E-01	3.896E-02	1.229E+00
+ H_2O from water injection	0.000E+00	0.000E+00	0.000E+00
= Flue gas	16.334	4.537	143.090
FG dew point temperature (K / °C)	325	52	
H_2O / N_2 in wet FG (vol%)	13.356	67.739	
Wet / dry FG mole weight (kg/kmole)	28.915	30.595	
Wet / dry FG density (kg/Nm^3)	1.290	1.365	

The “Gas conversion” sheet calculates the elementary weight fractions for a fuel gas for use as fuel composition input to Fuelsim - Average. The fuel gas composition can be inserted as either volume- or weight fractions.

Insert fuel gas composition as volume fractions

Push the “Copy input to Fuelsim - Average” push-button to copy the fuel gas elementary weight fractions, molecular weight, Upper Heating Value and specific heat capacity to Fuelsim - Average

Conversion from volume fraction to elemental fuel composition:

	1	Copy input to Fuelsim - Average					
	Input value	0.7172	0.2095	0.0132	0.0151	0.0451	1
Gases	Vol. fraction	XC	XH	XN	XS	XO	sum
O2	0.01	0	0	0	0	0.015044	0.015044
CO2	0.02	0.011294	0	0	0	0.030088	0.041382
H2O(g)	0	0	0	0	0	0	0
N2	0.01	0	0	0.01317	0	0	0.01317
SO2	0	0	0	0	0	0	0
C2H2	0	0	0	0	0	0	0

The “Gas conversion” sheet calculates the elementary weight fractions for a fuel gas for use as fuel composition input in Fuelsim - Average. The fuel gas composition can be either volume- or weight fractions.

Insert fuel gas composition as weight fractions

Push the “Copy input to Fuelsim - Average” push-button to copy the fuel gas elementary weight fractions, molecular weight, Upper Heating Value and specific heat capacity to Fuelsim - Average

Conversion from weight fraction to elemental fuel composition:

	1	Copy input to Fuelsim - Average					
	Input value	**0.7172**	**0.2095**	**0.0132**	**0.0151**	**0.0451**	1
Gases	Weight fraction	**XC**	**XH**	**XN**	**XS**	**XO**	sum
O2	0.015044011	0	0	0	0	0.015044	0.015044
CO2	0.041381937	0.011294	0	0	0	0.030088	0.041382
H2O(g)	0	0	0	0	0	0	0
N2	0.013170303	0	0	0.01317	0	0	0.01317
SO2	0	0	0	0	0	0	0
C2H2	0	0	0	0	0	0	0

The “Gas conversion” sheet can be modified by the user and new gas species can be added. For each species a number of input is needed: the species name, number of each element and thermodynamic data on CHEMKIN format.

Insert species name

Insert number of each element

The fuel gas molecular weight is calculated and used by Fuelsim - Average

									Mol.weight, fuel (kg/kmole)	
							Mol.weight	8.31432	For volume input:	**21.2701**
Gases		C	H	N	S	O	Mi, kg/kmole	R, kJ/kmoleK	Yi*Mi	Weight fraction
O2		0	0	0	0	2	31.9988	3.8486	0.319988	0.015044011
CO2		1	0	0	0	2	44.00995	5.2933	0.880199	0.041381937
H2O(g)		0	2	0	0	1	18.01534	2.1668	0	0
N2		0	0	2	0	0	28.0134	3.3693	0.280134	0.013170303
SO2		0	0	0	1	2	64.0628	7.7051	0	0
C2H2		2	2	0	0	0	26.03824	3.1317	0	0

The Upper Heating Value of the fuel gas is calculated from the heating values of each gas species, which is calculated from temperature dependent enthalpy expressions for each species.

Liquid water is included for determination of the Lower Heating Value of the fuel gas

The enthalpy expressions are given on CHEMKIN format and includes six coefficients, in both a high- and a low temperature range

Gases	Enthalpy H, kJ/kg	Low temperature range (< T_split) 8	9	10	11	12	13
H2O(l)	-15866.531	1.27E+01	-0.017663	-2.26E-05	2.08E-07	-2.41E-10	-37483.2000
O2	5.1074E-07	3.7824564	-0.002997	9.85E-06	-9.68E-09	3.24E-12	-1063.9436
CO2	-8941.1828	2.3567735	0.008985	-7.12E-06	2.46E-09	-1.44E-13	-48371.9697
H2O(g)	-13423.031	4.1986406	-0.002036	6.52E-06	-5.49E-09	1.77E-12	-30293.7267
N2	0.05104263	3.298677	0.001408	-3.96E-06	5.64E-09	-2.44E-12	-1020.8999
SO2	-4633.9947	2.911438	0.008103	-6.91E-06	3.33E-09	-8.78E-13	-36878.8100
C2H2	8763.83295	0.8086811	0.023362	-3.55E-05	2.80E-08	-8.50E-12	26428.9807

Also thermodynamic coefficients in the high temperature range are included. They are needed when very hot devolatilisation/gasification gas is defined as inlet fuel gas.

Enthalpy of liquid water is defined, and needed, only in the low temperature range

Gases	Enthalpy H, kJ/kg	Thermodynamic coefficients: High temperature range (> T_split) 1	2	3	4	5	6
H2O(l)	-15866.531						
O2	5.1074E-07	3.282538	0.001483	-7.6E-07	2.09E-10	-2.2E-14	-1088.46
CO2	-8941.1828	3.85746	0.004414	-2.2E-06	5.23E-10	-4.7E-14	-48759.2
H2O(g)	-13423.031	3.033992	0.002177	-1.6E-07	-9.7E-11	1.68E-14	-30004.3
N2	0.05104263	2.92664	0.001488	-5.7E-07	1.01E-10	-6.8E-15	-922.798
SO2	-4633.9947	5.254498	0.001979	-8.2E-07	1.58E-10	-1.1E-14	-37568.9
C2H2	8763.83295	4.14757	0.005962	-2.4E-06	4.67E-10	-3.6E-14	25936

The mean specific heat capacity in a temperature interval, in this case between the fuel gas temperature and the ambient temperature, is calculated for the fuel gas. The mean specific heat capacity times the temperature difference equals the enthalpy difference (h^0-$h^0_{,TAmb}$) for the two temperatures. The mean specific heat capacity is used as input to Fuelsim - Average.
Don't push the "Copy input to Fuelsim - Average" push-button before you have set the fuel gas temperature in Fuelsim - Average!

H2O(l)		1.9619	= specific heat capacity from volume fraction input
	at TFuel	1.9619	= specific heat capacity from weight fraction input
	Enthalpy	dH	
Gases	H, kJ/kg	H, kJ/kg	Thermodynamic data source
O2	9.189399	9.189398	GRI-Mech 3.0
CO2	-8932.69	8.488241	GRI-Mech 3.0
H2O(g)	-13404.4	18.65721	GRI-Mech 3.0
N2	10.43269	10.38165	GRI-Mech 3.0
SO2	-4627.74	6.253557	CHEMKIN Collection 3.6
C2H2	8780.869	17.0362	GRI-Mech 3.0

The validity range of the enthalpy expressions is defined between T_low and T_high. A temperature T_split is defined where the low temperature thermodynamic coefficients are valid between T_low and T_split, and the high temperature thermodynamic coefficients are valid from T_split to T_high. At T_split, both enthalpy expressions give the same value.

H2O(l)	273.15	1000	1000	-17180.144	
				at T_split:	
	T_low	T_high	T_split	H_low	H_high
Gases	K	K	K	kJ/kg	kJ/kg
O2	200	3500	1000	709.6	709.6
CO2	200	3500	1000	-8182.3	-8182.3
H2O(g)	200	3500	1000	-11979.7	-11979.7
N2	300	5000	1000	766.4	766.4
SO2	300	5000	1000	-4096.2	-4096.2
C2H2	200	3500	1000	10340.3	10340.3

Appendix 4

Fuelsim - Average examples

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August 2002

Fuelsim - Average v1.1
examples

by

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Documentation for v1.1 of Fuelsim - Average

Contents

The base case defaults used in the solid fuel combustion examples, unless stated otherwise, are:

Solid fuel composition:

C	H	O
0.5000	0.0600	0.4388
0.0007	0.1800	0.0005
N	H_2O	S

Ash fraction (dry fuel: 0.005)

Burning rate: 2 kg wet fuel/h

Oxidant
- (●) Air
- ( ) O2,N2,Ar,CO2,H2O mix

Fuel type
- (●) Solid or liquid
- ( ) Gas

Relative air humidity: 50%

Ambient temperature: 25ºC

and no preheating of air or fuel!

Other defaults (can be set by pushing the Defaults push-button):
- Normal condition: 273.15 K, 1 atm
- UHC expressed as C_3H_8 (original spreadsheet default is CH_4)
- Tar expressed as C_6H_6
- External preheating of Air and Fuel, if used

Example 1 - Determining the Upper and Effective Heating Value using the elemental fuel composition.

For solid fuels, the Upper (or Gross) and Effective (or Net) Heating Value can be estimated directly using the dry elemental fuel composition and an empirical expression

Make sure that the empirical expression is used by pushing the “Empirical” button!

Weigth fraction of ash in dry fuel / total ash (g/h)	0.005	8.241
Upper Heating Value of fuel (MJ/kg, daf)	19.981	Empirical
Upper Heating Value of fuel (MJ/kg, waf)	16.384	
Effective Heating Value of fuel (MJ/kg, waf)	14.870	

Answer

Example 2 - Determining the Effective Heating Value from a measured Upper Heating Value.

If you have measured the Upper Heating Value (in this case 21.5 MJ/kg) in a bomb calorimeter or know you have a more exact value than estimated by the empirical expression, you can insert the Upper Heating Value manually

Insert 21.5 here (even if the formula for the empirical expression shows)

Weigth fraction of ash in dry fuel / total ash (g/h)	0.005	8.241
Upper Heating Value of fuel (MJ/kg, daf)	21.500	Empirical
Upper Heating Value of fuel (MJ/kg, waf)	17.630	
Effective Heating Value of fuel (MJ/kg, waf)	16.116	

Answer

Example 3 - Determining the excess air ratio for a given flue gas composition.

You have measured 7 vol% O_2 in a dry flue gas. Find the excess air ratio

Insert 7 here (and set the other input flue gas volume fractions to zero)

O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0691	7.0000	70000
Excess air ratio (Lambda)	1.5	1.499	Set Lambda

Answer

Example 4 - Determining the excess air ratio for a given flue gas composition.

You have measured 7 vol% O_2 AND 5000 ppm CO in a dry flue gas. Find the excess air ratio

Insert 7 vol% O_2 and 0.5 vol% CO (and set the other input flue gas volume fractions to zero)

ppm

O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0591	7.0000	70000
CO in wet / dry FG (vol%) & ppm (dry FG)	0.4328	0.5000	5000

Excess air ratio (Lambda)	1.5	1.475	Set Lambda

Answer

Example 5 - Finding vol% O_2 in the dry flue gas for a given excess air ratio.

You would like to have an excess air ratio of 1.7. Find vol% O_2 in the dry flue gas

Insert 1.7 here (and set all, except O_2, input flue gas volume fractions to zero) and push the "Set Lambda" push-button. O_2 is now found by iteration

Excess air ratio (Lambda)	1.7	1.700	Set Lambda

O_2 in wet / dry FG (vol%) & ppm (dry FG)	7.6108	8.6540	86540

Answer

Example 6 - Finding the flue gas volume produced and the volume air added.

You have measured 7 vol% O_2 in a dry flue gas. Find the flue gas volume produced and the volume air added

Insert 7 here (and set the other input flue gas volume fractions to zero)

O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0691	7.0000	70000
Volume air added (Sm^3/h / Nm^3/h / Sm^3/s)	12.069	11.441	3.352E-03
Volume dry FG produced (Sm^3/h / Nm^3/h / Sm^3/s)	11.836	11.220	3.288E-03
+ Volume of water vapour from H (Nm^3/h)		1.094	
+ Volume of water vapour from H_2O in fuel (Nm^3/h)		0.448	
+ Volume of water vapour from H_2O in air (Nm^3/h)		0.179	
+ Volume of water vapour from water injection (Nm^3/h)		0.000	
= Total FG volume (Sm^3/h / Nm^3/h / Sm^3/s)	13.651	12.941	3.792E-03

Answer

Example 7 - Finding the flue gas volume produced and the volume air added.

Double the vol% O_2 in the dry flue gas in Example 6. Does the flue gas volume produced and/or the volume air added also double?

Insert 14 here (and set the other input flue gas volume fractions to zero)

O_2 in wet / dry FG (vol%) & ppm (dry FG)	12.9107	14.0000	140000
Volume air added (Sm^3/h / Nm^3/h / Sm^3/s)	24.184	22.925	6.718E-03
Volume dry FG produced (Sm^3/h / Nm^3/h / Sm^3/s)	23.761	22.524	6.600E-03
+ Volume of water vapour from H (Nm^3/h)		1.094	
+ Volume of water vapour from H_2O in fuel (Nm^3/h)		0.448	
+ Volume of water vapour from H_2O in air (Nm^3/h)		0.358	
+ Volume of water vapour from water injection (Nm^3/h)		0.000	
= Total FG volume (Sm^3/h / Nm^3/h / Sm^3/s)	25.766	24.425	7.157E-03

Answer

No, the flows does not double exactly! This is also the case if the excess air ratio had been doubled

Example 8 - Finding the burning rate when a volume has been measured.

You have measured a total flue gas volume of 25 Nm^3/h and 7 vol% O_2 in the dry flue gas. Find the burning rate

2) Select the option-buttons “wet FG” and “Nm3/h”. Insert 25 in the input cell and push the “Set, air, dry or wet FG” push-button

1) Insert 7 here (and set the other input flue gas volume fractions to zero)

O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0691	7.0000	70000

Select input flow: Air / dry FG / wet FG (selected: wet FG)

Select denomination: Sm3/h / Nm3/h / Sm3/s (selected: Nm3/h)

Input: 25 — [Set air, dry or wet FG]

= Total FG volume (Sm^3/h / Nm^3/h / Sm^3/s)	26.373	25.000	7.326E-03
Burning rate kg/h (dry / wet fuel) & kg/s (wet fuel)	3.168	3.864	1.073E-03

Answer

Example 9 - Finding the adiabatic combustion temperature.

What is the adiabatic combustion temperature at a vol% O_2 of 7, 11 and 14 in the dry flue gas?

Insert 7, 11 and 14 here (and set the other input flue gas volume fractions to zero) and make sure that there are no preheating of the fuel or inlet air. An automatic iteration procedure finds then the new adiabatic combustion temperature

O_2 in wet / dry FG (vol%) & ppm (dry FG)	6.0691	7.0000	70000
O_2 in wet / dry FG (vol%) & ppm (dry FG)	9.8748	11.0000	110000
O_2 in wet / dry FG (vol%) & ppm (dry FG)	12.9107	14.0000	140000

Answer

Adiabatic combustion temperature (K / °C)	1727.09	1453.94
Adiabatic combustion temperature (K / °C)	1407.59	1134.44
Adiabatic combustion temperature (K / °C)	1130.74	857.59

Note that ISO 110042-1, Gas turbines - Exhaust gas emission - Part 1: Measurement and evaluation, contains simplified expressions for conversion of emission levels between different denominations. Fuelsim - Average is based directly on the combustion equation, and contains no simplifications when converting emission levels between different denominations.

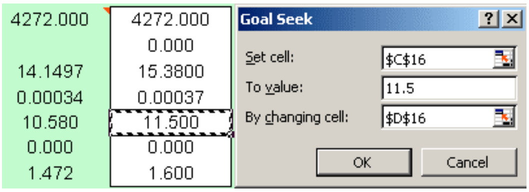
Gas turbine example 1 - LM2500 gas turbine with DLE (low NOx burner).

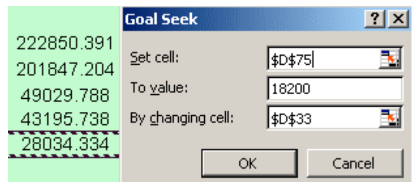
Problem: 1) Find the NOx emission level in the denominations; a) ppmvd at 15 vol%d O2, b) kg/h, c) g/kWh and d) g/kWhe when:
Fuel gas composition (vol%): 1.13N2 + 0.99CO2 + 78.1CH4 + 18.6C2H6 + 1.05C3H8 + 0.1C4H10 + 0.01C5H12 + 0.02C6H14
Flue gas composition: O2 = 15.38 vol%d, CO = 3.7 ppmvd, UHC (as CH4) = 1.6 ppmvd, CO2 = 3.07 vol%d and NOx = 11.5 ppmvw
Power output = 18.2 MW
Burning rate = 4272 kg/h, Ambient temperature = 25ºC, Relative air humidity = 85 %
2) Find NOx in kg/h if you know that the NOx level for this gas turbine is 25 ppmvd at 15 vol%d O2

Solution procedure: 1) The solution is quite straightforward but note that the NOx level in the flue gas is given on wet basis. Also, the power output is calculated on the basis of a combined turbine/generator el. efficiency, which has to be found. Hence, iterations is needed. The measured CO2 level is not needed in the calculation, but can be compared with the calculated CO2 level to check the measurement accuracy
2) The solution can be found by iteration

1) Solution steps:

- Push the “Defaults” push-button and restore the original defaults, which includes UHC given as CH4
- Insert the given dry flue gas composition in the Average sheet
- Set the level of the other (input) flue gas components to zero
- Set the burning rate
- Set preheating temperatures equal to ambient temperature (25ºC) and relative air humidity to 85%
- Insert the fuel gas composition in the Gas conversion sheet and push the “Copy input to Fuelsim - Average” push-button
- The input section should now look as Fig. 1
- Insert the given ppmvw NOx level as a starting value for the ppmvd NOx level, which now can be found by iteration. Use the Goal Seek function on the tools menu in Excel, as shown below. A NOx level of 12.500 ppmvd is now found
- Use the Goal Seek function again to find the combined turbine/generator el. efficiency (= 0.3246) that corresponds to a power output of 18200 kW, as shown below



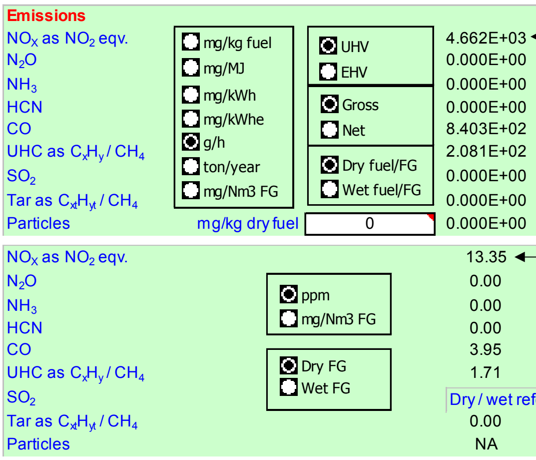


Fuel and flue gas (FG) properties		C	H	O
Fuel composition (weight fraction, daf)	Volume fraction	0.7422	0.2252	0.0163
(Moisture: waf)		0.0163	0.0000	0.0000
		N	H_2O	S
Burning rate kg/h (dry / wet fuel) & kg/s (wet fuel)		4272.000	4272.000	1.187E+00
Water injection rate kg/h & kg/s			0.000	0.000E+00
O_2 in wet / dry FG (vol%) & ppm (dry FG)		14.1497	15.3800	153800
CO in wet / dry FG (vol%) & ppm (dry FG)		0.00034	0.00037	3.7
NO in wet / dry FG (ppm)		0.000	0.000	Insert wet FG comp.
NO_2 in wet / dry FG (ppm)		0.000	0.000	
UHC as C_xH_y in wet / dry FG (ppm)		1.472	1.600	
SO_2 in wet / dry FG (ppm)		0.000	0.000	
N_2O in wet / dry FG (ppm)		0.000	0.000	
H_2 in wet / dry FG (vol%) & ppm (dry FG)		0.00000	0.00000	0.0
NH_3 in wet / dry FG (ppm)		0.000	0.000	
HCN in wet / dry FG (ppm)		0.000	0.000	
Tar as C_xH_y in wet / dry FG (ppm)		0.000	0.000	
Ambient air temperature (K / °C)		298.15	25.00	
Inlet primary air temperature (K / °C)		298.15	25.00	
Inlet secondary air temperature (K / °C)		298.15	25.00	
Weight fraction primary air of total air			0.5000	
Inlet fuel gas temperature (K / °C)		298.15	25.00	
Inlet water injection temperature (K / °C)		298.15	25.00	
Cp mean - fuel gas (kJ/kgK)			0.000	
Chimney inlet temperature (K / °C)		473.15	200.00	
Combined turbine/generator el. efficiency			0.5000	
Relative air humidity (%)	Oxidant: (●) Air ( ) O2,N2,Ar,CO2,H2O mix		85	

Fig. 1

1) Solution steps (continued):

- Set the reference O2 level to 15 vol%d
- The NOx emission levels can now be found by pushing their respective option-buttons, as shown below
- Answers:
  - a) 13.35 ppmvd at 15% O2, b) 4.662 kg/h
  - c) 0.08314 g/kWh (based on **EHV** and **Gross**), d) 0.2562 g/kWhe



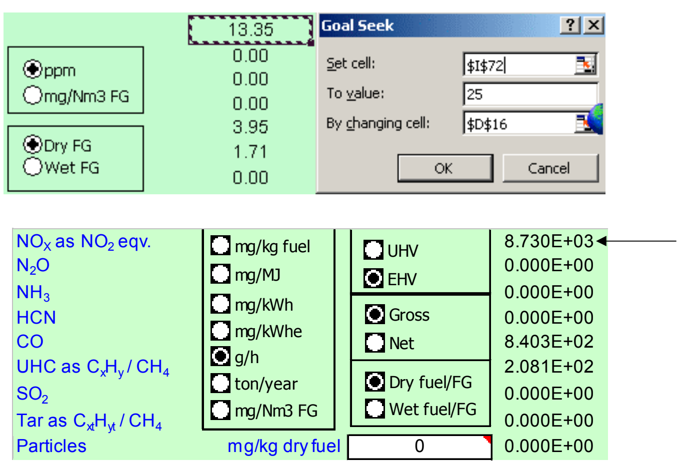
Gross: No heat losses is taken into account
Net: Heat loss due to incomplete combustion **and** chimney heat loss is accounted for

Note that the measured CO2 level (3.07 vol%d) deviates significantly from the calculated one (3.2879 vol%d), which can be due to measurement uncertainty

Dry / wet reference vol% O_2 15

2) Solution steps:

- Use the Goal Seek function to find kg/h NOx for 25 ppmvd at 15 vol%d O2, as shown below
- Answer:
  - 8.730 kg/h (Note that the power output decreased slightly)



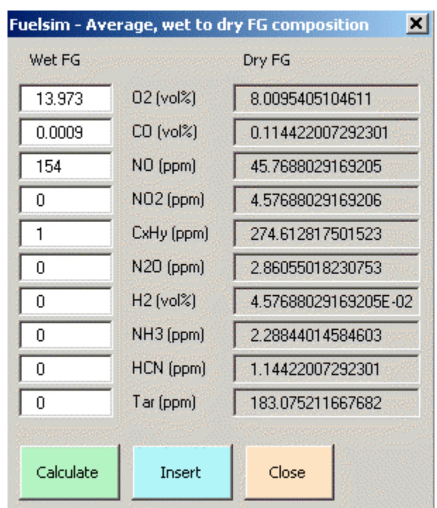
Gas turbine example 2 - LM2500 gas turbine with standard combustion chamber.

Problem: Find the NOx emission level in the denominations; a) ppmvd and ppmvw, b) kg/h, c) g/kWh and d) g/kWhe when:
Fuel gas composition (vol%): 6.07N2 + 0.67CO2 + 84.5CH4 + 5.58C2H6 + 2.05C3H8 + 0.78C4H10 + 0.18C5H12 + 0.17C6H14
Flue gas composition: O2 = 13.973 vol%w, CO = 9 ppmvw, UHC (as CH4) = 1 ppmvw, CO2 = 3.203 vol%w and NOx = 154 ppmvd at 15 vol%d O2
Power output = 22 MW
Burning rate = 4777 kg/h, Ambient temperature = 25ºC, Relative air humidity = 85 %

Solution procedure: The solution is quite straightforward but note that the NOx level in the flue gas is given on dry basis at a reference O2 level. Also, the power output is calculated on the basis of a combined turbine/generator el. efficiency, which has to be found. Hence, iterations is needed. The measured CO2 level is not needed in the calculation, but can be compared with the calculated CO2 level to check the measurement accuracy

Solution steps:

- Push the "Defaults" push-button and restore the original defaults, which includes UHC given as CH4
- Set the burning rate
- Set preheating temperatures equal to ambient temperature (25ºC) and relative air humidity to 85%
- Insert the fuel gas composition in the Gas conversion sheet and push the "Copy input to Fuelsim - Average" push-button
- Push the "Insert wet FG comp." push-button and insert the given wet flue gas composition in the Average sheet, as shown to the right. Use the given NOx level as a starting value for ppmvw NOx. Set the level of the other (input) flue gas components to zero. Push "Calculate", "Insert" and "Close"
- The input section should now look as Fig. 2

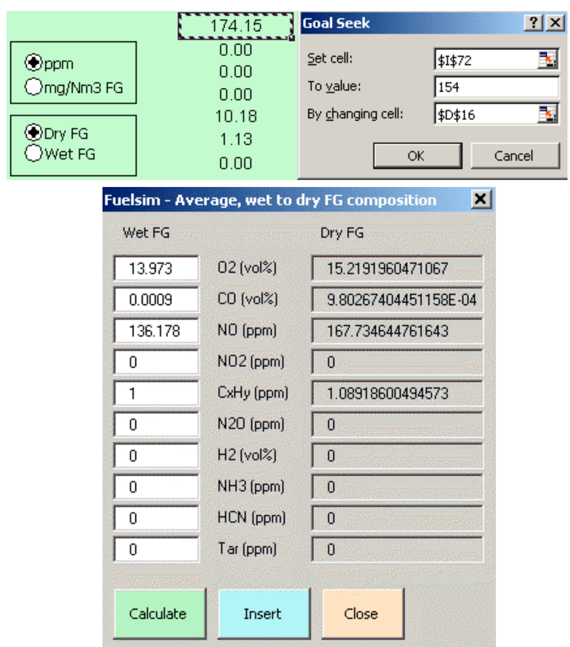


Fuel and flue gas (FG) properties		C	H	O
Fuel composition (weight fraction, daf)	Volume fraction	0.6846	0.2139	0.0114
(Moisture: waf)		0.0901	0.0000	0.0000
		N	H_2O	S
Burning rate kg/h (dry / wet fuel) & kg/s (wet fuel)		4777.000	4777.000	1.327E+00
Water injection rate kg/h & kg/s			0.000	0.000E+00
O_2 in wet / dry FG (vol%) & ppm (dry FG)		13.9730	15.2192	152192
CO in wet / dry FG (vol%) & ppm (dry FG)		0.00090	0.00098	9.8
NO in wet / dry FG (ppm)		154.000	167.735	Insert wet FG comp.
NO_2 in wet / dry FG (ppm)		0.000	0.000	
UHC as C_xH_y in wet / dry FG (ppm)		1.000	1.089	
SO_2 in wet / dry FG (ppm)		0.000	0.000	
N_2O in wet / dry FG (ppm)		0.000	0.000	
H_2 in wet / dry FG (vol%) & ppm (dry FG)		0.00000	0.00000	0.0
NH_3 in wet / dry FG (ppm)		0.000	0.000	
HCN in wet / dry FG (ppm)		0.000	0.000	
Tar as C_xH_y in wet / dry FG (ppm)		0.000	0.000	
Ambient air temperature (K / °C)		298.15	25.00	
Inlet primary air temperature (K / °C)		298.15	25.00	
Inlet secondary air temperature (K / °C)		298.15	25.00	
Weight fraction primary air of total air			0.5000	
Inlet fuel gas temperature (K / °C)		298.15	25.00	
Inlet water injection temperature (K / °C)		298.15	25.00	
Cp mean - fuel gas (kJ/kgK)			0.000	
Chimney inlet temperature (K / °C)		473.15	200.00	
Combined turbine/generator el. efficiency			0.3246	
Relative air humidity (%)	Oxidant: Air / O2,N2,Ar,CO2,H2O mix		85	

Fig. 2

Solution steps (continued):

- Set the reference O2 level to 15 vol%d
- Use the Goal Seek function on the tools menu in Excel to find ppmvd NOx at real vol%d O2 when you know that ppmvd NOx at reference O2 (15 vol%d) should be 154, as shown to the right. A NOx level of 148.324 ppmvd is now found
- The input volume fractions on wet basis have now changed slightly. Therefore, push the "Insert wet FG comp." push-button again and change the NO level to the calculated one (136.178 ppmvw), as shown to the right. Push "Calculate", "Insert" and "Close". The flue gas composition is now correct, while the NOx level at 15 vol%d O2 still is 154. Hence, we have now performed a "manual" iteration



Solution steps (continued):

- Use the Goal Seek function again to find the combined turbine/generator el. efficiency (= 0.3757) that corresponds to a power output of 22000 kW (see previous example)
- The NOx emission levels can now be found in the input section and by pushing their respective option-buttons (see previous example)
- Answers:
  - a) 148.324 ppmvd and 136.178 ppmvw, b) 56.59 kg/h
  - c) 0.9658 g/kWh (based on **EHV** and **Gross**), d) 2.572 g/kWhe

Gross: No heat losses is taken into account
Net: Heat loss due to incomplete combustion **and** chimney heat loss is accounted for

Note that the measured CO2 level (3.203 vol%w) deviates significantly from the calculated one (3.0432 vol%w), which can be due to measurement uncertainty

Gas turbine example 3.

Problem: Find a) vol% CO2 in dry flue gas, b) ppm NOx in dry flue gas at 15 vol% reference O2, c) excess air ratio, d) weight of air added (kg/h), e) weight of CO2 in flue gas (kg/h), f) weight of NOx as NO2 eqv. (kg/h), g) adiabatic combustion temperature (ºC) and h) vol% O2 calculated from vol% CO2 when:
Fuel gas composition (vol%): 1.01N2 + 1.15CO2 + 90.08C1 + 6.31C2 + 1.34C3 + 0.05IC4 + 0.06NC4
Flue gas composition: O2 = 16.4 vol%d, CO = 224.9 ppmvd, UHC (as C3) = 40.5 ppmvw, CO2 = 2.59 vol%d, NO = 24.7 ppmvd and NO2 = 20.13 ppmvd
Inlet air temperature = 273.73ºC, Inlet fuel gas temperature = 19.87ºC
Burning rate = 3141.8 kg/h, Ambient temperature = 6.5ºC, Relative air humidity = 75.4 %

Solution procedure: The solution is quite straightforward but note that the UHC level in the flue gas is given on wet basis. Hence, an iteration is needed
We assume that C1 = CH4, C2 = C2H6, C3 = C3H8 and IC4+NC4 = C4H10

Solution steps:

- Push the "Defaults" push-button and restore the original defaults, which includes UHC given as CH4. Your UHC is given as C3 (C3H8), so set "x in CxHy" equal to 3 and "y in CxHy" equal to 8
- Set the burning rate
- Set both primary and secondary air preheating temperatures equal to 273.73ºC, alternatively you can set only primary air preheating temperature and then set weight fraction primary air of total air equal to 1
- Set ambient temperature equal to 6.5ºC
- Set inlet fuel gas temperature equal to 19.87ºC
- Set relative air humidity equal to 75.4%
- Insert the fuel gas composition in the Gas conversion sheet and push the "Copy input to Fuelsim - Average" push-button
- Insert the given dry flue gas composition in the Average sheet. Use the given UHC level as a starting value for ppmvd UHC. Set the level of the other (input) flue gas components to zero
- Use the Goal Seek function on the tools menu in Excel to find ppmvd UHC for the given ppmvw UHC. A UHC level of 42.806 ppmvd is now found
- The input section should now look as Fig. 3

Fuel and flue gas (FG) properties		C	H	O
Fuel composition (weight fraction, daf)	Volume fraction	0.7312	0.2323	0.0207
(Moisture: waf)		0.0159	0.0000	0.0000
		N	H_2O	S
Burning rate kg/h (dry / wet fuel) & kg/s (wet fuel)		3141.800	3141.800	8.727E-01
Water injection rate kg/h & kg/s			0.000	0.000E+00
O_2 in wet / dry FG (vol%) & ppm (dry FG)		15.5166	16.4000	164000
CO in wet / dry FG (vol%) & ppm (dry FG)		0.02128	0.02249	224.9
NO in wet / dry FG (ppm)		23.370	24.700	Insert wet FG comp.
NO_2 in wet / dry FG (ppm)		19.046	20.130	
UHC as C_xH_y in wet / dry FG (ppm)		40.500	42.806	
SO_2 in wet / dry FG (ppm)		0.000	0.000	
N_2O in wet / dry FG (ppm)		0.000	0.000	
H_2 in wet / dry FG (vol%) & ppm (dry FG)		0.00000	0.00000	0.0
NH_3 in wet / dry FG (ppm)		0.000	0.000	
HCN in wet / dry FG (ppm)		0.000	0.000	
Tar as $C_{xt}H_{yt}$ in wet / dry FG (ppm)		0.000	0.000	
Ambient air temperature (K / °C)		279.65	6.50	
Inlet primary air temperature (K / °C)		546.88	273.73	
Inlet secondary air temperature (K / °C)		546.88	273.73	
Weight fraction primary air of total air			0.5000	
Inlet fuel gas temperature (K / °C)		293.02	19.87	
Inlet water injection temperature (K / °C)		298.15	25.00	
Cp mean - fuel gas (kJ/kgK)			2.066	
Chimney inlet temperature (K / °C)		473.15	200.00	
Combined turbine/generator el. efficiency			0.5000	
Relative air humidity (%)	Oxidant: Air / O2,N2,Ar,CO2,H2O mix		75.4	

Fig. 3

Solution steps (continued):

- The answers to question a) to g) can now be read off the Average sheet:

a) vol% CO_2 in dry flue = 2.622
b) ppm NO_x in dry flue gas at 15 vol% reference O_2 = 58.63
c) excess air ratio = 4.222
d) weight of air added (kg/h) = 217075.742
e) weight of CO_2 in flue gas (kg/h) = CO_2 + $CO_{2,Air}$ = 8303.611 + 103.1 = 8404.711. Hence, 1.23 % of the CO_2 is originating from the inlet air
f) weight of NO_x as NO_2 eqv. (kg/h) = 15.03
g) adiabatic combustion temperature (ºC) = 850.75

For question h) we first need to use the Goal Seek function, changing vol% O_2 in dry flue gas until calculated vol% CO_2 in dry flue gas is equal to 2.59. Ideally we should then find a new value for ppmvd UHC, since ppmvw UHC has changed slightly, and then repeat the first step. However, the two last steps does not change the result significantly, since the UHC level is this low

h) vol% O_2 calculated from vol% CO_2 = 16.4557

Appendix 5

Fuelsim - Average exercise

Øyvind Skreiberg

August 2002

Fuelsim - Average Exercise

6. January 2001

Start-up procedure:
1. Unzip the zip-file and place all files in the same directory
2. Start Fuelsim - Average by opening the Excel spreadsheet file FUELSIM-Average_v1.1.xls
3. Click the buttons “Introduction” and “Documentation” and read through them to get an introduction to Fuelsim - Average

Having done that, you should now be able to solve the following problems:

Problem 1 - Natural gas and methane combustion
Click the button “Examples” and go through the 2 given examples.
Replace the given fuel gas composition in Gas turbine example 1 with methane and solve the problem again. Did it make much difference?

Problem 2 - Solid and liquid fuel combustion

Mr. X has an old oil fired boiler. He is considering replacing the oil burner with a pellet burner instead. The oil burner has a nominal effect of 20 kW gross based on upper heating value (UHV). However, he never runs it at full load, usually only on 50% load and up to 75% load in the coldest winter days. The pellet burner has a nominal effect of 15 kW gross based on UHV.

The dry ash free elemental composition in weight % of fuel oil and pellets are given in the table below:

	C	H	O	N	S
Fuel oil	86.4	13.4	0	0	0.2
Pellets	50	6	43.89	0.1	0.01

The moisture content of the pellets is 7 weight % on wet basis.

Assume complete combustion, zero ash content, an excess air ratio of 1.5 and 1.2 for the pellet burner and the oil burner respectively, no preheating of air and fuel, ambient temperature of 25°C and a relative air humidity of 75%. Use ISO Standard air composition.

a) Determine UHV, lower heating value (LHV) and adiabatic combustion temperature (K) for both fuels using the empirical expression for UHV in Fuelsim - Average.
b) Determine the effective heating value (EHV) and the corresponding adiabatic combustion temperature (K) for the pellets.
c) Discuss the influence of the moisture content on the heating value and the adiabatic combustion temperature. How much energy is used for evaporation of the moisture content, and how much is this compared to the heat of evaporation for the water formed from H in both fuels?
d) Determine the flue gas volume in Nm^3/h for both fuels for a nominal effect of 15 kW gross based on UHV.
e) What is the corresponding flue gas volume in m^3/h and the combustion chamber residence time assuming a combustion chamber volume of 0.036 m^3 and a real combustion temperature of 65% and 70% of the adiabatic combustion temperature for the fuel oil and the pellets respectively?
f) Is the residence time for the pellets (15 kW) as long or longer than for fuel oil at the nominal effect (20 kW) the boiler has been designed for?
g) When replacing an oil burner with a pellet burner the general rule is that the nominal effect of the pellet burner needs to be significantly lower than for the original oil burner. Why do you think this is the case?
h) How low chimney inlet temperature (°C) is needed to achieve a thermal efficiency based on UHV of 85%, 90% and 95% for both fuels. How does this compare to the flue gas dew point temperature?
i) Determine the net reduction of CO_2 emissions to the atmosphere by replacing fuel oil with pellets in the boiler, assuming an average load through a whole year of 10 kW gross based on UHV.

Problem 3 - Emission conversion
Mr. Y and Z are arguing about emission levels, both claiming that their combustion unit is the one with the lowest emission levels. Mr. Y has a pellet stove and Mr. Z has a fuel oil burner, both standalone units with a nominal effect of 10 kW gross based on UHV.

Mr. Y says that the emission level of CO from his pellet stove is only 100 ppm at 15 vol%d O_2 and Mr. Z says that the emission level of CO from his oil burner is only 300 mg/Nm^3 at 7 vol%d O_2. Who are right? (Explain and discuss your assumptions!)

Answers:

Problem 1

1) a) 13.39 ppmvd at 15 vol%d O2, b) 4.940 kg/h, c) 0.08322 g/kWh (based on EHV and Gross), d) 0.2741 g/kWhe

2) 9.221 kg/h

Hence, using methane as a substitute for this natural gas composition has a significant effect on the calculated results. If known, the specific natural gas composition should always be used.

Problem 2

a)

Fuel oil: UHV=45.972 MJ/kg, LHV=43.046 MJ/kg, T=2100.68 K

Pellet: UHV=19.986 MJ/kg, LHV=18.676 MJ/kg, T=1808.22 K (LHV is found by setting the moisture content to zero)

b)

EHV=17.198 MJ/kg, T=1776.05 K

c)

Increasing moisture content decreases the heating value and the adiabatic combustion temperature due to heat of evaporation and subsequent heating of the water vapour. Water vapour has a much higher specific heat capacity than the other major flue gas components.

Energy needed for evaporation of the moisture content in the pellets: 0.171 MJ/kg wet fuel (0.92%)

Energy needed for evaporation of the water formed from H in the pellets: 1.218 MJ/kg wet fuel (6.56%)

Energy needed for evaporation of water formed from H in the fuel oil: 2.926 MJ/kg fuel (6.36%)

As can be seen, the effect of this relatively low moisture content is not large compared to energy needed for evaporation of the water formed from H in both fuels. Even though the hydrogen content in the fuel oil is more than twice as high as for the pellets, the percentage of the total heating value used to evaporate H2O formed from H in the fuel is somewhat lower than for the pellets.

d)

Fuel oil: 17.127 Nm^3/h, Pellets: 20.991 Nm^3/h

e)

Fuel oil: 85.617 m^3/h, 1.514 s, Pellets: 95.541 m^3/h, 1.356 s

f)

Fuel oil (20 kW): 114.16 m^3/h, 1.135 s

Hence, the residence time for the pellets at 15 kW is longer than for the fuel oil at 20 kW.

g)

First of all, the flame type for a fuel oil burner and a pellet burner is quite different. While the fuel oil burns in a stable concentrated flame, the pellet flame is less defined and more voluminous, with higher radiation loss. The higher excess air ratio usually needed for a pellet flame due to poorer mixing conditions will also lower the combustion temperature and increase the flue gas flow in Nm^3/h. However, the lower combustion temperature will decrease the real volume flow, giving a similar residence as for the fuel oil burner. Hence, the flame type and temperature is the governing differences.

h)

Fuel oil: 359.21°C (85%), 250.78°C (90%), 139.40°C (95%), dew point: 49.28°C

Pellets: 298.63°C (85%), 209.49°C (90%), 118.31°C (95%), dew point: 50.15°C

i)

Fuel oil (10 kW): 21.717 ton CO2/year = net CO2 reduction

Problem 3

Using the given fuel composition and defaults as for fuel oil and the pellets in Problem 2, the following table can be set up:

	Fuel oil	**Pellets**
ppm at 15 vol%d O2	102.37	100
mg/Nm^3 at 7 vol%d O2	300	293.07
kg/year	32.51	31.64
mg/MJ (EHV and Gross)	110.0	108.3
mg/MJ (UHV and Gross)	103.0	100.2
mg/MJ (EHV and Net) at 85% thermal efficiency based on UHV	131.1	129.4

Who are right is in general a question of priorities, whether it is volumetric concentrations, mass concentrations, total mass or emissions vs. total produced heat or net produced heat. In this case, the pellet stove has the lowest emission level of CO.

Appendix 6

Fuelsim - Average versus ISO 11042-1

Øyvind Skreiberg

August 2002

Fuelsim - Average v1.1

Fuelsim - Average versus ISO 11042-1

by

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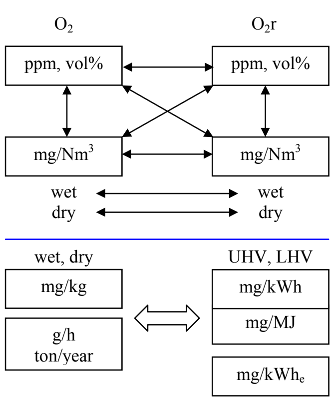
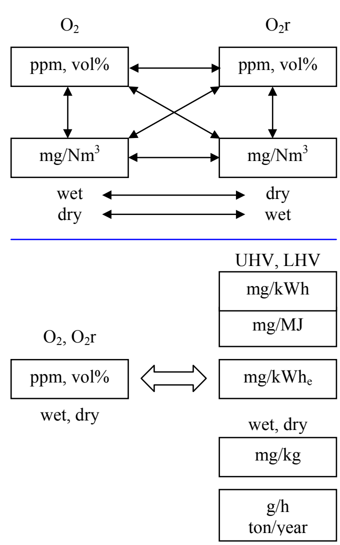
Documentation for v1.1 of Fuelsim - Average

Emission conversion: A trivial or challenging task?

Trivial:



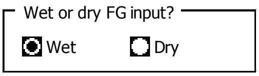
Challenging:



Fuelsim - Average provides the possibility to calculate the input data assumed known in the ISO 11042-1 emission conversion formulas

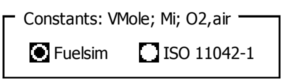
The emission conversion formulas given in ISO 11042-1 are compared to the Fuelsim - Average corresponding results in the ISO 11042-1 sheet. The ISO 11042-1 formulas are to some degree simplified and several input data needed in the conversion formulas are supposed to be known by measurement or calculation: vol% H_2O in wet flue gas, mass flow of wet flue gas and net produced electrical/mechanical output. Both vol% H_2O in wet flue gas and mass flow of wet flue gas are calculated in Fuelsim - Average, and also net produced electrical/mechanical output if a correct combined turbine/generator efficiency has been defined. Hence, Fuelsim - Average can be used both as a calculation tool for input to the ISO 11042-1 emission conversion formulas and as control tool for measured input data. In addition, the importance of deviations caused by the simplifications introduced in the ISO 11042-1 emission conversion formulas can be analysed. The ISO 11042-1 sheet has been made flexible, so that introduction of Fuelsim - Average constants and calculated results can be carried out in several steps.

Flue gas composition can be inserted on both wet and dry basis by clicking on the respective option buttons, as shown below.

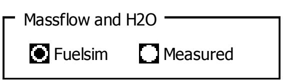


Choose to input wet or dry flue gas (FG) composition. However, vol% H_2O in wet flue gas must always be inserted!

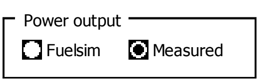
The options below in the ISO 11042-1 sheet can be selected independent of each other. The options are available for integration of Fuelsim constants/results into the ISO 11042-1 emission conversion formulas.



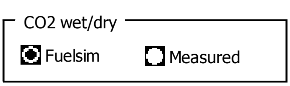
Choose to use ISO 11042-1 or Fuelsim constants: mole volume at normal condition, molecular weights and vol% O_2 in ISO 2533 dry air composition



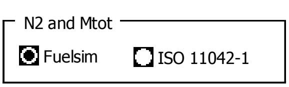
Choose to manually input measured wet flue gas mass flow and vol% H_2O in wet flue gas, or let Fuelsim calculate it for you



Choose to manually input measured net produced electrical/mechanical output, or let Fuelsim calculate it for you, based on a combined turbine/generator efficiency that you select



Choose to manually input measured vol% CO_2 in wet or dry flue gas, or use the value calculated by Fuelsim. Vol% CO_2 in wet flue gas is needed in the calculation of the wet flue gas vol% N_2 and mole weight in ISO 11042-1



Choose to use vol% N_2 in wet flue gas and wet flue gas mole weight as calculated by ISO 11042-1, or use the values calculated by Fuelsim

These species are not included in ISO 11042-1, and must be set to zero in the Average sheet

Set N2O, H2, NH3, HCN and Tar as zero in Average!

Wet or dry FG input? ◉ Wet ○ Dry

Constants: VMole; Mi; O2,air ◉ Fuelsim ○ ISO 11042-1

Power output ○ Fuelsim ◉ Measured

Massflow and H2O ◉ Fuelsim ○ Measured

Introduction and documentation

% deviation between Fuelsim and ISO 11042-1

			wet input ISO 11042-1	Fuelsim	%deviation
200	Test No.				
201	Time	min			
202	Time taken to measure one point	min			
203	Air temperature	°C		100	
204	Air pressure	kPa		101.325	
205	Relative air humidity	%		50	
206	Power output (mechanical/electrical)	kW	4.0147	4.0147	0
207	Fuel mass flow	kg/s		0.00056	
208	Exhaus gas mass flow (by measurement or calculation)	kg/s	0.004537358	0.00454	0
209	Exhaust gas mean temperature	°C		200	

Corresponds to ISO 11042-1 numbering

Optional manual input can be inserted in cells marked with yellow colour

Manual input can be inserted in the cells marked with white colour

Input cells marked with green colour are using the selected corresponding Fuelsim values instead of manual input

Only wet flue gas input, and calculated dry flue gas composition.

CO2 wet/dry ◉ Fuelsim ○ Measured

Note that UHC is expressed as CH4 in ISO 11042-1. Hence, UHC in the Average sheet must be set to CH4 if Fuelsim - Average calculated values are selected as input to the ISO 11042-1 sheet.

210	O_2	vol%	6.065068107	6.065	0
211	CO_2	vol%	11.84344697	11.843	0
212	H_2O	vol%	13.3561699	13.356	0
213	NO	ppm	43.32191505	43.322	0
214	NOx ($NO+NO_2$)	ppm	47.65410655	47.654	0
215	CO	ppm	866.438301	866.438	0
216	SOx ($SO_2 + SO_3$)	ppm	45.26991037	45.270	0
217	UHC (as CH_4)	ppm	259.9314903	259.931	0
	sum, excluding N_2	vol%	31.387	31.387	
300	**= Volumetric concentration of component i in dry exhaust gas**				
301	H_2O,wet	-	0.1336	0.1336	0
302	1/(1-H_2O,wet)	-	1.1542	1.1542	0
303	O_2,dry	vol%	7.000	7.000	0
304	CO_2,dry	vol%	13.669	13.669	0
305	NO,dry	ppm	50.000	50.000	0
306	NOx,dry ($NO+NO_2$)	ppm	55.000	55.000	0
307	CO,dry	ppm	1000.000	1000.000	0
308	SOx,dry ($SO_2 + SO_3$)	ppm	52.248	52.248	0
309	UHC,dry (as CH_4)	ppm	300.000	300.000	0
	sum, excluding N_2	vol%	20.810	20.810	

Only dry flue gas input, except for vol% H_2O in wet flue gas, and calculated wet flue gas composition.

CO2 wet/dry: Fuelsim / Measured

210	O_2	vol%	6.065	6.065	0
211	CO_2	vol%	11.843	11.843	0
212	H_2O	vol%	13.3561699	13.356	0
213	NO	ppm	43.322	43.322	0
214	NOx ($NO+NO_2$)	ppm	47.654	47.654	0
215	CO	ppm	866.438	866.438	0
216	SOx ($SO_2 + SO_3$)	ppm	45.270	45.270	0
217	UHC (as CH_4)	ppm	259.931	259.931	0
	sum, excluding N_2	vol%	31.387	31.387	
300	**= Volumetric concentration of component i in dry exhaust gas**				
301	H_2O,wet	-	0.1336	0.1336	0
302	1/(1-H_2O,wet)	-	1.1542	1.1542	0
303	O_2,dry	vol%	7	7.000	0
304	CO_2,dry	vol%	13.66911753	13.669	0
305	NO,dry	ppm	50	50.000	0
306	NOx,dry ($NO+NO_2$)	ppm	55	55.000	0
307	CO,dry	ppm	1000	1000.000	0
308	SOx,dry ($SO_2 + SO_3$)	ppm	52.24827933	52.248	0
309	UHC,dry (as CH_4)	ppm	300	300.000	0
	sum, excluding N_2	vol%	20.810	20.810	

Emissions are converted to a reference O_2 concentration in dry flue gas. Even though ISO 11042-1 only operates with 15 vol% O_2 in dry flue gas as reference O_2 concentration, the formulas used are generally valid for any reference O_2 concentration in dry flue gas. Hence, the possibility for manual selection of the reference O_2 concentration have been included in the ISO 11042-1 sheet.

Insert your choice of reference vol% O_2 in dry flue gas here

400	**$EV_{i,O2r,dry}$ = exhaust gas emission value as volumetric concentration related to an oxygen volume content of O2r vol% in dry exhaust gas**	11			
401	(O_2,air,dry-O2r)/(O_2,air,dry-O_2,dry)	-	0.7132	0.7132	0
402	$EV_{NO,O2r,dry}$	ppm	35.66		
403	$EV_{NOx,O2r,dry}$	ppm	39.23	39.23	0
404	$EV_{CO,O2r,dry}$	ppm	713.21	713.21	0
405	$EV_{SOx,O2r,dry}$	ppm	37.26	37.26	0
406	$EV_{UHC,O2r,dry}$	ppm	213.96	213.96	0

Emissions are also converted to mg/Nm^3 at the selected reference O_2 concentration, and g/kWh net produced electrical/mechanical output. Note that standard condition in ISO 11042-1 is equal to the default normal condition in Fuelsim!

500	**$EM_{i,O2r,dry}$ = exhaust gas emission value as volumetric concentration related to reference volume at standard condition**				
501	$EM_{NO,O2r,dry}$	mg/Nm^3	47.74		
502	$EM_{NOx,O2r,dry}$ (as NO_2)	mg/Nm^3	80.52	80.52	0
503	$EM_{CO,O2r,dry}$	mg/Nm^3	891.31	891.31	0
504	$EM_{SOx,O2r,dry}$ (as SO_2)	mg/Nm^3	106.51	106.51	0
505	$EM_{UHC,O2r,dry}$ (UHC as CH_4)	mg/Nm^3	153.15	153.15	0
600	**$EM_{i,P}$ = power output related emission value**				
601	N_2,wet	vol%	68.552	68.552	0
602	M_{tot},wet	kg/kmol	28.915	28.915	0
603	q_{mg7}/P	kg/kWs	0.0011302	0.0011302	0
604	$EM_{NO,P}$	g/kWh	0.1829		
605	$EM_{NOx,P}$	g/kWh	0.3085	0.3085	0
606	$EM_{CO,P}$	g/kWh	3.4151	3.4151	0
607	$EM_{SOx,P}$	g/kWh	0.4081	0.4081	0
608	$EM_{UHC,P}$	g/kWh	0.5868	0.5868	0

N2 and Mtot

(●) Fuelsim ( ) ISO 11042-1

ISO 11042-1 emission conversion formulas.

The emission conversion is based on use of ISO 2533 dry air composition and *knowledge of the H_2O concentration in the flue gas* (measured or calculated). When calculating the H_2O concentration a number of parameters must be known, see the textbox to the right. In addition water is formed from H in the fuel. The ISO 11042-1 standard includes formulas for conversion of measured concentrations (ppm) on wet or dry basis to concentrations at 15 vol% reference O_2 concentration in dry flue gas, together with conversion to mg/Nm^3 (15 vol% O_2 dry) and g/kWh_e. When converting emissions to g/kWh_e *must in addition net produced output and mass flow of wet flue gas be known*. The formulas used in ISO 11042-1 are given below:

ISO 11042-1: The water content is obtained by calculation or measurement to be agreed upon by the interested parties. Humidity of the air in the compressor inlet, water content in the fuel, as well as water of steam injection shall be considered.

From: / **To:**	ppm at O_2r	mg/Nm^3 at O_2r	g/kWh_e
$\varphi_{i,dry}$ or $\varphi_{i,wet}$ ppm at O_2 in dry or wet flue gas $\varphi_{i,dry} = \frac{\varphi_{i,wet}}{1-\frac{\varphi_{H_2O,wet}}{100}}$	$EV_{i,15,dry} = \frac{20.95-15}{20.95-\varphi_{O_2,dry}}\cdot\varphi_{i,dry} = \frac{5.95}{20.95-\varphi_{O_2,dry}}\cdot\varphi_{i,dry}$	$EM_{i,15,dry} = EV_{i,15,dry}\cdot\frac{M_i}{V_{mn}}$	$EM_{i,P} = 3.6\cdot\varphi_{i,wet}\cdot\frac{M_i}{M_{tot}}\cdot\frac{q_{m_{g7}}}{P}$

ISO 11042-1 emission conversion formulas (continued).

where:

- $\varphi_{i,dry}$ or $\varphi_{i,wet}$ are ppm NO, NOx ($NO+NO_2$), CO, SOx (SO_2+SO_3) or UHC (as CH_4) in dry or wet flue gas respectively
- $\varphi_{H_2O,wet}$ is vol% H_2O in wet flue gas
- 20.95 is approximated vol% O_2 in ISO 2533 dry air composition (20.9476)
- 15 is reference O_2 concentration in dry flue gas (vol%)
- $\varphi_{O_2,dry}$ is O_2 concentration in dry flue gas at operating conditions (vol%)
- M_i is mole weight of component i (kg/kmole)
- V_{mn} is mole volume at normal condition (Nm^3/kmole)
- M_{tot} is mole weight (kg/kmole) for wet flue gas based on the concentration of the main components O_2, CO_2, H_2O and N_2, where N_2 is calculated by difference:

$$\varphi_{N_2,wet} = 100 - \varphi_{O_2,wet} - \varphi_{CO_2,wet} - \varphi_{H_2O,wet} \text{ (vol\%)}$$

$$M_{tot} = \left(31.9988 \cdot \varphi_{O_2,wet} + 44.0098 \cdot \varphi_{CO_2,wet} + 18.0152 \cdot \varphi_{H_2O,wet} + 28.158 \cdot \varphi_{N_2,wet}\right)/100$$

where 28.158 is mole weight for N_2+Ar

- $q_{m_{g7}}$ is mass flow of wet flue gas (kg/s)
- P is net produced electrical/mechanical output (kW)

Comparison of constants used in Fuelsim and ISO 11042-1.

	Fuelsim	**ISO 11042-1**
Mole volume (Nm^3/kmole):		
V_{Mole}	22.414	
Mole weight (kg/kmole)		
O2	31.9988	31.9988
CO2	44.00995	44.0098
H2O	18.01534	18.0152
N2	28.0134	
Ar	39.948	
N2+Ar	28.1549	28.158
NO	30.0061	
NO2	46.0055	
CO	28.01055	
SO2	64.0628	
CH4	16.04303	
C	12.01115	
H	1.00797	
O	15.9994	
N	14.0067	
S	32.064	

	Fuelsim	**ISO 11042-1**
M_i/V_{mn} (kg/Nm^3):		
NO	1.3387	1.3387
NO2	2.05257	2.05255
CO	1.2497	1.2497
SO2	2.858	2.858
CH4	0.7158	0.7157
3.6*M_i:		
NO	108.02	108.02
NO2	165.62	165.64
CO	100.84	100.84
SO2	230.63	230.61
CH4	57.75	57.75