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

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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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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:

$$4C(s) + 5H_2(g) \rightarrow C_4H_{10}(g)$$

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

$4C(s) + 4O_2(g) \rightarrow 4CO_2(g)$	$\Delta H°_{298}$ = (4) (−393,509)
$5H_2(g) + 2\frac{1}{2} O_2(g) \rightarrow 5 H_2O(l)$	$\Delta H°_{298}$ = (5) (−285830)
$4CO_2(g) + 5 H_2O(l) \rightarrow C_4H_{10}(g) + 6\frac{1}{2}O_2(g)$	$\Delta H°_{298}$ = 2877396
$4C(s) + 5H_2(g) \rightarrow C_4H_{10}(g)$	$\Delta H°_{298}$ = -125790J

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

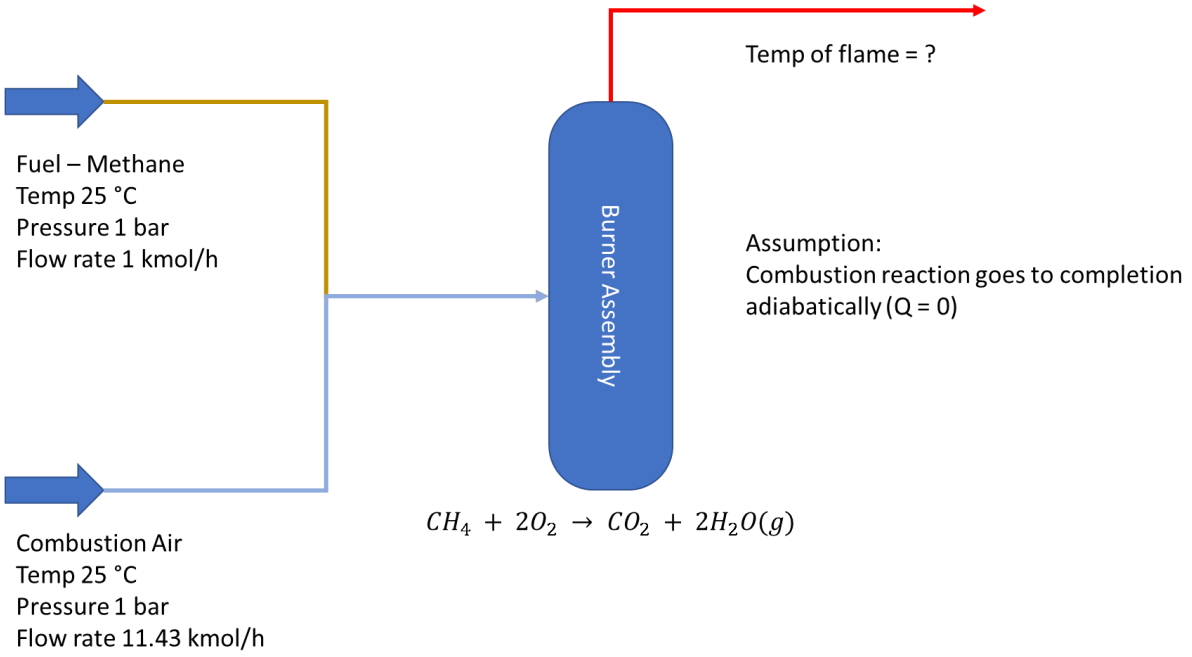

Figure 1 Problem Statement

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.

6. 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.

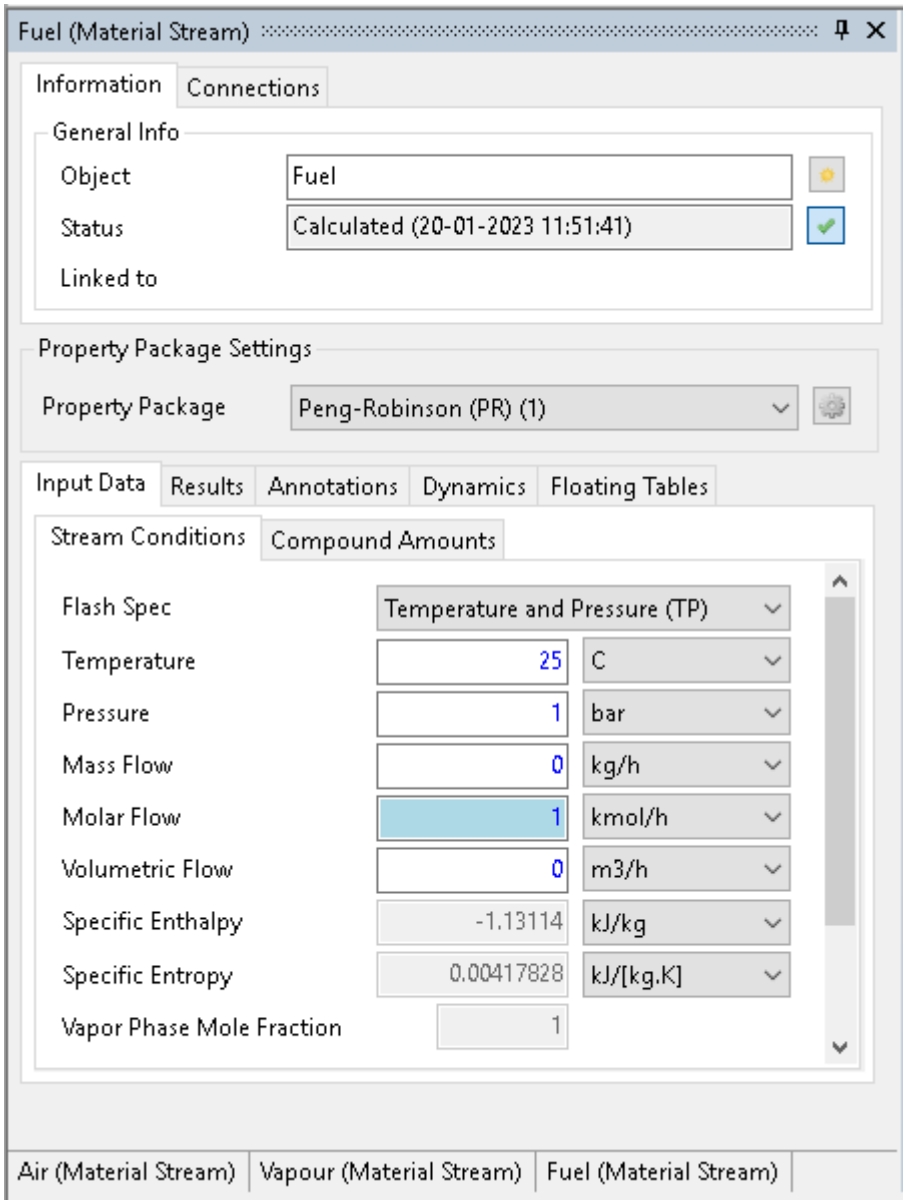

Figure 2 Fuel Stream Specs

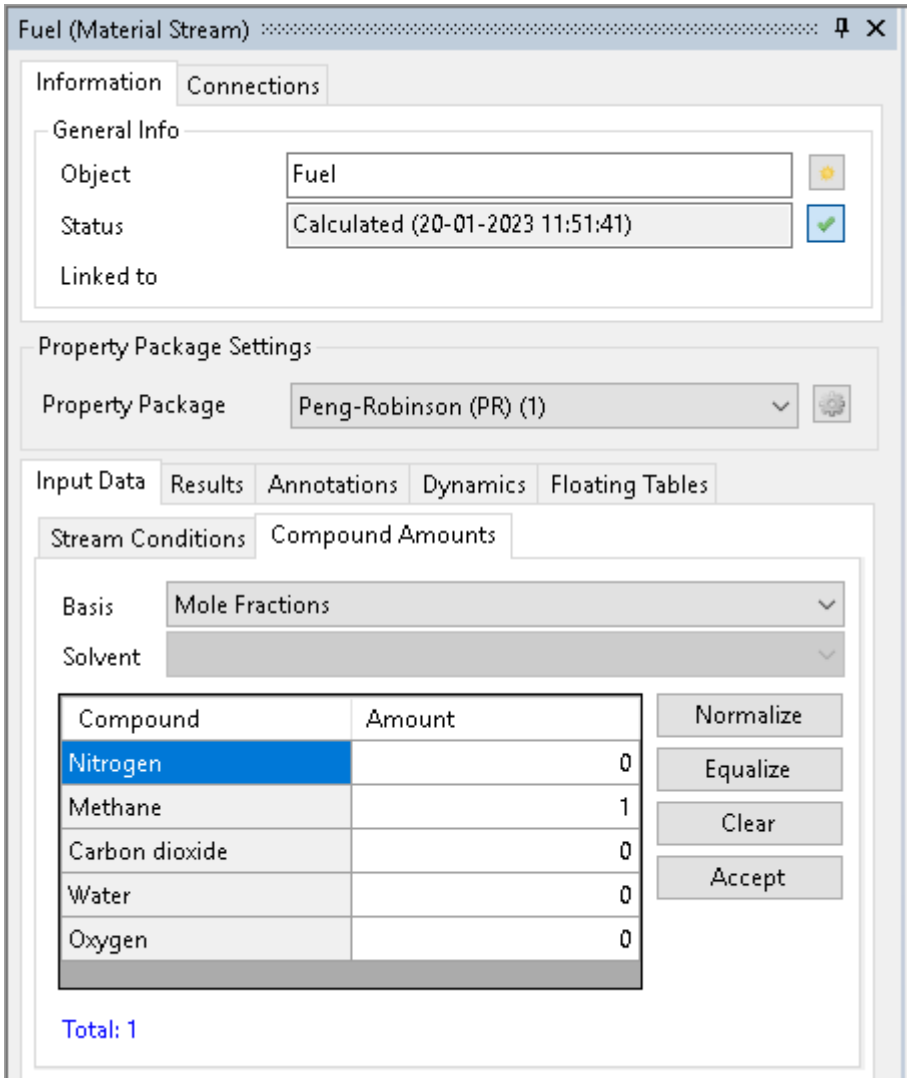

Figure 3 Fuel Stream Compound Amounts

7. 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.

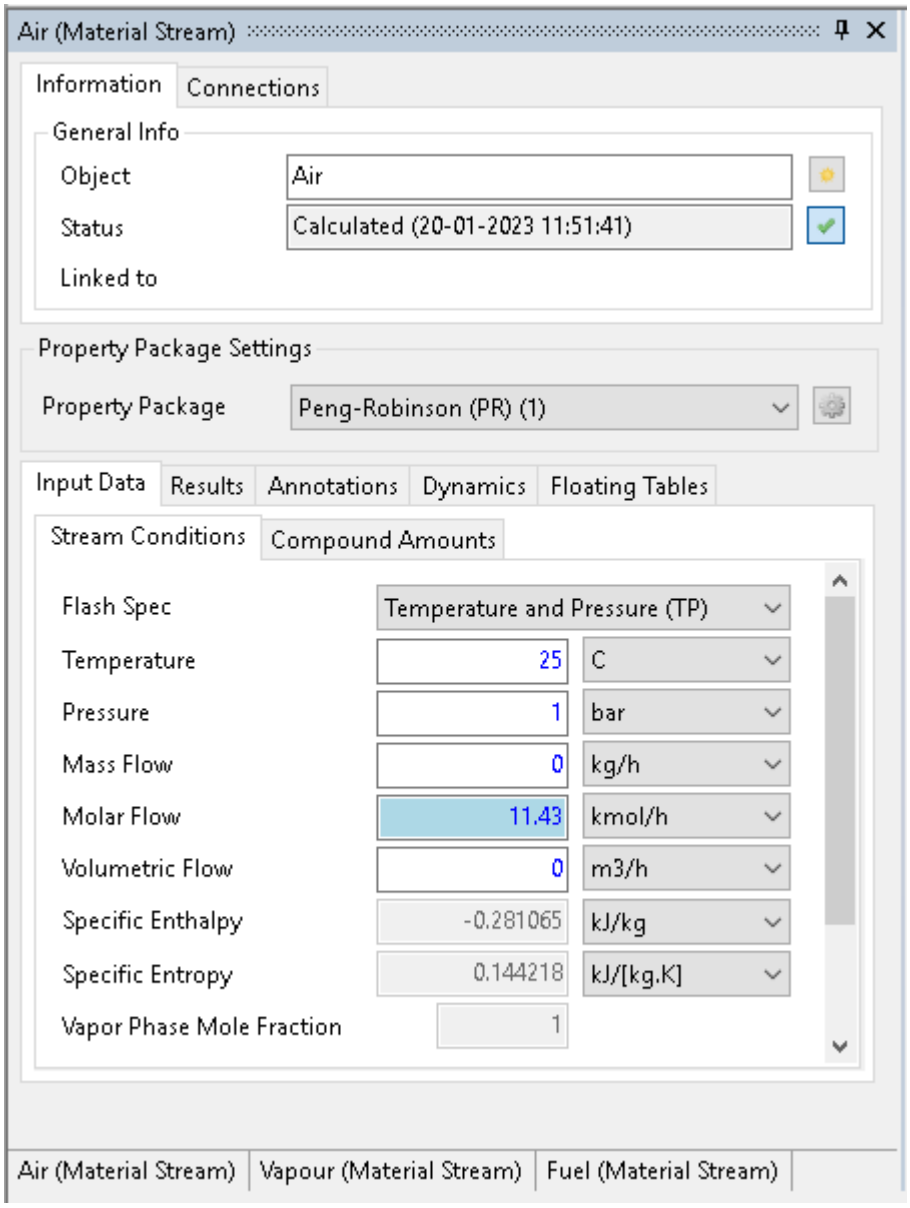

Figure 4 Air Stream Specs

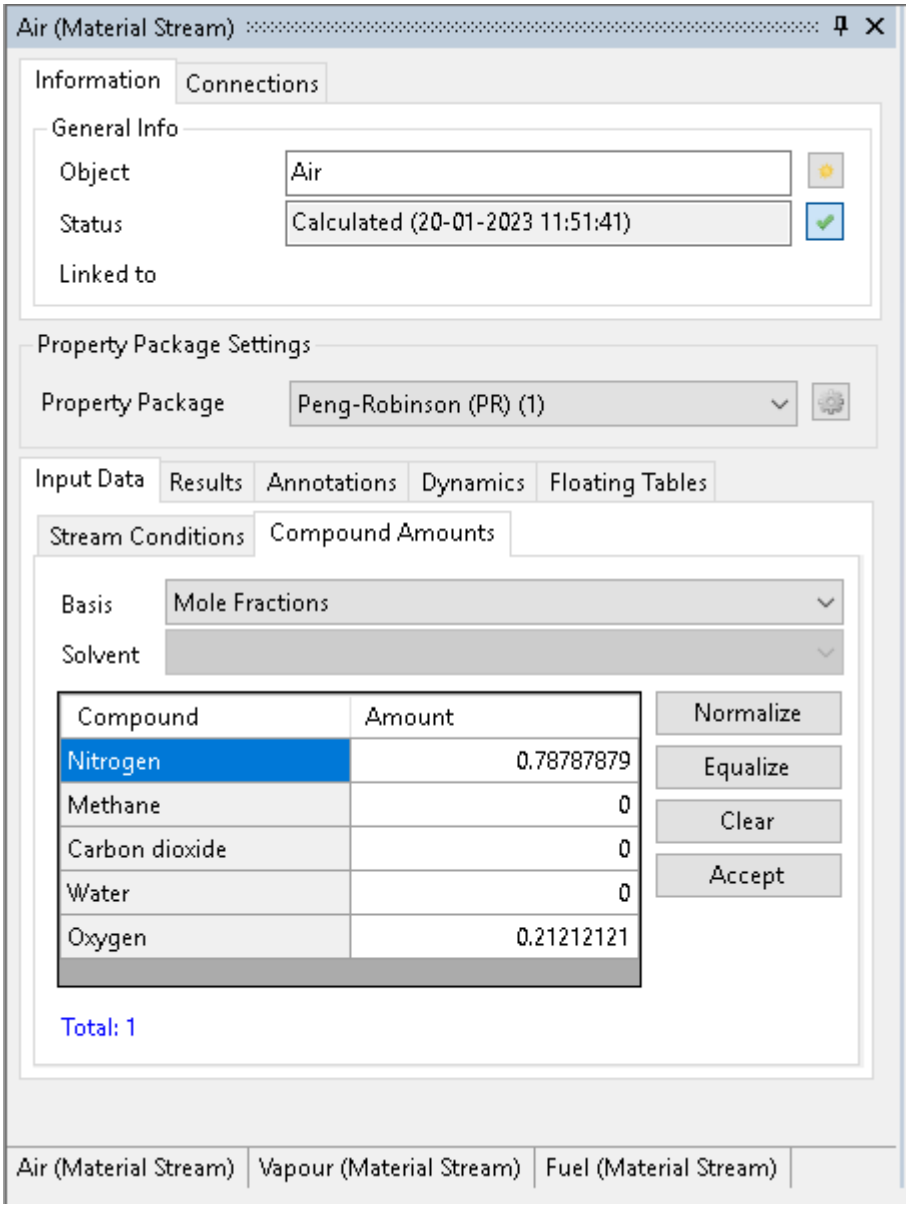

Figure 5 Air Stream Compound Amounts

8. 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.

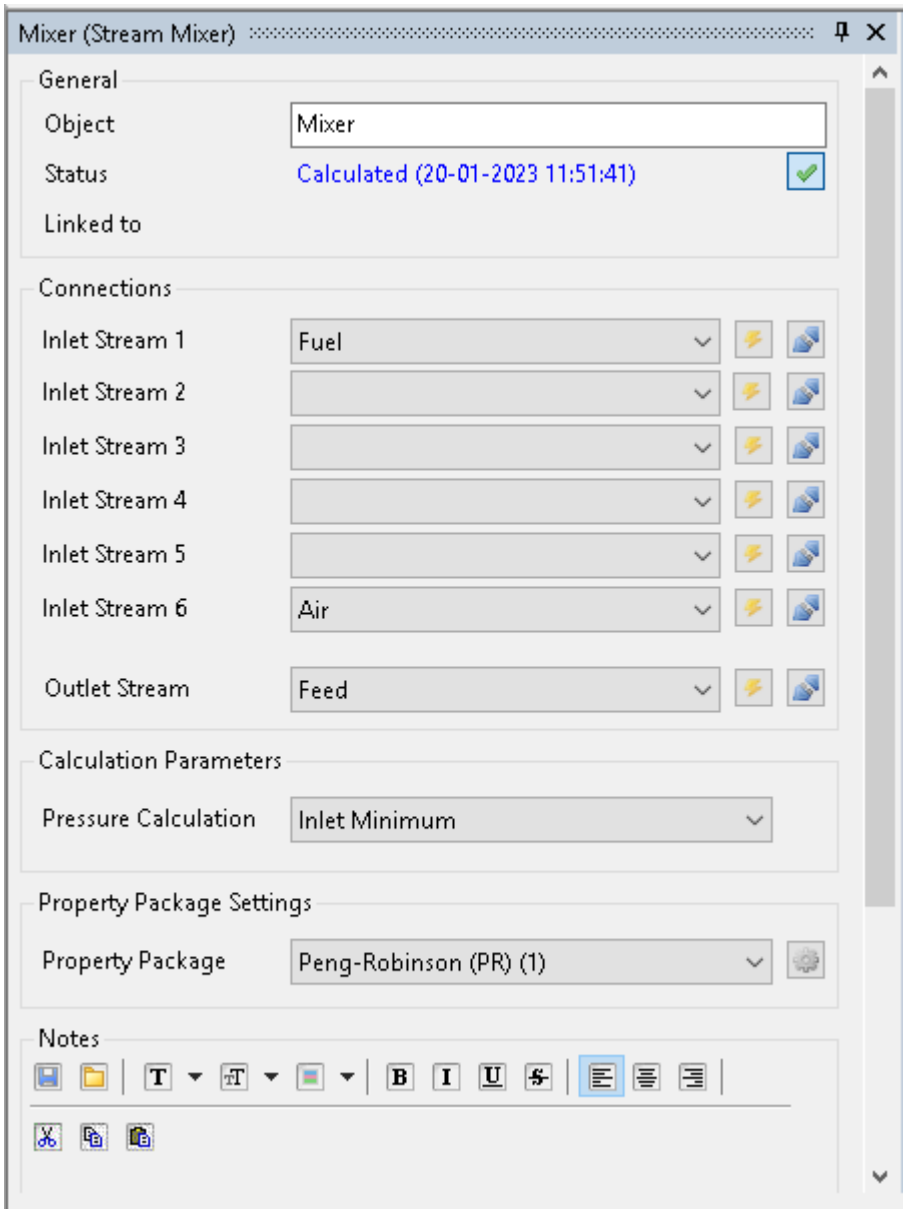

Figure 7 Mixer block Specs

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.

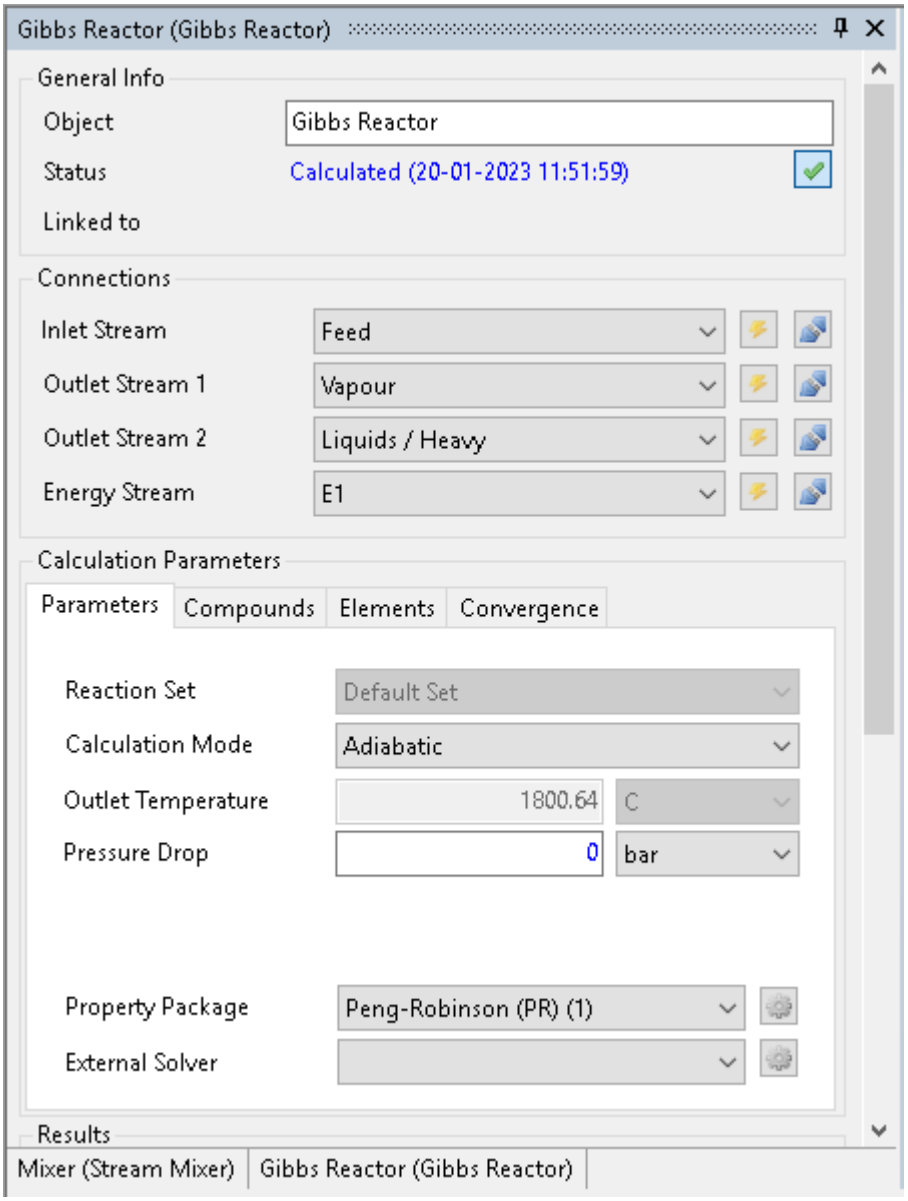

Figure 8 Gibbs Reactor Specs

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

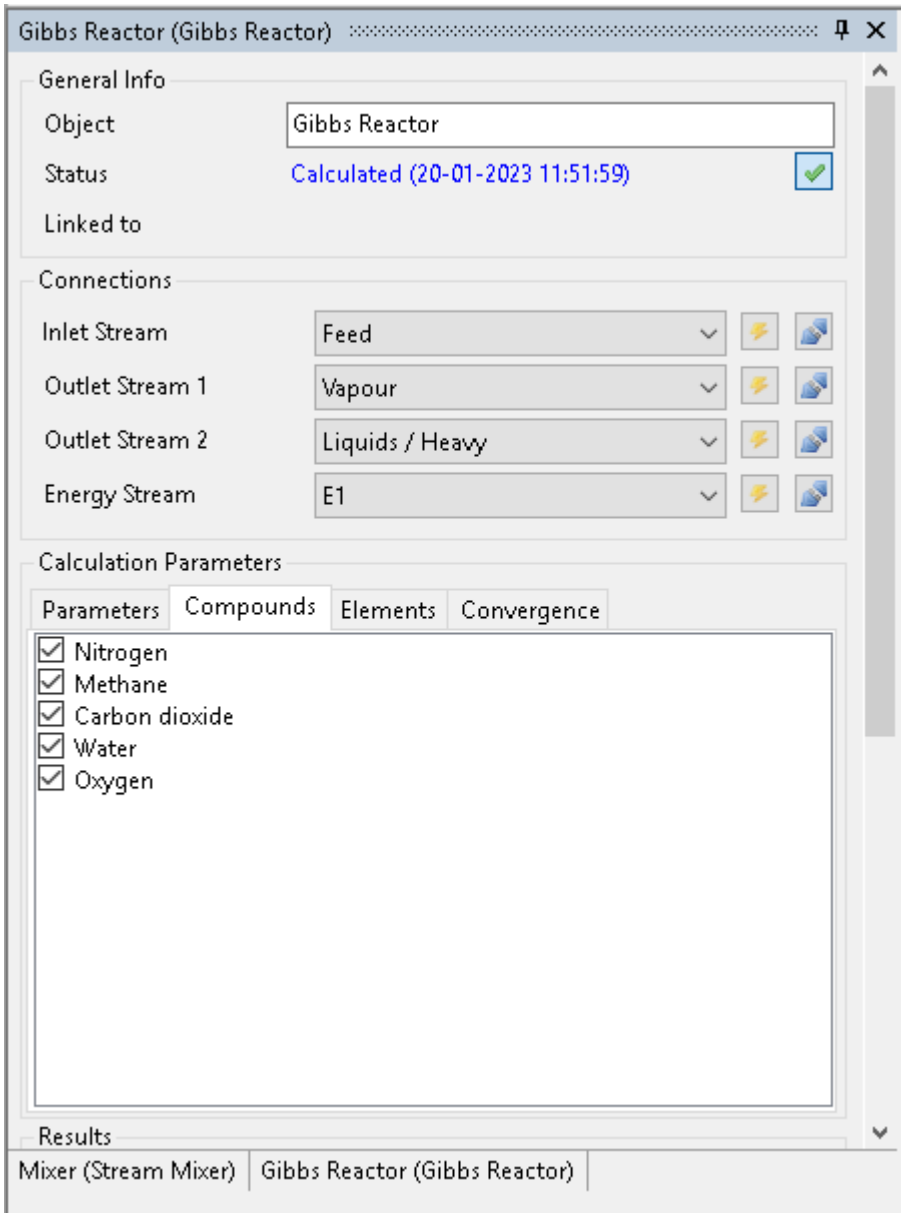

Figure 9 Compounds Selection

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

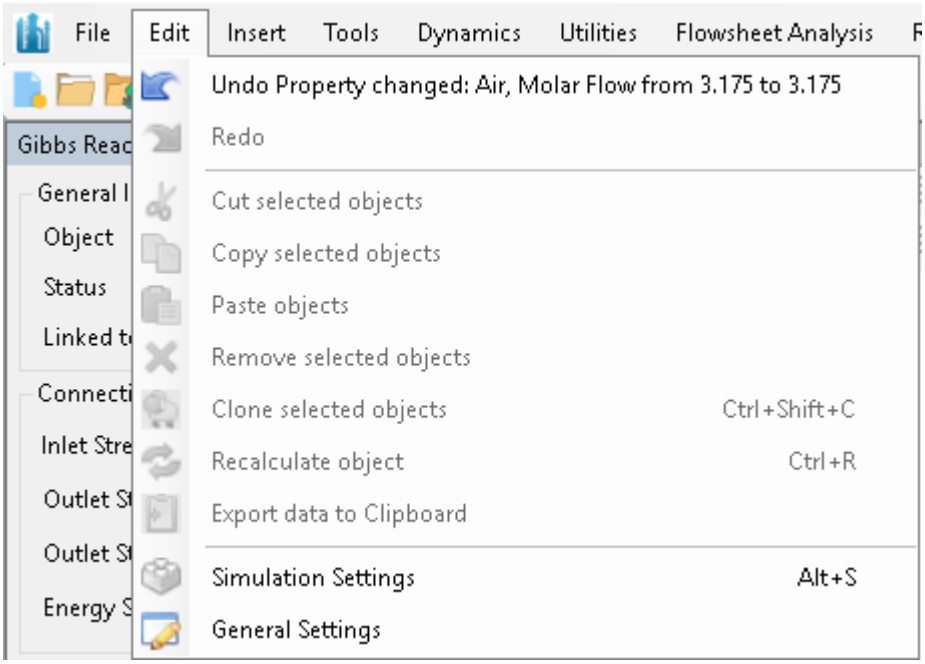

Figure 10 Simulation Settings

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

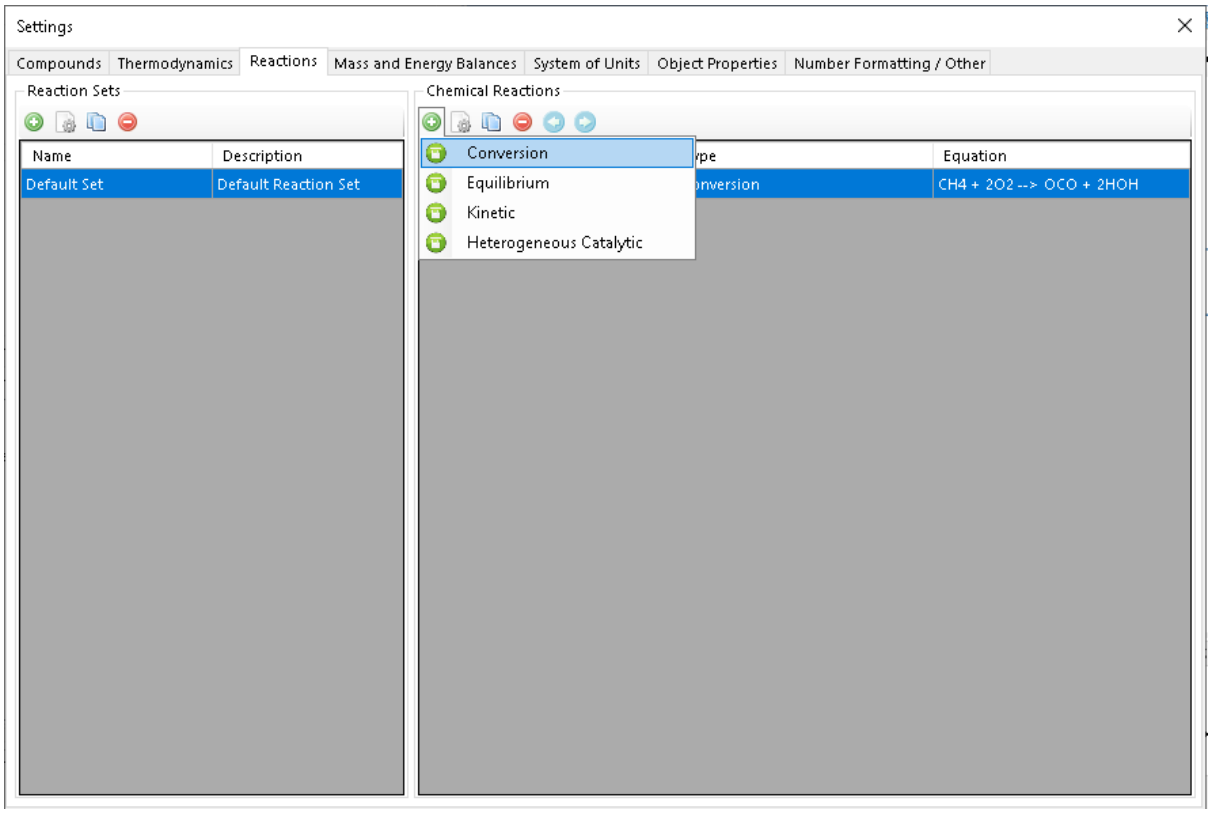

Figure 11 Conversion Reaction

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.

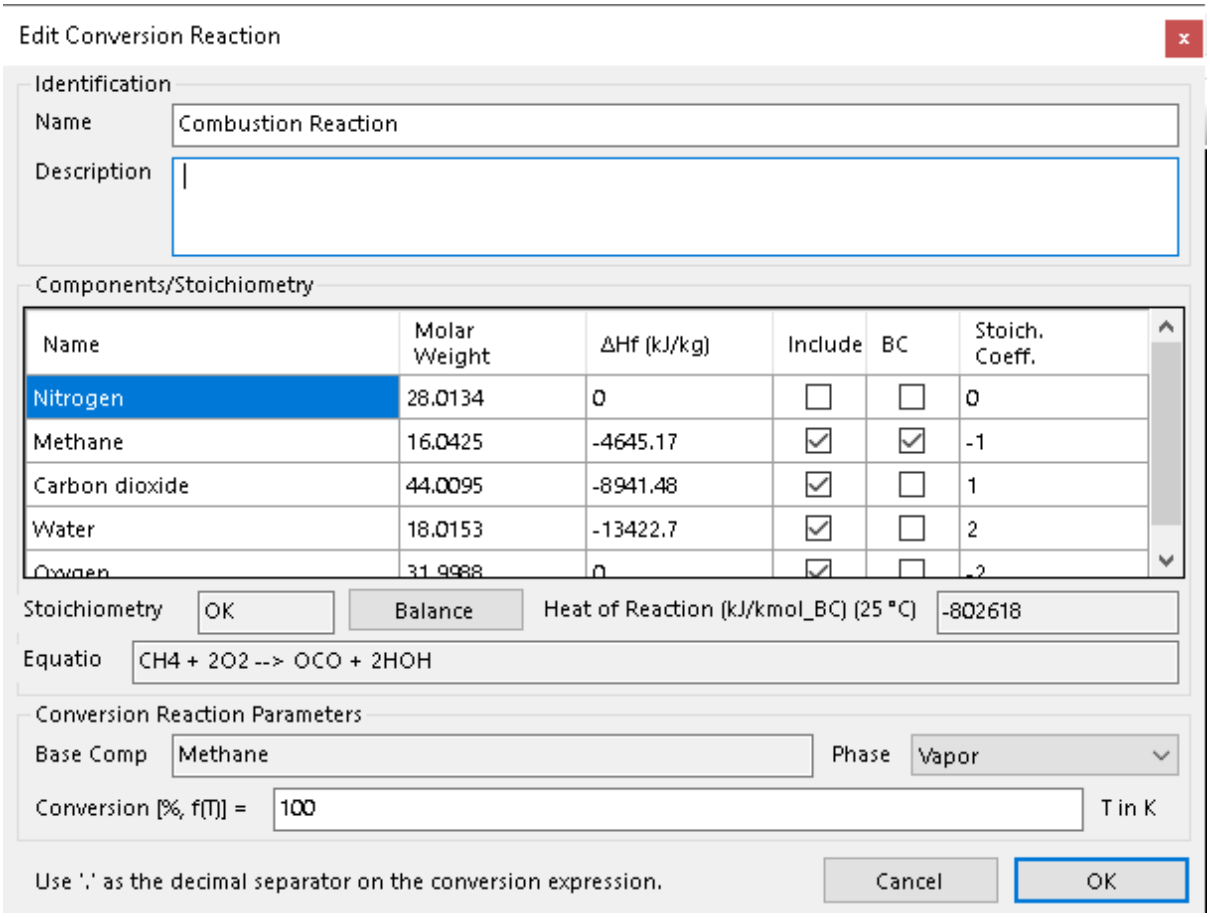

Figure 12 Conversion Reaction Specs

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

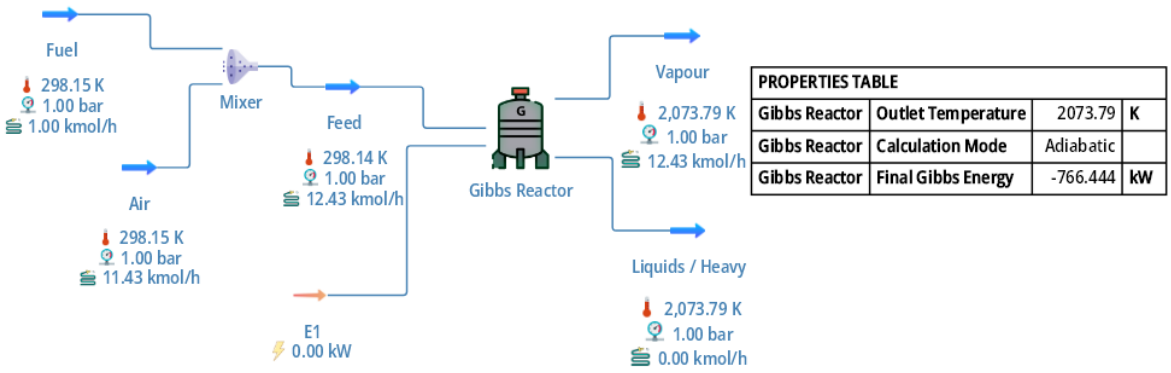

Figure 13 Flow Sheet

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 CH4 + 2O2 → CO2 + 2H2O(g) for which

Δ H 298

Elements	Stoichiometry Coeff (mol)	Δ H 298 (J/mol)	Δ H 298 x Stoichiometry Coeff (J/mol)
CH4	-1	-74520	74520
O2	0	0	0
CO2	1	-393509	-393509
H2O	2	-241818	-483636
Total			**-802625**

Constants	*Values*	*Units*
R	8.314	kJ/kmol K

Inputs		
Temp init	298.15	K
Pressure init	1	bar
CH4	1	mol
O2	2.4	mol
N2	9.03	mol

Products		
Pressure final	**1**	**bar**
Temp final	**2066.265322**	**K**
CO2	**1**	**mol**
H2O	**2**	**mol**
O2	**0.4**	**mol**
N2	**9.03**	**mol**

Calculations

$$\Delta H P^\circ = \langle C P^\circ \rangle H (T - 298.15)$$

$$\langle C P^\circ \rangle H \equiv \Sigma i \; ni \langle C Pi^\circ \rangle H$$

$$\langle C P^\circ \rangle H = \Sigma i \; ni \langle C Pi^\circ \rangle H = R [\Sigma i \; ni \; Ai + \Sigma i \; ni \; Bi \_ 2 \; (T - T0) + \; \Sigma i \; ni \; Di \_ T \; T0 \;]$$

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

τ	6.930287849	
⟨ C P ° ⟩ H	453.9438067	Error Fxn
Temp final	2066.265322	2.588E-09

Excel Calculations

5 REFERENCES

- Chapter 4 Heat Effects Pg 152
- Heat Capacities and properties