



# ADIABATIC FLAME TEMPERATURE CALCULATION USING DWSIM:

## A FREE AND OPEN-SOURCE CHEMICAL PROCESS SIMULATOR



By

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LEVEL: ADVANCED

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## PREFACE

The manual “Adiabatic Flame Temperature Calculation Using DWSIM” presents a set of “Adiabatic Flame Temperature Calculation Using DWSIM” exercise using a free and open-source chemical process simulator “DWSIM” and can be utilized to establish process simulation laboratory as part of undergraduate chemical engineering degree or in allied degree curriculum. The problem statements are of intermediate level.

### Prerequisite

- Must know about DWSIM UI/UX.
- Flow sheeting in DWSIM
- Selection of Thermodynamic Packages.
- Manipulating variables
- Combustion Calculations
- Advance Chemical Engineering Thermodynamics
- Basic Modules

Thanks

Viraj Desai

P.E. O&G

### Disclaimer

All the exercises are strictly restricted to learning only and not meant to be used in real world application.



## PROCESS SIMULATION USING DWSIM: A FREE AND OPEN-SOURCE CHEMICAL PROCESS SIMULATOR

### PREAMBLE

DWSIM is an open-source CAPE-OPEN compliant chemical process simulator. It features a Graphical User Interface (GUI), advanced thermodynamics calculations, reactions support and petroleum characterization / hypothetical component generation tools. DWSIM can simulate steady-state, vapor–liquid, vapor–liquid–liquid, solid–liquid and aqueous electrolyte equilibrium processes and has built-in thermodynamic models and unit operations (<https://en.wikipedia.org/wiki/DWSIM>). It is available for Windows, Linux and Mac OS.

The objective of the course is to create awareness of the open-source process simulator “DWSIM” among prospective graduates and practicing process engineers. The course will cover Intermediate aspects of create flow sheet in DWSIM and simulation of simple Pressure changing module like pipe segment, Compressor, etc.

### Target Audience

- Junior Interns in Process Firms
- III / Final year B. Tech. Chemical Engineering students
- M. Tech. Chemical Engineering students
- Practicing Process Engineers



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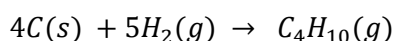
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# 1 STANDARD HEAT OF COMBUSTION

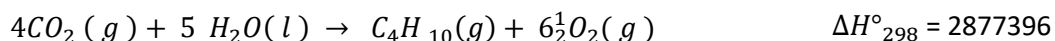
## 1.1 OVERVIEW OF STANDARD HEAT OF COMBUSTION

A combustion reaction is defined as a reaction of an element or compound with oxygen to form specified combustion products. For organic compounds consisting only of carbon, hydrogen, and oxygen, the products are carbon dioxide and water, but the state of the water may be either vapor or liquid. The value for liquid water product is called the higher heat of combustion, while that with water vapor as product is the lower heat of combustion. Data are always based on 1 mol of the substance burned.

A reaction such as the formation of n-butane:



is not feasible in practice. However, this equation results from combination of the following combustion reactions:



## 1.2 HEAT EFFECTS OF INDUSTRIAL REACTIONS

The preceding sections have dealt with the standard heat of reaction. Industrial reactions are rarely carried out under standard-state conditions. Furthermore, in actual reactions the reactants may not be present in stoichiometric proportions, the reaction may not go to completion, and the final temperature may differ from the initial temperature. Moreover, inert species may be present, and several reactions may occur simultaneously. Nevertheless, calculations of the heat effects of actual reactions are based on the principles already considered and are illustrated by the following examples, wherein the ideal-gas state is assumed for all gases.

## 2 ADIABATIC FLAME TEMPERATURE CALCULATION

### Objective

What is the maximum temperature that can be reached by the combustion of methane with 20% excess air? Both the methane and the air enter the burner at 25°C

### Data

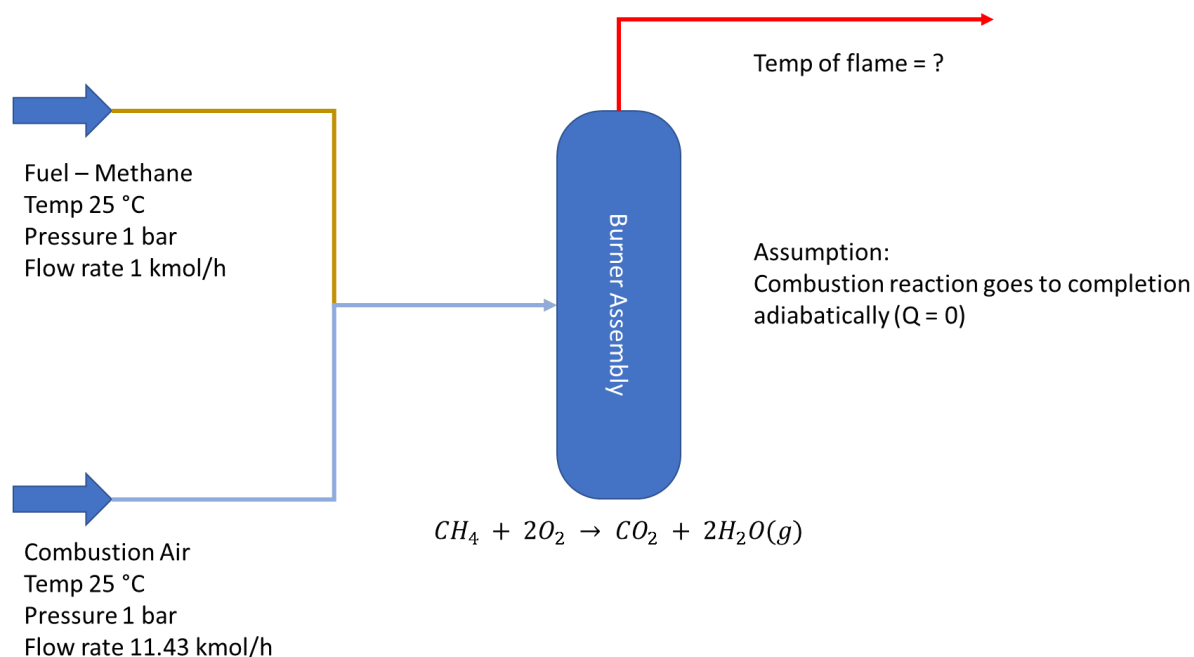


Figure 1 Problem Statement

### DWSIM Blocks Used

- Mixer
- Material Stream
- Energy Stream
- Gibbs Reactor

### Procedure

1. Start a new DWSIM Simulation (DWSIM VER 8.3.5 - CLASSIC UI). Click on “New steady state Simulation” as a template for new simulation.
2. The simulation configuration window will be opened. It shows a specification page. Add components required to solve the problem statement. In the present case, add methane, oxygen, nitrogen, carbon dioxide & water. Ensure the component is added from the same property database. For instance, in this case, both components are added from “ChemSep” database.
3. Specify the thermodynamic package as Peng-Robinson (PR) (1).
4. Customize the system of units for the simulation and click “Next”.
5. The flow sheeting section of simulation window will be opened. First, let provide fuel, air, feed, vapour, and liquids / heavy streams for the unit process to be performed.

- On clicking the "Fuel" stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, temperature, and pressure for the inlet streams. Once credentials are specified for the Fuel stream, the color of stream turns blue.

**Fuel (Material Stream)**

Information | Connections

General Info

Object: Fuel

Status: Calculated (20-01-2023 11:51:41)

Linked to:

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data | Results | Annotations | Dynamics | Floating Tables

Stream Conditions | Compound Amounts

Flash Spec: Temperature and Pressure (TP)

Temperature: 25 C

Pressure: 1 bar

Mass Flow: 0 kg/h

Molar Flow: 1 kmol/h

Volumetric Flow: 0 m3/h

Specific Enthalpy: -1.13114 kJ/kg

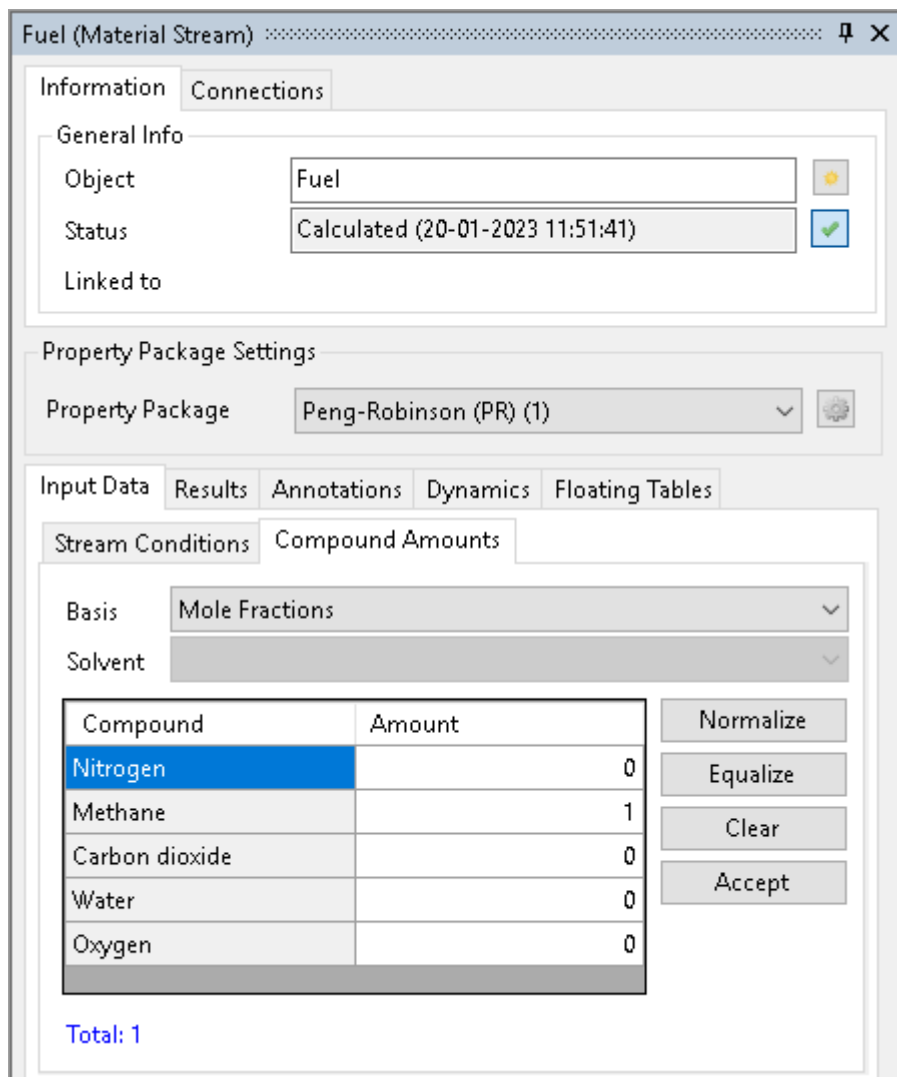
Specific Entropy: 0.00417828 kJ/[kg.K]

Vapor Phase Mole Fraction: 1

Air (Material Stream) | Vapour (Material Stream) | Fuel (Material Stream)

Figure 2 Fuel Stream Specs





**Fuel (Material Stream)**

Information | Connections

General Info

Object: Fuel

Status: Calculated (20-01-2023 11:51:41)

Linked to:

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data | Results | Annotations | Dynamics | Floating Tables

Stream Conditions | Compound Amounts

Basis: Mole Fractions

Solvent:

Compound	Amount
Nitrogen	0
Methane	1
Carbon dioxide	0
Water	0
Oxygen	0

Total: 1

Buttons: Normalize, Equalize, Clear, Accept

Figure 3 Fuel Stream Compound Amounts

- On clicking the “Air” stream, general information about the stream will be displayed on the left side of screen. Specify the feed compositions, temperature, and pressure for the inlet

streams. Once credentials are specified for the air streams, the color of stream turns blue.

Air (Material Stream)

Information

Connections

General Info

Object

Air

Status

Calculated (20-01-2023 11:51:41)

Linked to

Property Package Settings

Property Package

Peng-Robinson (PR) (1)

Input Data

Results

Annotations

Dynamics

Floating Tables

Stream Conditions

Compound Amounts

Flash Spec

Temperature and Pressure (TP)

Temperature

25

C

Pressure

1

bar

Mass Flow

0

kg/h

Molar Flow

11.43

kmol/h

Volumetric Flow

0

m3/h

Specific Enthalpy

-0.281065

kJ/kg

Specific Entropy

0.144218

kJ/[kg.K]

Vapor Phase Mole Fraction

1

Air (Material Stream)

Vapour (Material Stream)

Fuel (Material Stream)

Figure 4 Air Stream Specs

**Air (Material Stream)**

Information | Connections

General Info

Object: Air

Status: Calculated (20-01-2023 11:51:41)

Linked to:

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Input Data | Results | Annotations | Dynamics | Floating Tables

Stream Conditions | Compound Amounts

Basis: Mole Fractions

Solvent:

Compound	Amount
Nitrogen	0.78787879
Methane	0
Carbon dioxide	0
Water	0
Oxygen	0.21212121

Buttons: Normalize, Equalize, Clear, Accept

Total: 1

Air (Material Stream) | Vapour (Material Stream) | Fuel (Material Stream)

Figure 5 Air Stream Compound Amounts

- Below the Unit Operation tab on left, locate the Stream Mixer. Drag and drop into the flow sheet. Rename it as "Mixer".

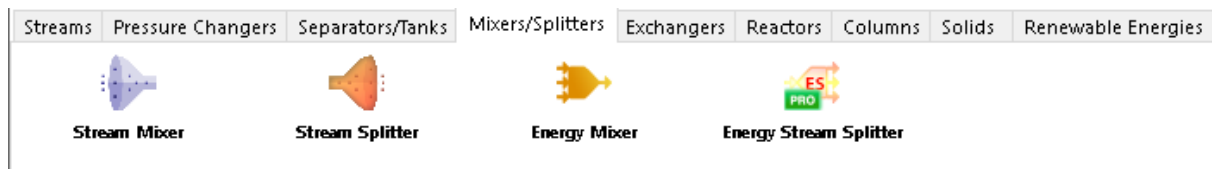


Figure 6 Mixer block

9. Under specification for Mixer add the data as follows.

Mixer (Stream Mixer)

General

Object: Mixer

Status: Calculated (20-01-2023 11:51:41) ☒

Linked to:

Connections

Inlet Stream 1: Fuel

Inlet Stream 2:

Inlet Stream 3:

Inlet Stream 4:

Inlet Stream 5:

Inlet Stream 6: Air

Outlet Stream: Feed

Calculation Parameters

Pressure Calculation: Inlet Minimum

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Notes

Rich text editor toolbar with icons for Bold, Italic, Underline, Strikethrough, Bulleted List, Numbered List, and Indentation.

Figure 7 Mixer block Specs

10. Below the Unit Operation tab on left, locate the Gibbs Reactor. Drag and drop into the flow sheet. Rename it as “Gibbs Reactor”. And select adiabatic mode in calculation parameter.

Gibbs Reactor (Gibbs Reactor)

General Info

Object: Gibbs Reactor

Status: Calculated (20-01-2023 11:51:59) ☒

Linked to:

Connections

Inlet Stream: Feed

Outlet Stream 1: Vapour

Outlet Stream 2: Liquids / Heavy

Energy Stream: E1

Calculation Parameters

Parameters | Compounds | Elements | Convergence

Reaction Set: Default Set

Calculation Mode: Adiabatic

Outlet Temperature: 1800.64 C

Pressure Drop: 0 bar

Property Package: Peng-Robinson (PR) (1)

External Solver:

Results

Mixer (Stream Mixer) | Gibbs Reactor (Gibbs Reactor)

Figure 8 Gibbs Reactor Specs

11. Make sure to select all compounds in Compounds ribbon of Gibbs Reactor

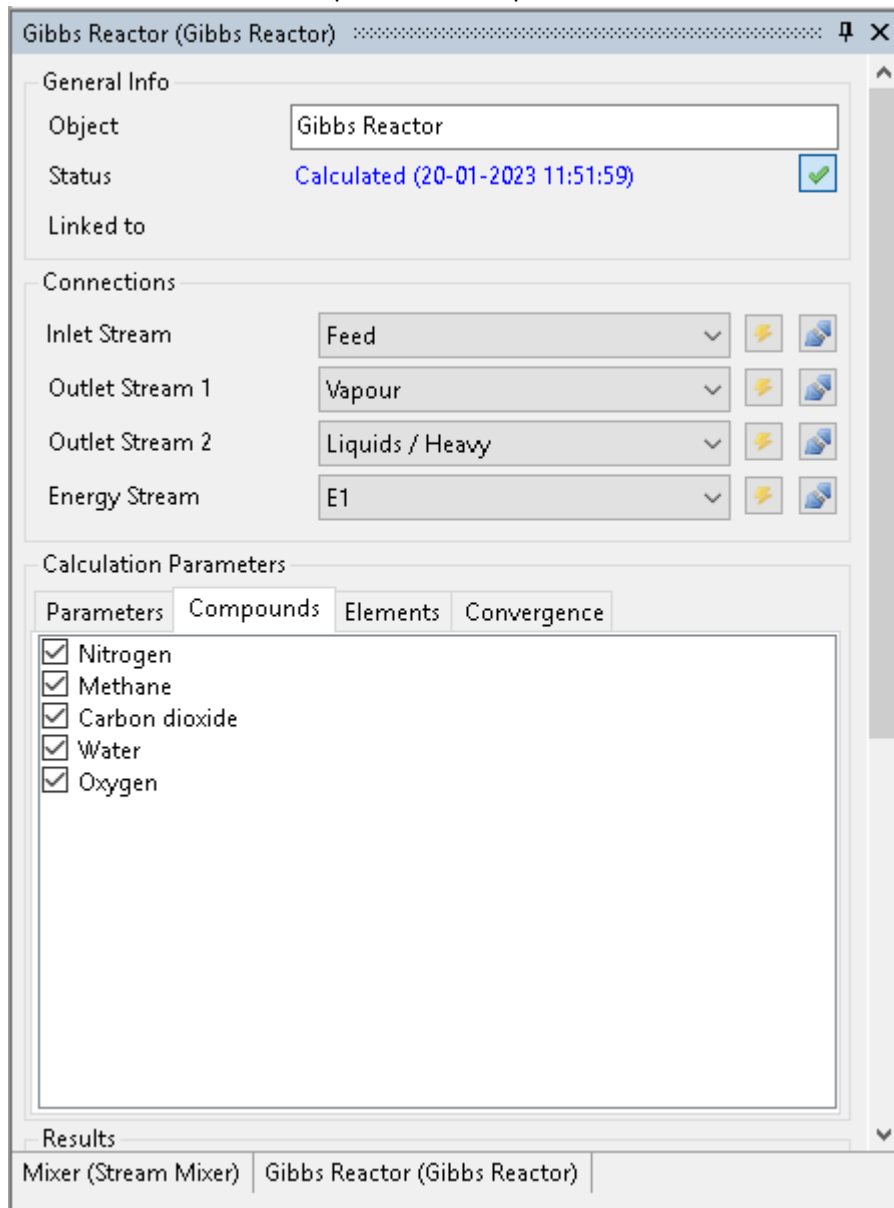


Figure 9 Compounds Selection

12. Click on edit ribbon and go into Simulation Settings or you may press “Alt + S”.

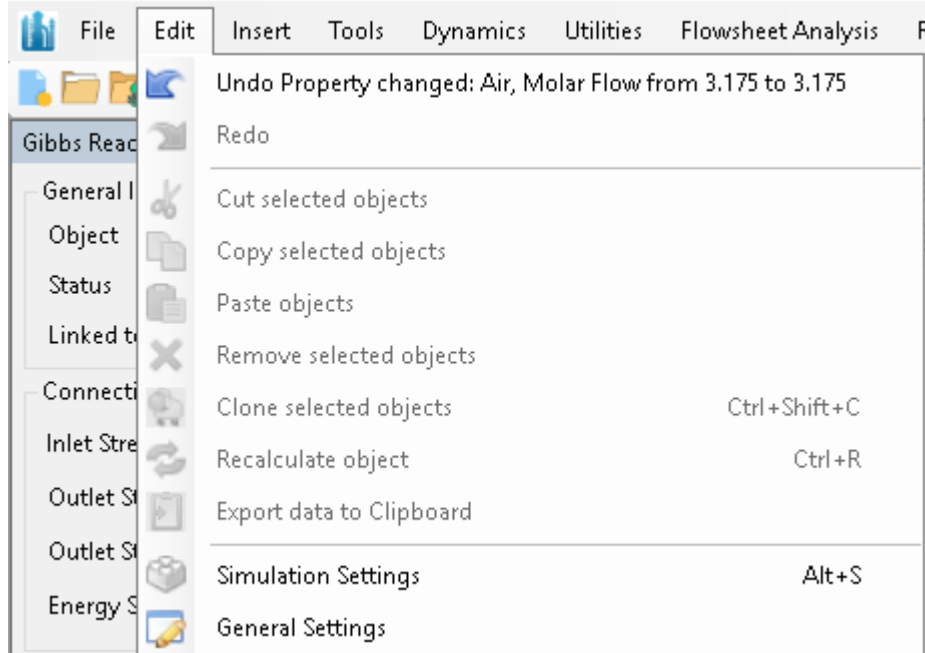


Figure 10 Simulation Settings

13. Click on Reaction ribbon and click on Conversion Reaction.

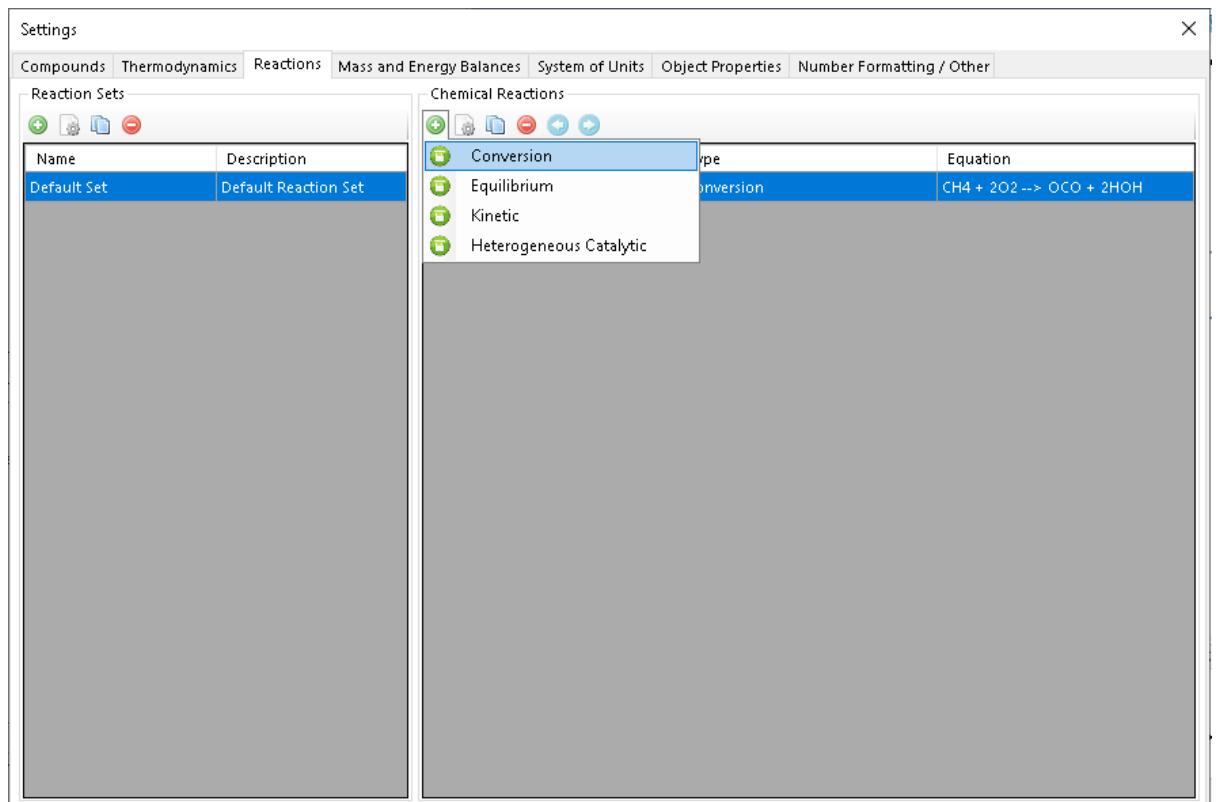


Figure 11 Conversion Reaction

14. Add the following specs as “-1” for methane, “-2” for Oxygen, “1” for Carbon Dioxide, “2” for Water. Select Methane as your base component and select vapour phase from the drop

down. And add 100% conversion.

Edit Conversion Reaction

Identification

Name: Combustion Reaction

Description:

Components/Stoichiometry

Name	Molar Weight	$\Delta H_f$ (kJ/kg)	Include	BC	Stoich. Coeff.
Nitrogen	28.0134	0	<input type="checkbox"/>	<input type="checkbox"/>	0
Methane	16.0425	-4645.17	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	-1
Carbon dioxide	44.0095	-8941.48	<input checked="" type="checkbox"/>	<input type="checkbox"/>	1
Water	18.0153	-13422.7	<input checked="" type="checkbox"/>	<input type="checkbox"/>	2
Oxygen	31.9988	0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	-2

Stoichiometry: OK Balance Heat of Reaction (kJ/kmol\_BC) (25 °C) -802618

Equatio:  $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$

Conversion Reaction Parameters

Base Comp: Methane Phase: Vapor

Conversion [%, f(T)] = 100 T in K

Use '.' as the decimal separator on the conversion expression.

Cancel OK

Figure 12 Conversion Reaction Specs

15. Run the simulation by pressing "Solve flow sheet" button on the top corner of the screen

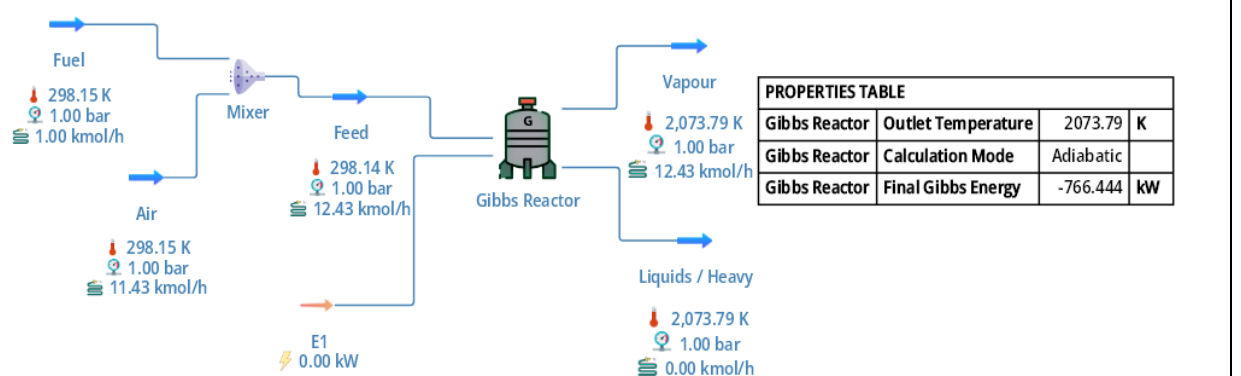


Figure 13 Flow Sheet



### 3 CROSS-CHECKING IN PYTHON CANTERA

```
%matplotlib inline
%config InlineBackend.figure_formats = ["svg"]
import cantera as ct
import numpy as np
import matplotlib.pyplot as plt

plt.rcParams["figure.dpi"] = 120

print(f"Using Cantera version: {ct.__version__}")

# Get all of the Species objects defined in the GRI 3.0 mechanism
species = {S.name: S for S in ct.Species.listFromFile("gri30.yaml")}

# Create an IdealGas object with species representing complete combustion
complete_species = [species[S] for S in ("CH4", "O2", "N2", "CO2", "H2O")]
gas1 = ct.Solution(thermo="IdealGas", species=complete_species)

phi = np.linspace(0.5, 2.0, 100)
T_complete = np.zeros(phi.shape)
for i in range(len(phi)):
    gas1.TP = 298, ct.one_atm
    gas1.set_equivalence_ratio(phi[i], "CH4", "O2:1, N2:3.76")
    gas1.equilibrate("HP")
    T_complete[i] = gas1.T

plt.plot(phi, T_complete, label="complete combustion", lw=2)
plt.grid(True)
plt.xlabel(r"Equivalence ratio, $\phi$")
plt.ylabel("Temperature [K]");

# Get all of the Species objects defined in the GRI 3.0 mechanism
species = {S.name: S for S in ct.Species.listFromFile("gri30.yaml")}

# Create an IdealGas object with species representing complete combustion
complete_species = [species[S] for S in ("CH4", "O2", "N2", "CO2", "H2O")]
gas1 = ct.Solution(thermo="IdealGas", species=complete_species)

phi = 2.0
gas1.TP = 298, ct.one_atm
gas1.set_equivalence_ratio(phi, "CH4", "O2:1, N2:3.76")
gas1.equilibrate("HP")
T_complete = gas1.T
T_complete
```

[Cantera Combustion Calculation Python Results](#)

## 4 MANUAL CALCULATION IN EXCEL

What is the maximum temperature that can be reached by the combustion of methane with 20% excess air? Both the methane and the air enter the burner at 25 °C.

The reaction is  $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}(\text{g})$  for which

$\Delta H_{298}$

Elements	Stoichiometry Coeff (mol)	$\Delta H_{298}$ (J/mol)	$\Delta H_{298} \times$ Stoichiometry Coeff (J/mol)
CH <sub>4</sub>	-1	-74520	74520
O <sub>2</sub>	0	0	0
CO <sub>2</sub>	1	-393509	-393509
H <sub>2</sub> O	2	-241818	-483636
Total			-802625

Constants	Values	Units
R	8.314	kJ/kmol K

Inputs		
Temp init	298.15	K
Pressure init	1	bar
CH <sub>4</sub>	1	mol
O <sub>2</sub>	2.4	mol
N <sub>2</sub>	9.03	mol

Products		
Pressure final	1	bar
Temp final	2066.265322	K
CO <sub>2</sub>	1	mol
H <sub>2</sub> O	2	mol
O <sub>2</sub>	0.4	mol
N <sub>2</sub>	9.03	mol

### Calculations

$$\Delta H_P^\circ = \langle C_P^\circ \rangle_H (T - 298.15)$$

$$\langle C_P^\circ \rangle_H \equiv \sum_i n_i \langle C_{Pi}^\circ \rangle_H$$

$$\langle C_P^\circ \rangle_H = \sum_i n_i \langle C_{Pi}^\circ \rangle_H = R \left[ \sum_i n_i A_i + \sum_i n_i B_i - \frac{1}{2} (T - T_0) + \sum_i n_i D_i - \frac{T_0}{T} \right]$$

## Manual calculation in Excel

12 February 2023

By Viraj Desai, Process Engineer

A			
CO2	1	5.457	5.457
H2O	2	3.47	6.94
O2	0.4	3.639	1.4556
N2	9.03	3.28	29.6184
			43.471

B	0.001		
CO2	1	1.045	0.001045
H2O	2	1.45	0.0029
O2	0.4	0.506	0.0002024
N2	9.03	0.593	0.00535479
			0.00950219

C	0.000001		
CO2	1	0	0
H2O	2	0	0
O2	0.4	0	0
N2	9.03	0	0
			0

D	100000		
CO2	1	-1.157	-115700
H2O	2	0.121	24200
O2	0.4	-0.227	-9080
N2	9.03	0.04	36120
			-64460

$\tau$	6.930287849	
$\langle C P^\circ \rangle H$	453.9438067	Error Fxn
Temp final	2066.265322	2.588E-09

[Excel Calculations](#)

## 5 REFERENCES

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- [Chapter 4 Heat Effects Pg 152](#)
- [Heat Capacities and properties](#)