

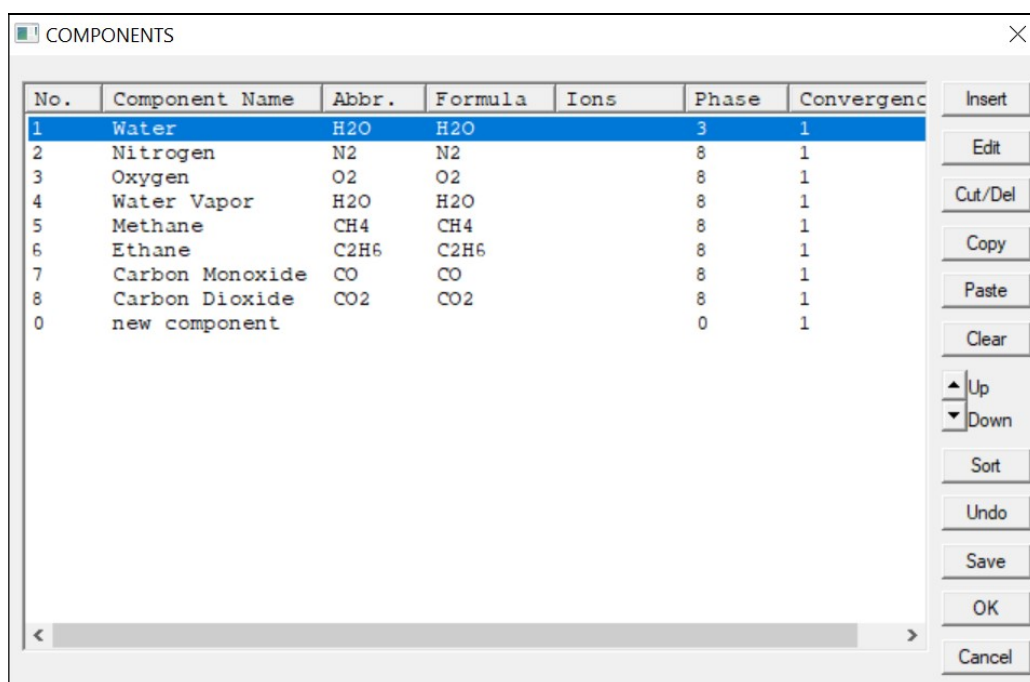
## NATURAL GAS BURNER EXAMPLE

The following example is designed to demonstrate METSIM® fundamentals, simple chemistry, heat balancing, and the use of feedback controls in a flowsheet.

1. In *Model Parameters*, under the *Project* tab, type 'Natural Gas Burner Example' for the Title and 'Training' for the Case. Also, under the *Calc Parameters* tab, change the units for this example to *metric tonne*.
2. From the *Comp* menu at the top of the screen, select *DBAS Component Database* to select the desired components. For this example, you will need to add the following components (do not include the YAWS database): CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>, CO, and CO<sub>2</sub> (recall that H<sub>2</sub>O<sub>(l)</sub>, N<sub>2</sub>, O<sub>2</sub>, and H<sub>2</sub>O<sub>(v)</sub> are defaulted in the component list).

Note: When there are two (2) identical components in the database within the same phase, the first listed is written with the newest data available and there are slight variations between them. In most occasions, the first component listed is the desirable selection.

3. From the *Comp* menu, select *ICOM Edit Components* and sort the component list in the following order (using the Up and Down buttons, alternatively sort by phase by clicking on the column name "Phase"):



No.	Component Name	Abbr.	Formula	Ions	Phase	Convergence
1	Water	H2O	H2O		3	1
2	Nitrogen	N2	N2		8	1
3	Oxygen	O2	O2		8	1
4	Water Vapor	H2O	H2O		8	1
5	Methane	CH4	CH4		8	1
6	Ethane	C2H6	C2H6		8	1
7	Carbon Monoxide	CO	CO		8	1
8	Carbon Dioxide	CO2	CO2		8	1
0	new component				0	1

Note: Always check that Water is first in the aqueous phase and Nitrogen is first in the gas phase

- From the *GEN* screen object button, select a *MIX Stream Mixer* and add it to the palette area (increase the size of the unit operation by first clicking on the *Change Object Size* button and left clicking on the unit operation number). Connect three (3) streams, two inputs and one output (numbered 1 and 2 for inputs; 3 for output). Before stream compositions can be entered, enter 1 MT/HR for the respective phases (in this case - GAS). The stream compositions can be entered by first clicking the *Edit Object Data* and then left clicking on the stream number of each stream and should be set up as follows:

Stream 1 – 20% w/w CH<sub>4</sub>; 80% w/w C<sub>2</sub>H<sub>6</sub>

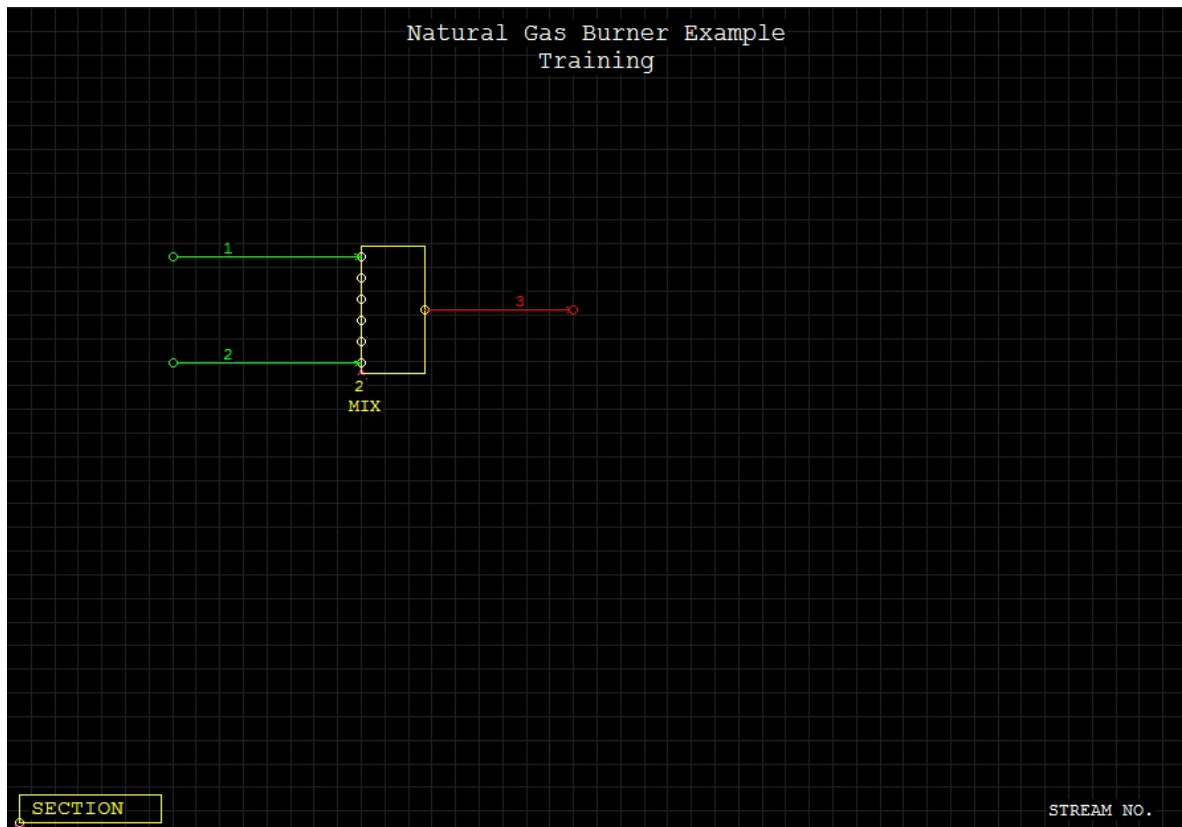
	Wt. Frac	Mol. Frac	KG/HR
H2	0	0	0
O2	0	0	0
H2O	0	0	0
CH4	0.2	0.3190726	0.2
C2H6	0.8	0.6809273	0.8
CO	0	0	0
CO2	0	0	0

Stream 2 – Air – 23% w/w O<sub>2</sub>; 1% w/w H<sub>2</sub>O<sub>(v)</sub> (the remainder will default to N<sub>2</sub>)

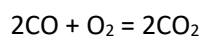
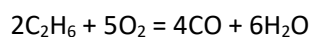
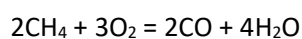
	Wt. Frac	Mol. Frac	KG/HR
H2	0.76	0.7779682	0.76
O2	0.23	0.2061143	0.23
H2O	0.01	0.0159173	0.01
CH4	0	0	0
C2H6	0	0	0
CO	0	0	0
CO2	0	0	0

Note: When entering assays for input streams, the fraction of the flow remaining will default to the component at the top of the list for the respective phases present (ie. H<sub>2</sub>O and N<sub>2</sub>).

The model should appear as follows:



5. Click on the *Edit Object Data* button so that the *Stream Mixer* may be edited. Left click on the unit operation number of the *Stream Mixer* and in the *Reactions* tab the following three chemical reactions are entered to simulate the burning of natural gas. This is achieved by first clicking on +React to add the reactants; then click on +Prod to add the products; and finally clicking on Balance to add the stoichiometry of the reaction.



Note: The reaction extent for each reaction is to be set at 1 (default).

6. Calculate the *Stream Mixer*. The result should be 2 metric tonnes of natural gas consisting of 38%w/w  $\text{N}_2$ , 9.1%w/w  $\text{H}_2\text{O}$ , 6.2%w/w  $\text{CH}_4$ , 40%w/w  $\text{C}_2\text{H}_6$ , and 6.7%w/w  $\text{CO}$ . The temperature should be  $20^\circ\text{C}$ .
7. In *Model Parameters*, under the *Calc Options* tab, select the *Heat Balance* option and recalculate the *Stream Mixer*. The temperature of Stream 3 should now be  $629.2^\circ\text{C}$ .

8. In order to control the excess oxygen injected, the next step is to put a *Feedback Controller (FBC)* on the air stream (stream 2). From the *CTL* button, select the *FBC* and put it on stream 2. The input sheets should be set-up as shown:

FEEDBACK CONTROLLER	
FBC 1	FBC 2   Notes
FEEDBACK CONTROLS simulate PID controls and other constraints.	
ON	<input checked="" type="checkbox"/> Controller On
CN	<input type="text" value="1"/> Control Loop Number, (use with VCTL value functions).
TY	<input type="text" value="FBC"/> Controller Type: FRC, FFC, PSC, FBC
Controller Description	
ID	<input type="text" value="Excess Air Controller"/>
OP	<input type="text" value="2"/> * Unit operation no. where set point is calculated.
NO	<input type="text" value="2"/> * Unit operation no. where controlled variable is used.
ADJUSTED STREAM OR MANIPULATED VARIABLE:	
SN	<input type="text" value="s2"/> * If a stream or streams are to be adjusted, enter number(s) or a predefined vector of the numbers. If parameter 'vn' or a reaction extent is to be adjusted, enter 0, And: Enter 'vn-VCTL CN' in the unit op 'Controls CtB' field, Or: Enter 'VCTL CN' in the reaction 'EXPRESSION FOR EXTENT.' Also: Enter the starting value in the output field below.
OV	<input type="text" value="0"/> Output value of adjusted variable.
LV	<input type="text" value="1"/> * Lower limit of adjusted variable.
HV	<input type="text" value="100"/> * Upper limit of adjusted variable.

FEEDBACK CONTROLLER

FBC 1 **FBC 2** Notes

VALUE FUNCTION for CONTROLLED/MEASURED VARIABLE \_SET POINT:  
APL expression for the current value of the set point variable.

VF

SP  \* Set Point

DB  Not used

SL  Proportionality Switch

\* If VF increases with an increase in Controller Output, enter '1'.  
If VF decreases with an increase in Controller Output, enter '-1'.

PID USED FOR DYNAMIC SIMULATION ONLY

CO  PID Method

PROPORTIONALITY CONSTANTS: PID control, KP \_KI required, KD optional

KP  \* Proportional gain

KI  \* Integral tuning constant

KD  Derivative tuning constant

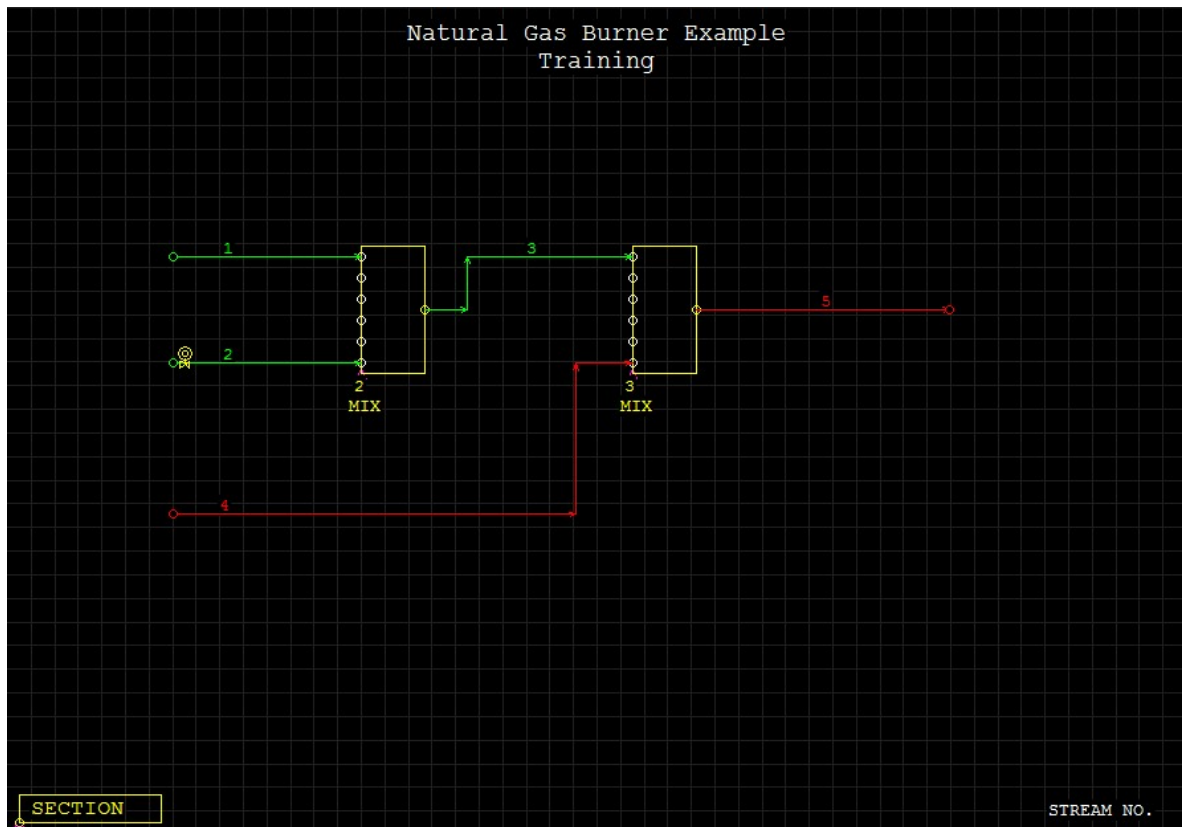
CONTROLLER TUNING PARAMETERS

EE	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	- Controller Factors
PG	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	- Controller Outputs
PV	<input type="text" value="0"/>	<input type="text" value="0"/>	<input type="text" value="0"/>	- Set Point Values

Now, calculate the *Stream Mixer* again. The air flow (stream 2) should have been set to 19.5 MT/HR by METSIM®, and the temperature of stream 3 should now be 1863°C.

- Add a second *MIX Stream Mixer* and connect stream 3 as an input. Also add stream 4 as an input to the new *Stream Mixer* as well as an output stream, stream 5 (as seen below).

Note: The most effective way to add stream 3 as an input to the second *MIX* is to *Edit* the second *MIX* and enter a '3' in the *Feed 1* field. Then, simply move the stream as desired.



10. Using the *Copy Object Data* button, copy the stream information from stream 2 and paste it into stream 4. Ensure that *Replace Data* is selected on the *Data Copying* tab and that all the *Stream Values to be Copied* boxes are checked on the *Switches* tab. After clicking *OK*, left click on stream 2 and right click on stream 4 (the streams should turn violet as they are selected). Redraw the flowsheet.
11. Calculate the Section. The temperature of stream 5 should read 1044°C.
12. To control the temperature of stream 5 to 345°C, place a *Feedback Control* on stream 4 using the following parameters:  
  
OP = 3; NO = 3; SN = s4; LV = 1; HV = 150; VF = VTEM s5; SP = 345; SL = -1
13. Calculate the section. Stream 4 should be set to 113 MT/HR and stream 5 should be 345°C.
14. To simulate Free Energy Reactors, in which the chemical reactions written earlier are disregarded, change the *Unit Operation Code* from *MIX* to *FEM* for both *Stream Mixers*. The inputs for this unit operation are different from the *MIX*, and therefore will alter the stream routes. The streams may be re-routed using the *Move Object* button.
15. Set the parameters in both FEM unit operations as seen below:

GIBBS FREE ENERGY EQUILIBRIUM								
	Labor	Materials		Reagents		Notes		
FEM	Parameters	Phase Splits	Components	Reactions	Equil.	Heat Bal	Logic	Controls
CO	<input type="text" value="1-Calculate equilibrium temperature"/> * Calculation Option Recommend setting temperature until stability is achieved							
TE	<input type="text" value="0"/>	0 Equilibrium temperature °C						
PR	<input type="text" value="0"/>	* Pressure in kPa						
IN	<input checked="" type="checkbox"/> * Use last FEM solution for initial estimate							
LE	<input checked="" type="checkbox"/> * Perform Gibb's Free Energy leveling							
TR	<input checked="" type="checkbox"/> * Allow Gibb's data extrapolation outside temp range							
AC	<input type="checkbox"/> * Calculate activity coefficients							
AC2	<input type="checkbox"/> * Calculate 2nd activity coefficients							
AN	<input type="text"/>	* Name of activity coefficient subroutine						
DX	<input type="checkbox"/> * Display intermediate calculations							
ER	<input type="checkbox"/> - Math error occurred during calculations							
PA	<input type="text" value="10"/>	- Convergence parameter						
TS	<input type="text" value="0.5"/>	- Temperature step						

16. Add the following components to the *Component List* using the *DBAS Component Database*: NO, NO<sub>2</sub>, NO<sub>3</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>3</sub>, N<sub>2</sub>O<sub>4</sub> (gas), and N<sub>2</sub>O<sub>5</sub>
17. Calculate the section. Stream 5 should now contain various NO<sub>x</sub> components.