NATURAL GAS BURNER EXAMPLE

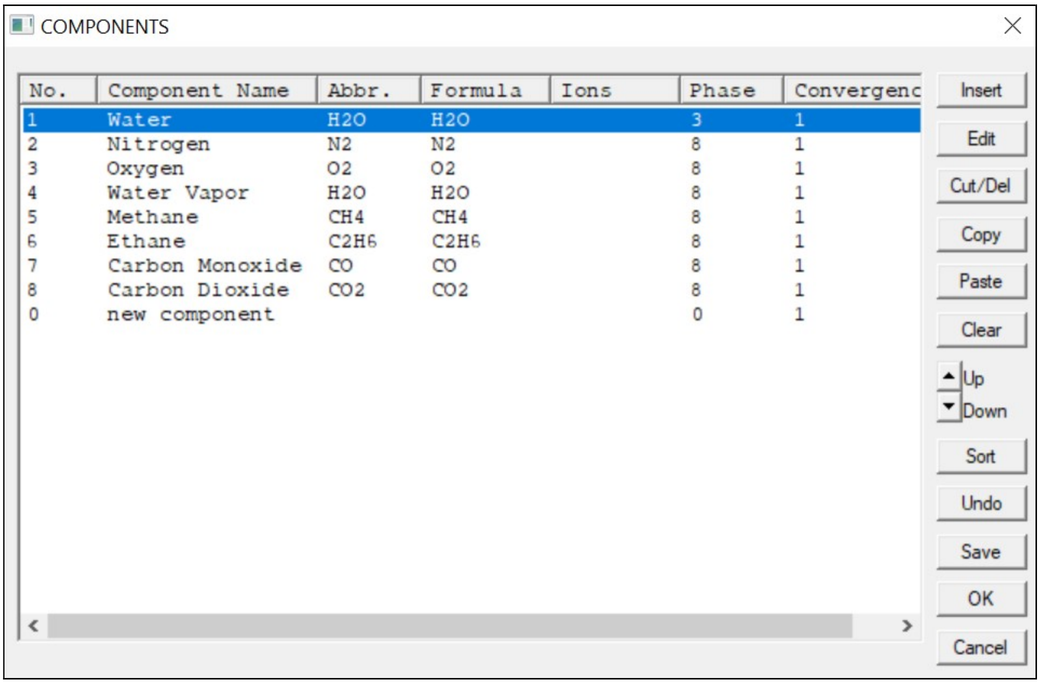
The following example is designed to demonstrate METSIM® fundamentals, simple chemistry, heat balancing, and the use of feedback controls in a flowsheet.

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_4, C_2H_6, CO, and CO_2 (recall that $H_2O_{(l)}$, N_2, O_2, and $H_2O_{(v)}$ 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"):

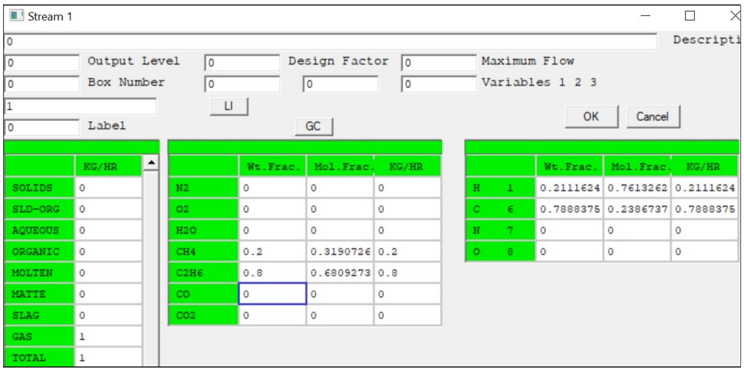


No.	Component Name	Abbr.	Formula	Ions	Phase	Convergenc
1	Water	H2O	H2O		3	1
2	Nitrogen	N2	N2		8	1
3	Oxygen	O2	O2		8	1
4	Water Vapor	H2O	H2O		8	1
5	Methane	CH4	CH4		8	1
6	Ethane	C2H6	C2H6		8	1
7	Carbon Monoxide	CO	CO		8	1
8	Carbon Dioxide	CO2	CO2		8	1
0	new component				0	1

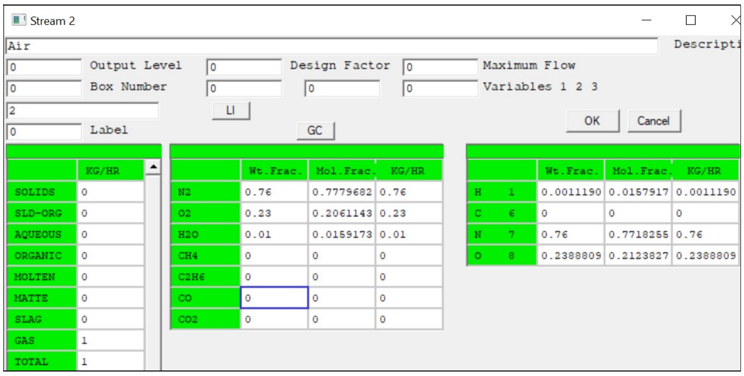
Note: Always check that Water is first in the aqueous phase and Nitrogen is first in the gas phase

4. 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_4; 80% w/w C_2H_6

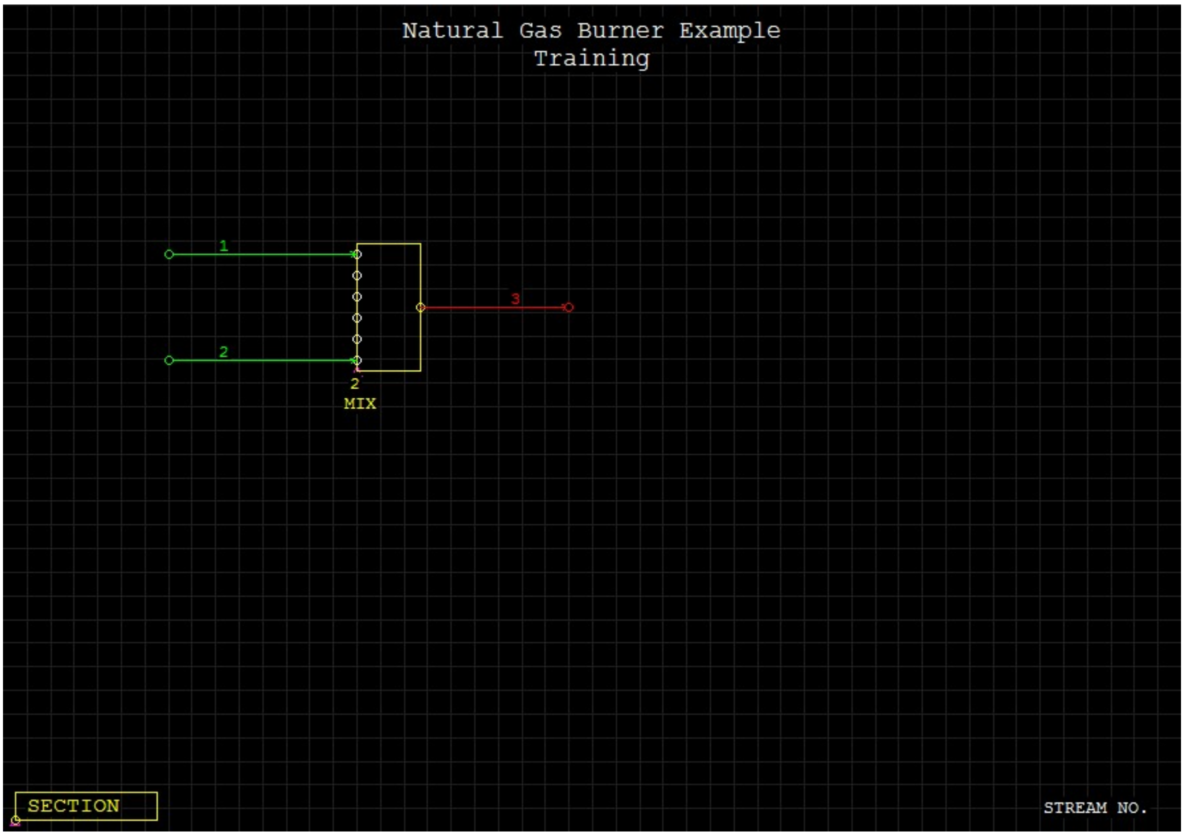


Stream 2 – Air – 23% w/w O_2; 1% w/w $H_2O_{(v)}$ (the remainder will default to N_2)



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_2O and N_2).

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.

   $2CH_4 + 3O_2 = 2CO + 4H_2O$

   $2C_2H_6 + 5O_2 = 4CO + 6H_2O$

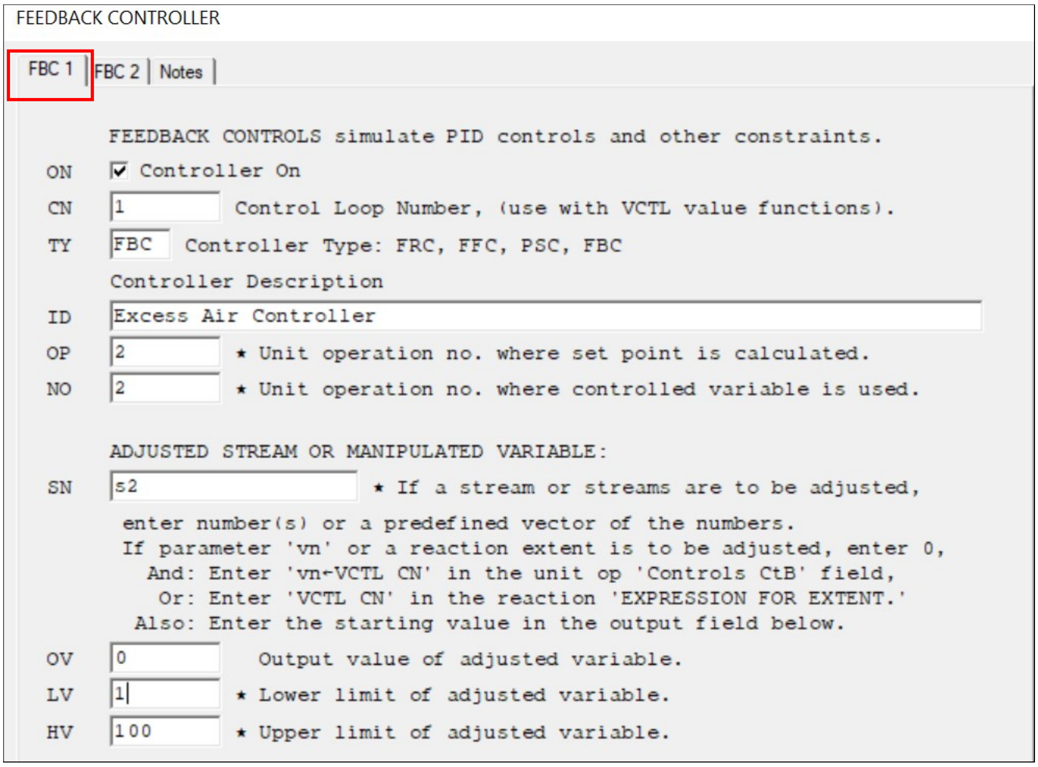
   $2CO + O_2 = 2CO_2$

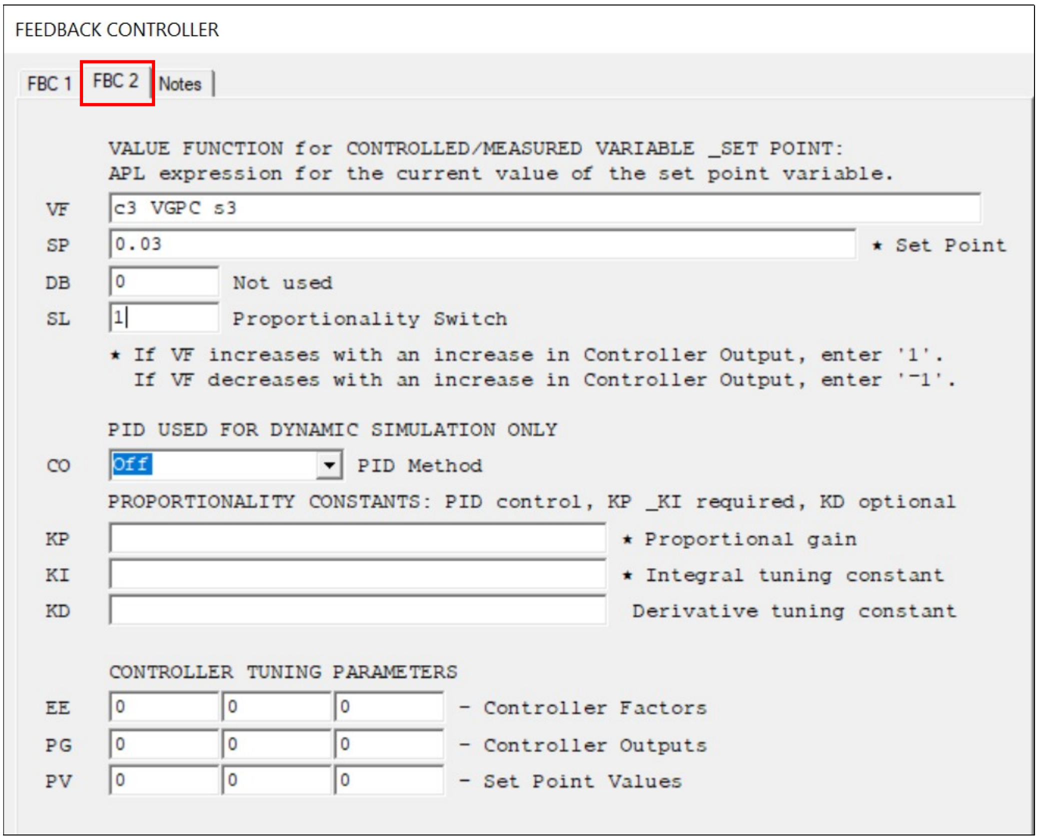
   Note: The reaction extent for each reaction is to be set at 1 (default).

6. Calculate the *Stream Mixer*. The result should be 2 metric tonnes of natural gas consisting of 38%w/w N_2, 9.1%w/w H_2O, 6.2%w/w CH_4, 40%w/w C_2H_6, and 6.7%w/w CO. The temperature should be 20°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°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:

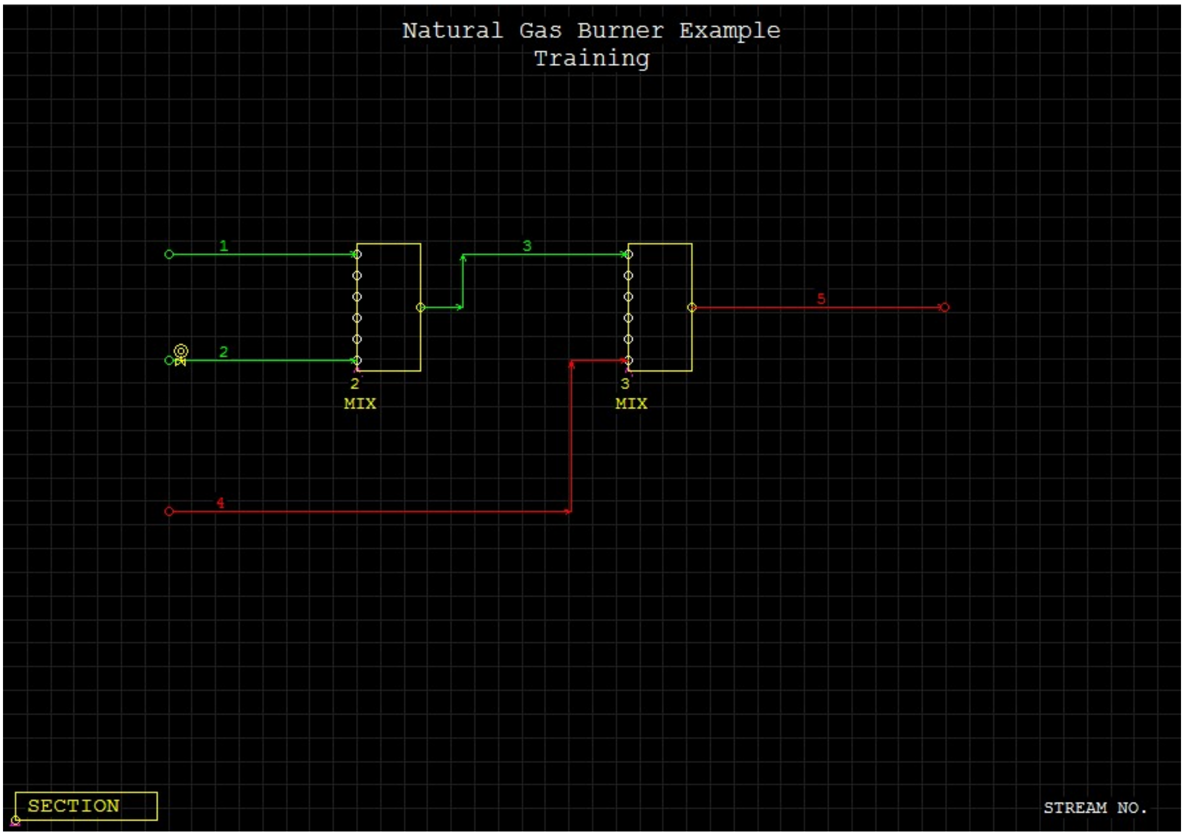




Now, calculate the *Stream Mixer* again. The air flow (stream 2) should have been set to 19.5 MT/HR by METSIM®, and the temperature of stream 3 should now be 1863°C.

9. 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 allthe *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.

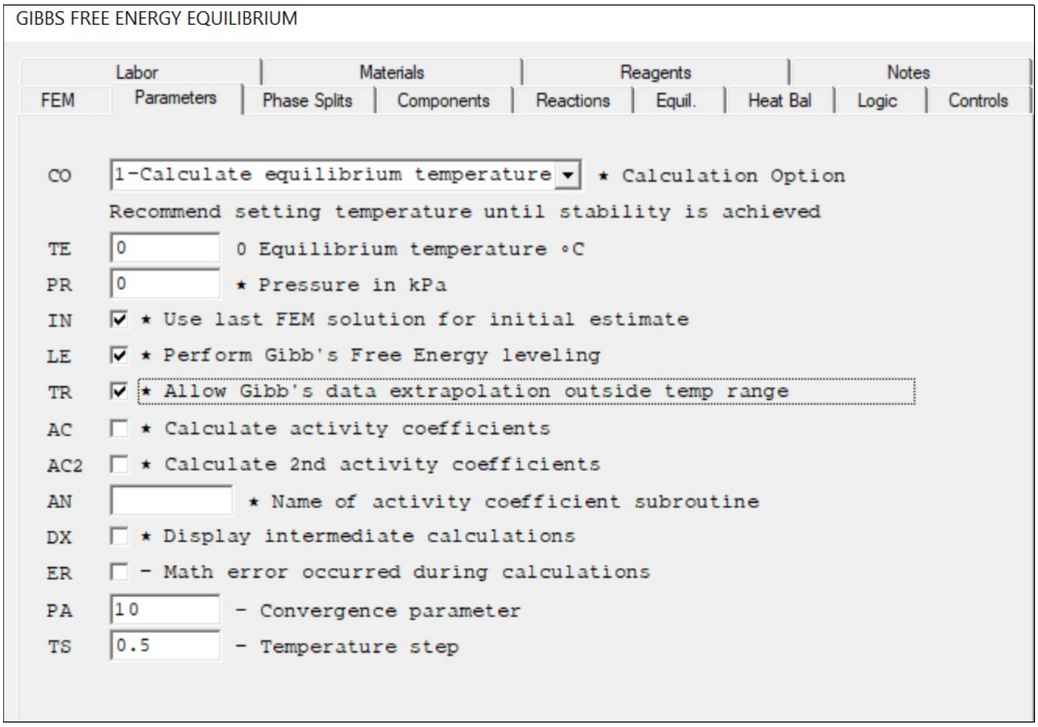
12. To control the temperature of stream 5 to 345°C, place a *Feedback Control* on stream 4 using the following parameters:

    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:



16. Add the following components to the *Component List* using the *DBAS Component Database*: NO, NO2, NO3, N2O, N2O3, N2O4 (gas), and N2O5

17. Calculate the section. Stream 5 should now contain various NO_X components.