NATURAL GAS COMBUSTION MODELING

This case study demonstrates the use of Flownex® to model and analyse a natural gas combustion process. Several compound components have been developed to assist and simplify the modelling process.

OIL AND GAS INDUSTRY

Challenge:

The main challenge in this case study is the application of Flownex® to:

- conveniently and easily specify and model natural gases;
- analyze natural gas properties;
- conveniently and easily specify ambient conditions, using ambient air as the oxidant;
- perform the combustion process and extract meaningful results; and
- analyze the flue gas emissions.

Benefits:

By creating compound components for the specification and analysis of gas compositions, and by wrapping the Flownex® *Adiabatic Flame* model and some associated scripts in another compound component, Flownex® may be used to perform extremely powerful combustion modeling in a very simple and efficient manner. Furthermore, this basic combustion model may be used in conjunction with other heat transfer and fluid flow processes to create very comprehensive, yet easy to use models of industrial applications. This combined capability of modeling combustion, fluid flow and heat transfer is not commonly available in other design tools.

Solution:

Flownex® could effectively be used to model natural gas combustion processes.

"There are several dedicated software tools available on the market to model combustion processes; however none of them - except maybe full-fledged 3D CFD models which are not likely to be reusable and user friendly - are able to also model the fluid flow, thermodynamics and heat transfer processes in a single environment. The power and convenience of Flownex has been demonstrated in that a comprehensive, but simple to use combustion model, could be developed and implemented with some simple, reusable compound elements that I could develop myself."
Hannes van der Walt
Principal Thermal Engineer
Gasco Pty Ltd

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Introduction

The Flownex® *Adiabatic Flame* model is based on the *NASA Glenn Chemical Equilibrium Program CEA2* and supports a large range of fuels. The development of the natural gas combustion model has only attempted to implement a combustion model for typical natural gas compositions. It would be easy to add capabilities for other fuel components, whether gaseous or liquid.

The development of this model essentially comprised of three basic fields of development. Firstly, some effort went into defining fluid tables for the selected natural gas components (listed in Table 2) in such a way that accurate interpolation would result at low partial pressures and at temperatures exceeding those expected during combustion. Secondly, a suite of compound components were developed to assist with the convenient specification and analysis of the gas components. Thirdly, a Simple Burner model was developed by wrapping the Flownex *Adiabatic Flame* model in a compound component together with a script to enable the specification and calculation of typical natural gas burner performance parameters.

"Using a few simple compound components, the capabilities of Flownex® has been extended easily to include natural gas combustion processes. It has been shown that the results obtained are accurate and in close agreement with other available software. This extension enables Flownex® to be utilised as a complete heat and mass balance tool whilst simultaneously performing as a fluid dynamics, thermodynamics and heat transfer tool in this industry. The ability to extend the capability of Flownex® for any particular task through simple compound components sets Flownex® apart from other tools in the industry."

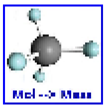
Model

The gas tables were created in Aspen HYSYS for each component and range in pressure from 0.0001 kPa to 200 kPa. The assumption is that the combustion process itself will be atmospheric, around 100 kPa (abs). Similarly, the gasses are defined between -10ºC and 2500ºC, so care should be taken to ensure gas inlet temperatures are not sub-zero to be safe.

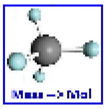
Unfortunately, only hydrocarbon gasses up to Octane (C8) are supported by the NASA Glenn Chemical Equilibrium Program CEA2 on which this model is based. The combustion model also produces NO, O and OH. These fluids are not in the fluid mixture, so a warning will be produced as a result. The mass (and mol) fractions of these fluids are added to that of Argon and hence the mass fraction of Argon will appear to increase from inlet to outlet.

Flownex® deals with combustion gas mixtures via the specification of the mixture mass fractions at the boundaries. Similarly, the combusted flue gas may be analysed at any node downstream of the *Adiabatic Flame* model. As gas compositions are commonly specified in mol fractions rather than mass fractions, a suit of 5 scripts, each wrapped in a compound component for convenience has been developed. These serve as inputs and outputs of information to and from the burner compound component.

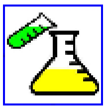
Air Psychrometry. This component calculates the ambient air composition in mass and mol percentage given the site elevation, the atmospheric temperature and the relative humidity. This component may be used to specify the oxidant (air) composition at the inlet boundary via a data transfer link.



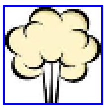
NG Mol to Mass. This component may be used to specify the fuel gas composition in mol percent. It will then calculate the equivalent mass percentage for each of the constituents. These results (mass percentages) may then be transferred from the component to the fuel gas inlet boundary via a data transfer link.



NG Mass to Mol. This component performs the reverse calculation of the one above. It may be used to convert a given composition anywhere in the network (nodes typically) from mass percent to mol percent.



NG Combustion Props. This component provides the user with an analysis of the specified fuel properties such as heating values, molar mass, standard density, stoichiometric air-fuel ratios (dry and wet) etc. It may be connected to either of the two components above (it accepts inputs in mol percent) or it may be used on its own as a calculation tool.



NG Flue Gas Analysis. This component is used to analyze flue gasses. It accepts inputs in mass percent from any node in the network and converts the flue gas to mol percent for convenience. Based on the water and SO_2 fractions present in the flue gas, it also estimates the water and SOx dew point temperatures.

Basic Burner. This component is a simple compound wrapped around the *Adiabatic Flame* model. It includes a script which calculates the burner heat release (HHV) from the flue mass flow rate and the inlet and outlet enthalpies.

CASE STUDY

As an example, a hypothetical natural gas which contains all the gas species supported by the model is combusted using wet atmospheric air as the oxidant. The results are then compared with the results of other available software.

Data Specification

The example uses the following data specification:

Table 1: Input Data

Property	Unit	Value
Fuel gas flow rate	kg/hr	10
Fuel inlet temperature	°C	30
Excess air	%	25
Site elevation	m	35
Atmospheric temperature	°C	24
Atmospheric air relative humidity	%	80

The hypothetical natural gas composition is shown in Table 3 below.

Results Comparison & Discussion

Air Psychrometry

The simplest compound component in the natural gas combustion suite is the *Air Psychrometry* component which implements equations from ASHRAE. Given typical site conditions – altitude, temperature and relative humidity – this component aims to calculate the ambient pressure and ambient air composition. This information is then assigned to the combustion system's air inlet boundary component. Using the inputs given in the table above, calculations from this component are compared with results from other software in the following table:

Table 2: Atmospheric and Psychrometric Calculations

Air Properties	Unit	Flownex	WinBurn (1)	Ashrae (2)	Psychro Calc (3)
Pressure	kPa	100.905	-	100.9	100.9
Density	kg/Sm^3	1.172	-	1.155	1.173
Dew point temperature	°C	20.6	-	20.4	20.5
Air Composition:					
N_2 – Nitrogen	Mol%	76.208	76.195		
O_2 - Oxygen	Mol%	20.443	20.494		
CO_2 – Carbon Dioxide	Mol%	0.038	0.0293		
Ar – Argon	Mol%	0.909	0.9178		
H_2O – Water vapor	Mol%	2.402	2.365		
Molar mass	kg/kmol	28.702	-		

1 WinHeat Thermal Rating Suite
2 ASHRAE Dayton Chapter (www.daytonashrae.org/psychrometrics.shtml)
3 Psychrometric Calculator (www.psychrometric-calculator.com)

It is shown that the Flownex® *Air Psychrometry* component provides accurate calculations of atmospheric air properties as well as composition.

NG Mol to Mass

The following results were obtained using the Flownex® model's *NG Mol to Mass* compound component to convert the gas composition as supplied by the user from mol% to mass% and assign it to the fuel gas inlet boundary. This conversion has been repeated in HYSYS and is compared below:

Table 3: Natural Gas Composition Conversion from Mol% to Mass%

Gas Component	Input	Flownex	HYSYS
	Mol%	Mass %	Mass %
CH_4 - Methane	78.2	58.1508	58.15
C_2H_6 - Ethane	10.0	13.9379	13.94
C_3H_8 - Propane	5.0	10.2199	10.22
C_4H_{10} - Butane	2.0	5.3883	5.39
C_5H_{12} - Pentane	0.6	2.0066	2.01
C_6H_{14} - Hexane	0.5	1.99725	2.0
C_7H_{16} - Heptane	0.4	1.85787	1.86
C_8H_{18} - Octane	0.3	1.58846	1.59
H_2 - Hydrogen	0.1	0.00934	0.01
H_2S - Hydrogen Sulfide	1.1	1.73743	1.74
CO - Carbon Monoxide	0.2	0.25967	0.26
CO_2 - Carbon Dioxide	1.0	2.03992	2.04
N_2 - Nitrogen	0.3	0.38954	0.39
Ar - Argon	0.1	0.185166	0.19
O_2 - Oxygen	0.1	0.148326	0.15
H_2O - Water	0.1	0.0835	0.08
Molar Mass	kg/kmol	21.574	21.57

It is shown that the mol% to mass% conversion agrees well with the same conversion done in HYSYS.

NG Combustion Props

The gas composition is also supplied to the *NG Combustion Props* compound component via a data transfer link to calculate the gas heating values and other properties. The results are tabled below and compared to results from HYSYS (amongst others)

Table 4: Natural Gas Properties

Gas Property	Unit	Flownex	HYSYS (1)	HMB (2)
Standard density	kg/Sm^3	0.934	0.916	0.912
Relative density	-	0.762	0.748	0.744
Compressibility Z at STP	-	0.977	0.995	-
Higher Heating Value (HHVm)	MJ/kg	50.910	51.327	51.4
Lower Heating Value (LHVm)	MJ/kg	46.211	46.577	46.6
Higher Heating Value (HHVv)	MJ/Sm^3	47.568	47.017	46.9
Lower Heating Value (LHVv)	MJ/Sm^3	43.177	42.665	42.5

1 Aspen HYSYS
2 Heat & Mass Balance by Phillip Dane, ABM Combustion Pty Ltd

These properties are not used in the actual combustion calculations implemented by the *Basic Burner* compound component as it relies on the underlying NASA Glenn Chemical Equilibrium Program CEA2. Although the results are reasonably close, they only serve to assist the user with additional information.

The small differences between the heating values may be attributed to the Flownex *NG Combustion Props* component being based on the GPSA Data Book gas property tables (www.gpsa.gpaglobal.org).

The *NG Combustion Props* component also performs air-fuel ratio calculations, the results of which are used to specify the combustion airflow at the combustion air inlet boundary. As such, the required excess air flow percentage is also specified in this component. These air-fuel ratio calculations have been compared against the results of other commercial software, the results of which are presented below.

Table 5: Natural Gas Air-Fuel Ratio Requirements

Gas Property		Flownex®	WinBurn	HMB
Air-fuel ratio (stoichiometric, dry)	-	15.954	-	-
Air-fuel ratio (stoichiometric, wet)	-	16.198	16.168	16.0
Air-fuel ratio (excess air, wet)	-	20.248	20.210	-
Fuel gas flow rate	kg/hr	10	10	-
Required air flow rate	kg/hr	202.5	202.1	-

As shown, good agreement is also achieved between the Flownex *NG Combustion Props* component and WinBurn. Further verification of the air-fuel ratio calculation is also provided below with the combustion calculation comparison, using WinBurn and HMB.

Basic Burner & NG Flue Gas Analysis

As previously discussed, the *Basic Burner* compound component is simply a wrapper around the Flownex *Adiabatic Flame* element, which itself simply implements the NASA Glenn Chemical Equilibrium Program CEA2. The results of the *Basic Burner* component is the heat release and of course the conversion of the natural gas components to products of combustion. The results of the *Basic Burner* and *NG Flue Gas Analysis* components are therefore best verified together.

This *NG Flue Gas Analysis* compound component is used to analyse natural gas products of combustion. The flue gas composition is transferred from a node downstream of the *Basic Burner* via a data transfer link. The component will then convert the results from mass% to mol% for presentation as well as calculating the flue gas molar mass and water dew point temperature. In cases where hydrogen sulfide is present in the fuel gas, the SOx acid dew point temperature is also calculated. The SOx dew point temperature depends on an assumed SO_3 to H_2SO_4 conversion rate which may be specified in the component. The default value of 5% is frequently assumed in the gas industry. For the example at hand, the results compare as follows:

Table 6: Combustion Performance and Flue Gas Analysis

Property	Unit	Flownex	WinBurn	HMB
Fuel flow rate	kg/hr	10	-	10
Air flow rate	kg/hr	202.5		202.5
Combustion Heat Release (HHV)	kW	140.7		145
Adiabatic flame temperature	°C	1697.3		1718
Flue Gas Composition:				
N_2 Nitrogen	Mol%	70.716	70.733	71.6
O_2 Oxygen	Mol%	3.653	3.803	3.8
CO Carbon Monoxide	Mol%	0.044	0.0	-
CO_2 Carbon Dioxide	Mol%	8.152	8.184	8.2
SO_2 Sulfur Dioxide	Mol%	0.067	0.155	0.067
Ar Argon	Mol%	1.135	0.852	-
H_2 Hydrogen	Mol%	0.014	0.0	-
H_2O Water	Mol%	16.220	16.273	16.3
Molar Mass	kg/kmol	27.997	27.949	-
Water dew point temperature	°C	55.8	-	-
SOx acid dew point temperature	°C	149.7	-	-

The HMB model does not perform any psychrometric calculations, hence the combustion air composition was simply copied from the Flownex® calculations. Furthermore, the Winburn and HMB models do not calculate the production of CO and HMB does not account for the production of Argon or Hydrogen. The Flownex combustion model also produces very small amounts of other combustion products including NO, O and OH which are not included in the gas definition, and these have been added to Argon for simplicity. This explains why the amount of Argon has increased and is higher than what WinBurn calculates.

The dew point calculation is checked against ES Flue Gas which is a dedicated software to calculate flue gas properties.

Table 7: Dew Point Calculations

Property	Unit	Flownex	ESFG (1)
Water dew point temperature	°C	55.8	55.9
SOx acid dew point temperature (5% SO3 conversion rate)		149.7	-
SOx acid dew point temperature (3.9% SO3 conversion rate)			
Okkes method	°C	146.3	145.9
Verhoff method	°C		150.2

1 ES_FlueGas by ENGSoftware.

It is shown that accurate dew point temperatures are predicted by the *NG Flue Gas Analysis* compound component and that a 5% SO_3 conversion rate is a conservative estimate.

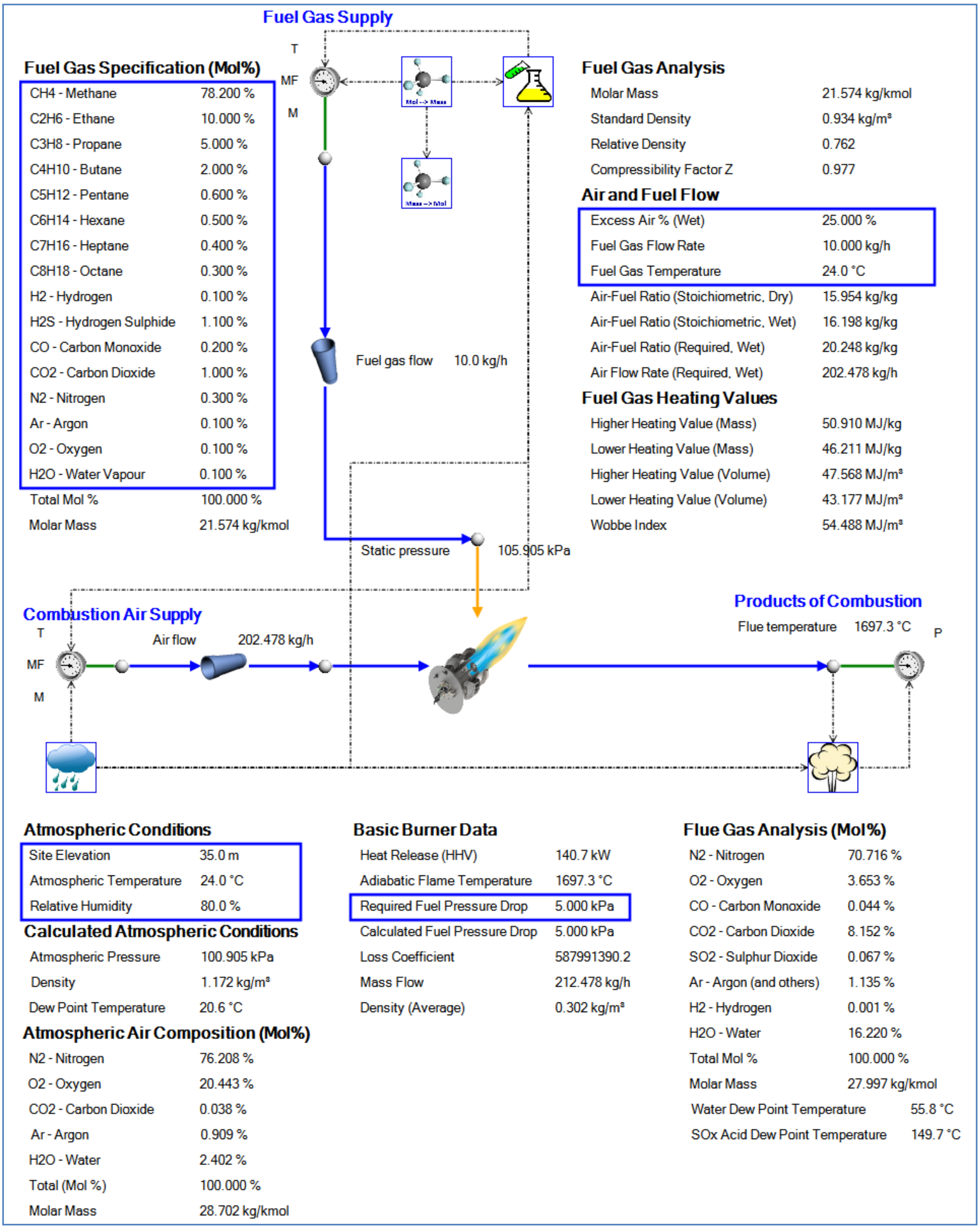


Figure 1: Flownex® Model.

Summary

Using a few simple compound components, the capabilities of Flownex® has been extended easily to include natural gas combustion processes. It has been shown that the results obtained are accurate and in close agreement with other available software. This extension enables Flownex® to be utilised as a complete heat and mass balance tool whilst simultaneously performing as a fluid dynamics, thermodynamics and heat transfer tool in this industry. The ability to extend the capabilities of Flownex® for any particular task through simple compound components sets Flownex® apart from other tools in the industry.

Case Study Flownex Model Availability

The Flownex model discussed in this case study is available in the user project downloads area located at:

http://www.flownex.com/projectlibrary