MBR data treatment

May 7, 2009, Trondheim

by

Øyvind Skreiberg

Content

- Introduction
- Theory
- Data treatment procedure
- Demonstration
- Tasks to be carried out

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).

With optional preheating

Solid or liquid fuel:
C,H,N,S,O,H_2O(l)

or

Fuel gas:
Any gas mixture only containing C,H,N,S,O
+ water injection

+

With optional preheating

Oxidant:
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

=

Adiabatic temperature

Products:
Combustion, gasification or pyrolysis gas products:
O_2, CO, NO, NO_2, UHC, SO_2, N_2O, H_2, NH_3, HCN, Tar, CO_2, N_2, Ar and H_2O

Conservation of mass and energy

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.

Emission conversion

Emissionconversions are carried out using the Fuelsim- Average fuel composition, heating value and the selected defaults

Input: UHV / EHV — Input: Dry fuel/FG / Wet fuel/FG

Convert from O_2 7 vol% dry

to O_2r 11 vol% dry

Convert | Insert

Input: ppm (dry)

Output: ppm (dry) at O2r

Output: UHV / EHV — Output: Dry fuel/FG / Wet fuel/FG

	Input	Output
CO	1000	713.21
UHC as C_xH_y	300	213.96
Tar as $C_{xt}H_{yt}$	200	142.64
NO	50	35.66
NO_2	5	3.57
N_2O	3	2.14
NH_3	2	1.43
HCN	1	0.71
H_2	500	356.61
SO_2	25	17.83

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:

Convert from O_2	7	vol% dry

Push-button:

Volume fraction

Pull-down menu:

ppm (dry)

Option-button:

UHV

EHV

Input box:

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

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, Norwegian University of Science and Technology, Department of Energy and Process Engineering, NO-7491 Trondheim, Norway, e-mail: Oyvind.Skreiberg@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.ieabcc.nl/

Theory

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

Theory

See FUELSIM-Average_v1.2.xls

See Average-Report-v1.1.pdf

Procedure for treatment of experimental results

- Convert log files to proper input data in pre-prepared Excel spreadsheet
- Remove data points that does not belong there (not necessarily easy)
- Insert the useful log files data in the proper place in the pre-prepared Excel spreadsheet:
  - FTIR data in sheet "SEARCHRESULTS"
  - Temperature data in sheet "SEARCHRESULTS"
- Insert the fuel composition in sheet "Matrix"
- Delete excess rows in sheet "SEARCHRESULTS" and sheet "Experiment" if your experiment has less data points than the one existing in the pre-prepared Excel spreadsheet
- or copy rows/formulas down if your experiment has more data points than the one existing in the pre-prepared Excel spreadsheet
- Perform the calculations (by pushing the "RUN" button in sheet "Experiment")
- Selected pre-prepared graphs can be viewed directly in sheet "Figures" when the calculations have finished
- Check the figures for:
  - Calculated CO2 versus measured CO2 and calculated H2O versus measured H2O
  - Errors or unexpected results
- Add graphs or calculations if wished for

Demonstration

of one experiment

You can try the other one afterwards

Tasks to be carried out

- Convert the raw data into useful and quality controlled results using pre-prepared Excel worksheet (explanation/theory and demonstration on Thursday)

- Extract the following key data for each fuel
  - Burning rate
  - Excess air ratio
  - Emissions levels of NOx, N2O, SO2 and HCl
  - Conversion factors for fuel N, S and Cl
  - Emission levels of NOx as a function of excess air ratio
  - Axial temperature profile in the reactor at each experimental condition

- Compare the above data for the two fuels

- Suggest explanations for differences in the results

- Discuss within your group: How would you design an experimental setup for improved constant operating conditions?