Semester Long Internship Report

On

Modelling of Methane Steam Reforming Unit in OpenModelica

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Contents

Nomenclature

ϵ Void fraction of the bed

ρ_g Density of the fluid, $\frac{kg}{m^3}$

ρ_c Density of catalyst, $\frac{kg}{m^3}$

A Cross-sectional area of the bed, m^2

C_p Heat capacity of water , $\frac{J}{kgK}$

D Diameter of bed, m

d_p Diameter of the particles, m

Ea Activation Energy, $\frac{J}{mol}$

g_c Gravitational constant, $\frac{m}{s^2}$

H_r Heat of reaction, $\frac{J}{mol}$

K_1 Equilibrium constant of MSR reaction

k_1 Rate Constant of MSR reaction

K_2 Equilbrium Constant of WGS reaction

k_2 Rate constant of WGS reaction

K_3 Equilbrium Constant of Overall reaction

k_3 Rate constant of Overall reaction

K_i Adsorption equilibrium constant of component i

L Length of bed, m

mu Dynamic viscosity of the fluid, $atmhr$

P Total Pressure, Pa

P_i Partial Pressure of component i

R Universal Gas Constant, $\frac{J}{molK}$

T Temperature of the water in the reactor, K

T_w Wall temperature of the reactor, K

U Overall heat transfer coefficient, $\frac{W}{m^2 K}$

u Superficial velocity, $\frac{m}{hr}$

1   Introduction

1.1   Introduction to OpenModelica

An open-source simulation and modelling environment for complex dynamic systems and cyber-physical systems is called OpenModelica. Users can build models, simulate system behavior, and assess system effectiveness. OpenModelica offers a flexible platform for academics, engineers, and students to design and test models in a variety of areas with features such as multi-domain simulation, code generation, optimization, and integration with other tools. It encourages cooperation and creativity in system modelling and simulation because it is publicly accessible as open-source software. Expressions, equations, functions, and algorithms are compiled into C code by Open-Modelica. A run-time library, a library of utility functions, and a numerical Differential-Algebraic Equation (DAE) solver are added to the resulting C code. The integrated Graphical User Interface (GUI) of OpenModelica for graphical modelling and editing is called OMEdit, or OpenModelica Connection Editor. OMEdit has a number of libraries for many subject areas, including Electrical, Magnetic, Math, Thermal, etc. It offers a number of user-friendly features, such as the representation of a model as block diagrams. Custom models may be built using OMEdit, which may also be used to edit or connect the model interfaces. Users can also use it to plot graphs comparing model simulation parameter values.

1.2   Introduction to Methane Steam Reforming

The main goal of this project was to create a thorough model of the methane steam reforming process that precisely forecasts the system's behavior and gives significant insight into the fundamental physical and chemical phenomena. We intended to comprehend the complicated interactions among the reactants, catalyst, and reactor design factors by modelling the reforming unit in OpenModelica.

It is impossible to exaggerate the value of methane steam reforming in industrial applications. This method yields hydrogen as its primary byproduct, which has a wide range of potential applications in transportation, energy production, and chemical synthesis. Hydrogen is a clean and adaptable energy carrier. Furthermore, the abundance of methane as a feedstock and the accessibility of proven catalytic technology makes methane steam reforming an appealing method for hydrogen synthesis.

The report is organized to give a thorough summary of the research done and the results obtained. A review of the prior research on methane steam reforming is presented before getting started. This review provides the framework for our work and aids in locating any gaps or restrictions in the body of previous research, giving our

modelling method some context.

The process we used to create the model with OpenModelica is described in the methodology and literature review section. We provide an overview of the data collection techniques used and talk about the mathematical models, equations, and presumptions that were used to accurately replicate the behavior of the reforming unit. The background information required to comprehend the ensuing model construction and analysis is provided in this section.

The parts and subsystems that make up the model are thoroughly described in section on the model development. We briefly discuss the factors and parameters taken into account, highlighting their importance in capturing the salient features of the reforming process in form of Code. We also address any simplifications or assumptions used throughout the modelling process as well as the numerous interactions and reactions occurring within the reforming unit.

The output and conclusions from our simulations are presented in the results and analysis section. We examine the influence of various factors on the process performance and describe the system's projected behavior under various operating situations.

2 Methodology

2.1 Process Description

The steam methane reformer, also known as the methane steam reforming unit (SMR), is an essential feature of many industries, especially those that produce synthesis gas and hydrogen. In fields including petrochemicals, ammonia production, refineries, and hydrogen fuel cell technology, it is frequently used. The capacity of the methane steam reforming unit to catalytically change methane, which is the main component of natural gas, into hydrogen gas is what gives it its fundamental significance. In numerous industrial processes, hydrogen is a crucial feedstock and a crucial component for many different applications. It is extensively utilised in the production of methanol for chemical synthesis, ammonia for fertiliser production, and hydrodesulfurization and hydrocracking operations in refineries.
Moreover, hydrogen is a promising energy carrier and plays a vital role in fuel cell technologies for clean and efficient power generation.

The methane steam reforming unit enables the efficient and large-scale production of hydrogen by utilizing steam and a catalyst to break down methane molecules into hydrogen and carbon monoxide. This process is typically carried out at elevated temperatures and pressures to optimize the reaction kinetics. The produced synthesis gas (a mixture of hydrogen and carbon monoxide) can then be further processed and utilized in various downstream processes based on industry requirements. Methane is reacted with high-temperature steam with the aid of a catalyst, commonly made of nickel, at temperatures between 700 and 900 degrees Celsius. The following equation can be used to model the reaction:

$$CH_4 + H_2O \longleftrightarrow CO + 3H_2; \Delta H_{R,298K} = 206\frac{kJ}{mol} \tag{1}$$
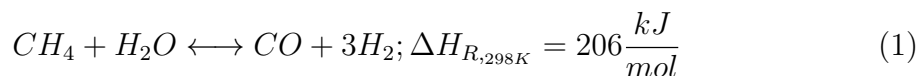
The WGS reaction is typically used to minimize carbon monoxide and improve hydrogen output after the reforming or gasification process. It is an exothermic, reversible reaction that takes place in two reactors operating in series at 400 and 210°C, respectively.

$$CO + H_2O \longleftrightarrow CO_2 + H_2 \Delta H_{R,298K} = -40.6\frac{kJ}{mol} \tag{2}$$
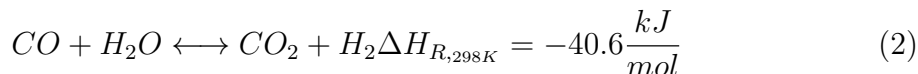
Hence, the overall reaction involves the methane reacting with steam to produce carbon dioxide and hydrogen gas. The reaction is typically carried out in the presence of a catalyst and at high temperatures and pressures.

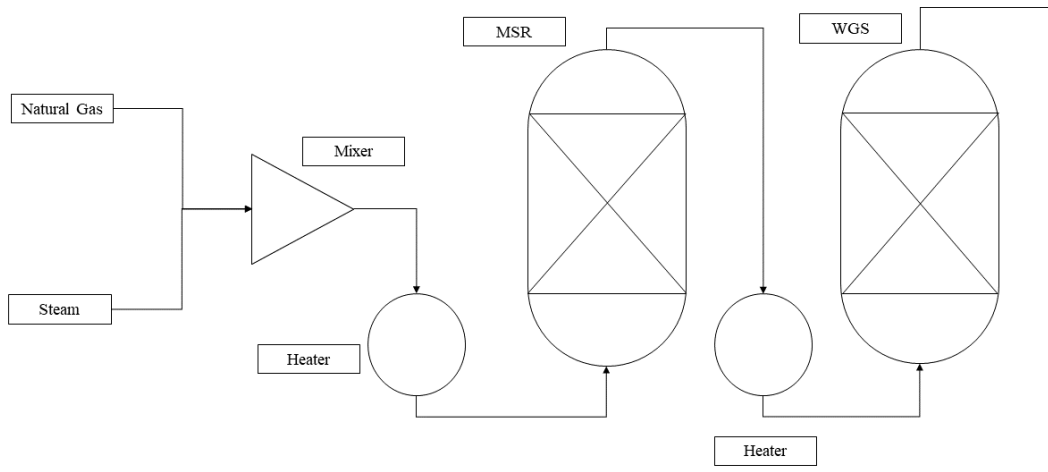$$CH_4 + 2H_2O \longleftrightarrow CO_2 + 4H_2 \tag{3}$$
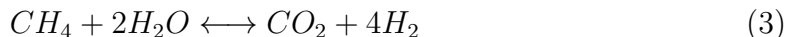
Figure 1: Schematic of MSR and WGS

The relationship between the rate of a chemical reaction and the concentrations of the reactants is expressed mathematically by a rate equation. It gives important details regarding how reactant concentrations affect reaction rate.

The rate equation, which is usually generated from experimental data, is represented in terms of the rate at which the concentration of a specific reactant or product changes over time.

The rate equation offers a mathematical link between the rate of the reaction and the concentrations of the reactants, which aids in determining the conversion. We may calculate the conversion of the reactants as a function of time by integrating the rate equation over time. The rate expression for the MSR reaction, RMSR based on Langmuir-Hinshelwood (LHHW) reaction mechanism on Nickel catalyst is as follows:

$$RMSR = \frac{\frac{k_1}{P_{H_2}^{2.5}}\left[P_{CH_4}P_{CO} - \frac{P_{H_2}^3 P_{CO}}{K1}\right]}{DEN^2} \tag{4}$$

where,

$$DEN = 1 + K_{CO}P_{CO} + K_{H2}P_{H2} + K_{CH_4}P_{CH_4} + \frac{K_{H2O}P_{H2O}}{P_{H2}} \tag{5}$$

The kinetic coefficient and equilibrium constants of MSR are shown in Table 1.

The kinetic model for reaction in Eq(2) is based on a LHHW reaction mechanism.

Parameter	Pre-exponential	Ea (J/mol)
k1	$4.2248 \times 10^{15}(mol * atm^{0.5}/g * h)$	2,40,100
K1	$7.846 \times 10^{12}(atm^2)$	2,20,200
KCH4	$6.65 \times 10^{-4}(atm^{-1})$	-38,280
KH2O	$1.77 \times 10^5(atm^{-1})$	88,680
KH2	$6.12 \times 10^{-5}(atm^{-1})$	-82,900
KCO	$8.23 \times 10^{-5}(atm^{-1})$	-70,650

The rate reaction, RWGS is given by:

$$R_{WGS} = \frac{\frac{k_2}{P_{H_2}}[P_{CO}P_{H_2O} - \frac{P_{H_2}P_{CO_2}}{K2}]}{DEN^2} \tag{6}$$

The kinetic coefficient and equilibrium constants of WGS are shown in Table 2.

Parameter	Pre-exponential	Ea (J/mol)
k2	$1.955 \times 10^{-6}(mol/gh)$	67130
K2	1.412×10^{-2}	-37720

Two key variables, the Ea and the Pre-exponential factor, can be used to derive the rate constant of a chemical reaction using the Arrhenius equation. In the Arrhenius equation, k stands for the rate constant, R is the ideal gas constant, and T is the temperature in Kelvin. This equation is written as k = A * exp(-Ea/RT). We may find the rate constant for a given temperature by entering the temperature of interest, the values of Ea and A, and the Arrhenius equation. Hence, all the parameters were calculated using the experimental data available from literature.

The rate expression for the overall reaction, ROC based on Langmuir-Hinshelwood (LHHW) reaction mechanism on Nickel catalyst is as follows:

$$R_{OC} = \frac{\frac{k_3}{P_{H_2}^{3.5}}[(P_{CH_4}P_{H_2O}^2) - \frac{P_{H_2}^4 P_{CO_2}}{K_3}]}{DEN^2} \tag{7}$$

where,

$$DEN = 1 + K_{CO}P_{CO} + K_{H_2}P_{H_2} + K_{CH_4}P_{CH_4} + K_{H_2O}\frac{P_{H_2O}}{P_{H_2}} \tag{8}$$

The kinetic coefficient and equilibrium constants of ROC are shown in Table 3.

Parameter	Pre-exponential	Ea (J/mol)
k3	$1.0202 \times 10^{15} (mol * atm^{0.5}/g * h)$	243900
K3	1.11×10^{11}	18240

Two key variables, the Ea and the Pre-exponential factor , can be used to derive the rate constant of a chemical reaction using the Arrhenius equation. In the Arrhenius equation, k stands for the rate constant, R is the ideal gas constant, and T is the temperature in Kelvin. This equation is written as k = A * exp(-Ea/RT). We may find the rate constant for a given temperature by entering the temperature of interest, the values of Ea and A, and the Arrhenius equation. Hence, all the parameters were calculated using the experimental data available from literature

We may calculate the conversion of methane by dividing the current molar flow rate of the gas by the initial molar flow rate, then subtracting the result from 1. The amount of methane that has been transformed or consumed throughout the reaction is indicated by the conversion value. A conversion of 0 means that no methane has been converted, whereas a conversion of 1 means that all methane has been converted.

By changing the relevant numbers for the molar flow rates, we can use this equation to calculate the conversion of methane. The molar flow rate of methane at a particular point in the process is represented by the numerator, FlowRateCH4. The initial molar flow rate of methane at the start of the process is represented by the denominator, InitialFlowrateCH4.

In the following equation, the molar flow rate of methane at a given time is represented by FlowRateCH4, and the initial molar flow rate of methane is denoted by InitialFlowrateCH4.

The amount of methane that is yet unconverted can be found by deducting the ratio of the current molar flow rate of methane (FlowRateCH4) to the initial molar flow rate (InitialFlowrateCH4) from 1. The portion of methane that hasn't reacted or been converted into other products is represented by the difference.

$$X_{CH_4} = 1 - \frac{F_{CH_4}}{F^0_{CH_4}} \tag{9}$$

In order to comprehend how quickly carbon dioxide is produced or consumed in a chemical process, it is crucial to grasp the derivative of the carbon dioxide conversion (XCH4). We can examine the rate of change of XCH4 with respect to time by computing the derivative, which reveals information about the reaction kinetics and rate of carbon dioxide production. This derivative assists in the optimisation and

control of the reaction process by allowing us to evaluate how the conversion of carbon dioxide is changing over time.

$$\frac{dX_{CH_4}}{dz} = \frac{\rho_c A(RMSR + ROC)}{F_{CH_4}^0} \tag{10}$$

Water (H2O) conversion in a chemical reaction is calculated using the equation below. In this equation, the initial molar flow rate of methane (InitialFlowrateCH4) is divided by the molar flow rate of water at a particular moment, denoted by FlowRateH2O. The amount of water that is yet unconverted is found by deducting this ratio from 1. The resulting percentage or fraction of water that has not been converted is represented by the value. We can calculate the conversion of water by subtraction the fraction of unconverted water from 1.

$$X_{H_2O} = 1 - \frac{F_{H_2O}}{F_{CH_4}^0} \tag{11}$$

Understanding the rate at which water is consumed or created in a chemical reaction depends on the derivative of the conversion of water (XH2O). We may learn more about the reaction kinetics by computing the derivative to get the rate at which XH2O changes with respect to time. This derivative enables us to analyse the reaction rate by enabling us to comprehend how the conversion of water is changing over time.

$$\frac{dX_{H_2O}}{dz} = \frac{\rho_c A(RMSR + WGS + 2ROC)}{F_{CH_4}^0} \tag{12}$$

The conversion of hydrogen (H2) in a chemical reaction is calculated using the equation below. Here, the initial molar flow rate of methane (InitialFlowrateCH4) is divided by the molar flow rate of hydrogen at a particular period, denoted by FlowRateH2. The proportion or percentage of hydrogen that has undergone conversion is directly provided by this ratio. It is an indicator of how much methane has been converted to hydrogen.

$$X_{H_2} = 1 - \frac{F_{H_2}}{F_{CH_4}^0} \tag{13}$$

The rate of hydrogen creation or consumption in a chemical reaction is mostly determined by the derivative of the conversion of hydrogen (XH2). We can examine the rate of change of XH2 with respect to time by computing the derivative, which reveals information about the reaction kinetics and hydrogen production rate. This

derivative assists in the improvement and management of the reaction process by allowing us to evaluate how the conversion of hydrogen is changing over time.

$$\frac{dX_{H_2}}{dz} = \frac{\rho_c A(3RMSR + WGS + 2ROC)}{F_{CH_4}^0} \tag{14}$$

The carbon monoxide (CO) conversion in a chemical reaction is calculated using the equation below. In this equation, the initial molar flow rate of methane (InitialFlowrateCH4) is divided by the molar flow rate of carbon monoxide at a particular period, denoted by FlowRateCO. The fraction or percentage of carbon monoxide that has undergone conversion is obtained by this division. It shows how much methane has been transformed into carbon monoxide.

$$X_{C_O} = 1 - \frac{F_{C_O}}{F_{CH_4}^0} \tag{15}$$

Understanding the rate at which carbon monoxide is produced or consumed in a chemical reaction requires knowledge of the derivative of the conversion of carbon monoxide (XCO). By calculating the derivative, we can calculate the rate at which XCO changes over time and gain knowledge about the kinetics of the process as well as the rate at which carbon monoxide is produced. This derivative helps with reaction process optimisation and monitoring by enabling us to analyse how the conversion of carbon monoxide is changing over time.

$$\frac{dX_{C_O}}{dz} = \frac{\rho_c A(RMSR - WGS)}{F_{CH_4}^0} \tag{16}$$

The carbon dioxide (CO2) conversion in a chemical reaction is calculated using the equation below. Here, the total molar flow rate of all the reactants in the reaction (FlowRate) is divided by the molar flow rate of carbon dioxide at a particular moment, denoted as FlowRateCO2. We are able to determine how much carbon dioxide has been converted by doing this. It designates how much of the reactants have been converted into carbon dioxide.

$$X_{CO_2} = 1 - \frac{F_{CO_2}}{F_{CH_4}^0} \tag{17}$$

In order to comprehend how quickly carbon dioxide is produced or consumed in a chemical process, it is crucial to grasp the derivative of the carbon dioxide conversion (XCO2). We can examine the rate of change of XCO2 with respect to time by computing the derivative, which reveals information about the reaction kinetics and

rate of carbon dioxide production. This derivative assists in the optimisation and control of the reaction process by allowing us to evaluate how the conversion of carbon dioxide is changing over time.

$$\frac{dX_{CO_2}}{dz} = \frac{\rho_c A(WGS + ROC)}{F^0_{CH_4}} \tag{18}$$

For caluclation of rate equations the individual pressure terms are calculated using Ergun equation, which offers a framework for computing the total pressure term in a given system. The overall pressure drop is calculated using the Ergun equation, which also considers variables like fluid velocity, particle size, and bed porosity. The equation provides a thorough understanding of the pressure behaviour of the system when these parameters are taken into account. Individual pressures within the system can be determined from this overall pressure term, offering important insights into the pressure distribution and allowing the evaluation of particular pressure points or regions of interest.

The pressure drop in packed bed systems is measured by the Ergun equation, a commonly used empirical equation in fluid dynamics and chemical engineering. The pressure drop, fluid velocity, and bed properties like particle size and bed porosity are all related in this passage. Viscous resistance and inertial resistance are two different mechanisms that are considered in the equation. While the inertial resistance term captures the pressure drop brought on by fluid acceleration and deceleration around the particles, the viscous resistance factor accounts for the frictional losses brought on by fluid flow through the interstitial spaces between particles.

$$\frac{dP}{dL} = -\frac{\rho_g u}{\rho_g g_c d_p}\frac{1-\epsilon}{\epsilon^3}\frac{150(1-\epsilon)mu}{d_p} + 1.75\rho_g u \tag{19}$$

3   Code

```
1  package SteamReformer
2  function Compressibilty
3  input Integer N;
4  input Real w[N];
5  input Real T;
6  input Real P;
7  input Real X[N];
8  input Real Tc[N];
9  input Real Pc[N];
10 input Real K[N, N];
11 output Real tr[N];
12 output Real a[N];
13 output Real b[N];
14 output Real am;
15 output Real bm;
16 output Real A;
17 output Real B;
18 algorithm
19 for i in 1:N loop
20 tr[i] := T / Tc[i];
21 a[i] := (1 + (0.3764 + 1.54226 * w[i] - 0.26992 * w[i] ^ 2) * (1 -
       tr[i] ^ 0.5)) ^ 2 * (8.314 ^ 2 * Tc[i] ^ 2 * 0.45724 / Pc[i]);
22 b[i] := 0.07780 * 8.314 * Tc[i] / Pc[i];
23 end for;
24 am := 0;
25 bm := 0;
26 for i in 1:N loop
27 for j in 1:N loop
28 am := am + (a[i] * a[j]) ^ 0.5 * X[i] * X[j] * (1 - K[i, j]);
29 end for;
30 end for;
31 for i in 1:N loop
32 bm := bm + X[i] * b[i];
33 end for;
34 A := am * P / (8.314 ^ 2 * T ^ 2);
35 B := bm * P / (8.314 * T);
36 end Compressibilty;
37
38
39   model Reformer
40   extends Modelica.Constants;
41   import data = ChemsepDatabase;
42   parameter data.Methane Meth;
```

```
43   parameter data.Water Wat;
44   parameter data.Hydrogen Hyd;
45   parameter data.Carbonmonoxide CarbM;
46   parameter data.Carbondioxide CarbD;
47   parameter data.GeneralProperties comp[5] ={Meth, Wat, Hyd,
      CarbM, CarbD};
48   parameter Integer N = 5;
49   // Kinetic coefficients of Methane Stean Reforming (MSR)
      reactions
50   Real k1(unit = "mol*atm^0.5/g*h");
51   Real K1(unit = "atm^2");
52   Real KCO(unit = "1/atm");
53   Real KH2(unit = "1/atm");
54   Real KCH4(unit = "1/atm");
55   Real KH2O(unit = "1/atm");
56   // Kinetic coefficient of Water Gas Shift (WGS) reactions
57   Real k2 (unit = "mol/g*h");
58   Real K2(unit = "1/atm");
59   Real k3(unit = "mol*atm^0.5/g*h");
60   Real K3(unit = "atm^2");
61   // Predefined values for MSR reaction
62   parameter Real InitialFlowrateCH4 (unit = "kmol/hr") = 49.75;
63   parameter Real k10 (unit ="mol*atm^0.5/gm*hr") = 4.2248e15 ;
64   parameter Real Ea1 (unit ="J/mol") = 240100 ;
65   parameter Real K10 (unit ="atm^2") = 7.846e12 ;
66   parameter Real Ea2 (unit ="J/mol")= 220200 ;
67   parameter Real Kch4 (unit ="1/atm") = 6.65e-4 ;
68   parameter Real Ea3 (unit ="J/mol")= -38280 ;
69   parameter Real Kh2o (unit ="1/atm") = 1.77e5 ;
70   parameter Real Ea4 (unit ="J/mol")= 88680 ;
71   parameter Real Kh2 (unit ="1/atm")= 6.12e-9 ;
72   parameter Real Ea5 (unit ="J/mol")= -82900 ;
73   parameter Real Kco (unit ="1/atm")= 8.23e-5 ;
74   parameter Real Ea6 (unit ="J/mol")= -70650 ;
75   parameter Real gc  (unit = "m/s^2")= 9.81 ;
76   // Predefined values for WGS reaction
77   parameter Real k20 (unit ="mol/gm*hr")= 1.955e6 ;
78   parameter Real Ea7 (unit ="J/mol")= 67130 ;
79   parameter Real K20 = 1.412e-2 ;
80   parameter Real Ea8 (unit ="J/mol")= -37720 ;
81   parameter Real k30 (unit ="mol*atm^0.5/gm*hr") = 1.0202e5 ;
82   parameter Real Ea9 (unit ="J/mol")= 243900 ;
83   parameter Real K30 (unit ="atm^2")= 1.11e11 ;
84   parameter Real Ea10 (unit ="J/mol")= 18240 ;
85   // Ergun Equation
86   parameter Real D (unit ="m") = 1.128 "Diameter of the bed" ;
```

```
87   parameter Real L (unit ="m") = 1 "Length of the bed";
88   parameter Real epsilon = 0.4 "Void fraction of the bed";
89   parameter Real rhoc (unit ="kg/m^3")= 2.355 "Density of the
      catalyst";
90   parameter Real mu (unit ="atm*hr")=  0.0000353147 "Dynamic
      viscosity of the fluid";
91   parameter Real dp (unit ="m")= 2 "Diameter of the particles";
92   parameter Real Ar (unit ="m^2")= 3.14 * D^2 / 4 "Cross-sectional
       area of the bed" ;
93   // Temperature profile in PFR
94   parameter Real cp (unit ="J/kg*K")= 4186 "Heat capacity of water
      ";
95   parameter Real U (unit ="W/m^2*K")= 100 "Overall heat transfer
      coefficient";
96   parameter Real Hr (unit ="J/mol")= -286000 "Heat of reaction for
       methane steam reforming";
97   parameter Real R (unit ="J/mol*K")= 8.314 "Universal Gas
      Constant";
98    //Variables
99   Real VolumePFR(unit = "m3")"Volume of PFR";
100  Real MolarFlow(unit="kmol/hr") "Molar Flowrate";
101  Real Fr[5](each unit = "kmol/h") "Molar flowrate of CH4, H20,
      H2, CO and CO2 respectively";
102  Real y[5] "Mole fraction of CH4, H20, H2, CO and CO2
      respectively";
103  Real PP[5] (each unit = "atm") "Partial pressure of CH4, H20,
      H2, CO and CO2 respectively";
104  Real Massflowrate[5] "Molar Flowrate of CH4, H20, H2, CO and CO2
       respectively ";
105  Real X[5] "Conversion of CH4, H20, H2, CO and CO2 respectively";
106  Real RMSR;
107  Real DEN;
108  Real WGS;
109  Real ROC;
110  Real P (unit ="atm") "Total Pressure in tubular reactor";
111  Real rhog (unit ="kg/m^3")"Density of gas";
112  Real PSI (unit ="Pa") "Pressure calculated from Ergun's Equation
      ";
113  Real TotalMassflowrate (unit ="Kg/hr") "Total Massflowrate
      flowing through tubular reactor";
114  Real TotalVolumetricflowrate (unit ="m^3/hr") "Total
      Volumetricflowrate flowing through tubular reactor";
115  Real u "Superficial Velocity";
116  Real z[3,2] "Compressibilty factor";
117  Real A;
118  Real B;
```

```
119    Real a[5];
120    Real b[5];
121    Real am;
122    Real bm;
123    Real w[5] "Accessing the accentric factor of CH4, H20, H2, CO
        and CO2 respectively";
124    Real Tc[5] "Accessing the Critical Temperature of CH4, H20, H2,
        CO and CO2 respectively";
125    Real Pc[5] "Accessing the Critical Pressure of CH4, H20, H2, CO
        and CO2 respectively";
126    Real MW[5] "Molecular Weight of CH4, H20, H2, CO and CO2
        respectively";
127    Real tr[5];
128    Real H[4];
129    Real Zi[3];
130    Real Zf;
131    Real MassFrac[5] "Mass Fraction of CH4, H20, H2, CO and CO2
        respectively";
132    Real avgMW "Average Molecular Weight";
133    parameter Real K[5,5] = {
134    {0,0.5,0.0263,0.03,0.0793},
135    {0.5,0,0,0,-0.12155},
136    {0.0263,0,0,0.0919,-0.1622},
137    {0.03,0,0.0919,0,0},
138    {0.0793,-0.12155,-0.1622,0,0}
139     };
140    parameter Real T (unit ="K")= 1003.15 "Temperature of the water
        in the reactor";
141    parameter Real Tw (unit ="K")= 700.15 "Wall temperature of the
        reactor";
142    initial equation
143    P = 1;
144    Fr[1] = 49.75;
145    Fr[2] = 49.75;
146    Fr[3] = 0.5;
147    equation
148    // Calculating values of preexponential factor for MSR reaction
149    k1 = k10 * exp(-Ea1 / (R * T));
150    K1 = K10 * exp(-Ea2 / (R * T));
151    KCH4 = Kch4 * exp(-Ea3 / (R * T));
152    KH20 = Kh2o * exp(-Ea4 / (R * T));
153    KH2 = Kh2 * exp(-Ea5 / (R * T));
154    KCO = Kco * exp(-Ea6 / (R * T));
155    // Calculating values of preexponential factor for MSR reaction
156    k2 = k20 * exp(-Ea7 / (R * T));
157    K2 = K20 * exp(-Ea8 / (R * T));
```

```
158  k3 = k30 * exp(-Ea9 / (R * T));
159  K3 = K30 * exp(-Ea10 / (R * T));
160  VolumePFR = pi*(D/2)^2*L;
161  MolarFlow = sum(Fr[:]);
162  for i in 1:N loop
163  y[i] = Fr[i]/MolarFlow;
164  end for;
165  // Ergun equation
166  u = TotalVolumetricflowrate / (3600*Ar);
167  der(PSI)/der(L) = -(rhog*u*(1-epsilon)*((150*(1-epsilon)*mu/dp)
      +1.75*rhog*u))/(rhog*gc*dp*epsilon^3);
168  P = PSI/101325;
169  // Calculation of RMSR
170  DEN = 1.0 + KCO * PP[4] + KH2 * PP[3] + KCH4 * PP[1] + (KH2O *
      PP[2] / PP[3]);
171  RMSR = (k1*((PP[1] * PP[2]) - ((PP[3]^3 * PP[4])/K1))/ PP
      [3]^2.5) / DEN^2;
172  WGS = (k2*((PP[4]*PP[2])-(PP[3]*PP[5]/K2))/PP[3])/DEN^2;
173  ROC = (k3*(PP[1]*PP[2]^2)-(PP[3]^4*PP[5]/K3)/PP[3]^3.5)/DEN^2;
174  // Conversion values of all components
175  X[1] = 1 - Fr[1] / InitialFlowrateCH4;
176  X[2] = 1- (Fr[2]/InitialFlowrateCH4);
177  X[3] =  Fr[3]/InitialFlowrateCH4;
178  X[4] =  Fr[4]/InitialFlowrateCH4;
179  X[5] =  Fr[5]/InitialFlowrateCH4;
180  // Variations of Moles of Components
181  der(X[1]) = rhoc * Ar * (RMSR + ROC)/InitialFlowrateCH4;
182  der(X[2]) = rhoc*Ar*(RMSR+WGS+2*ROC)/InitialFlowrateCH4;
183  der(X[3]) = (3*RMSR+WGS+2*ROC)*Ar*rhoc*3 /InitialFlowrateCH4;
184  der(X[4]) = (RMSR-WGS)*Ar*rhoc/InitialFlowrateCH4;
185  der(X[5]) = (WGS+ROC)*Ar*rhoc/InitialFlowrateCH4;
186  // Massflowrates of Components
187  for i in 1:N loop
188  Massflowrate[i] = Fr[i].*MW[i];
189  end for;
190  // Calculations for TotalVolumetricflowrate
191  TotalMassflowrate = Massflowrate[1]+Massflowrate[2]+Massflowrate
      [3]+Massflowrate[4]+Massflowrate[5];
192  rhog = PSI*avgMW/(1000*R*Zf*T);
193  TotalVolumetricflowrate = TotalMassflowrate/(rhog);
194  for i in 1:N loop
195  PP[i] = y[i].*P;
196  end for;
197  H[1] = 1;
198  H[2]= B-1;
199  H[3]=(A-(3*B^2)-2*B);
```

```
200   H[4]= -(A*B)+(B^2)+(B^3);
201   // Compressibility factor
202   z = Modelica.Math.Polynomials.roots(H);
203   for i in 1:3 loop
204   Zi[i]= z[i,1];
205   end for;
206   Zf = max(Zi);
207   (tr, a, b, am, bm, A, B) = Compressibilty( N, w, T, PSI, y, Tc,
       Pc, K);
208   for i in 1:N loop
209   w[i] = comp[i].ChaoSeadAF ;
210   Tc[i] = comp[i].Tc ;
211   Pc[i] = comp[i].Pc ;
212   MW[i] = comp[i].MW ;
213   end for;
214   for i in 1:N loop
215   MassFrac[i] = Massflowrate[i]/TotalMassflowrate ;
216   end for;
217   avgMW = 1/sum(MassFrac[:]./MW[:]);
218   end Reformer;
219 end SteamReformer;
```

4   Results and Discussion

The user must define the variables given in the table below in accordance with their particular needs in order to properly run the model and produce the appropriate outcome. Each variable has a significant impact on the simulation's behaviour and outcome. Users can customise these variables to fit their personal needs, allowing them to explore different scenarios and get the desired outcomes. In order to effectively accomplish the desired outcomes and precisely depict the system being simulated, it is crucial to thoroughly evaluate and specify each variable.

Variable	Value
D	0.1
L	10
ϵ	0.4
ρ_c	2.355
μ	3.53147E-05
D_p	0.01
A	$\pi * D^2/4$
C_p	4186
U	100
H_r	-28600
R	8.314
T	1003.15
T_w	700.15

The simulation was run with methane, water, and traces of hydrogen as inputs, and the findings show that hydrogen was present in the output along with traces of carbon monoxide and carbon dioxide. The attached graph, which shows the conversion of separate components and the corresponding partial pressures, clearly illustrates these results. We can see the conversion rates and variations in partial pressures over time by looking at the graph, which shows how the individual components changed throughout the experiment. By examining this graph, we may learn important things about how the system behaves and how the various parts of the simulated process are distributed.
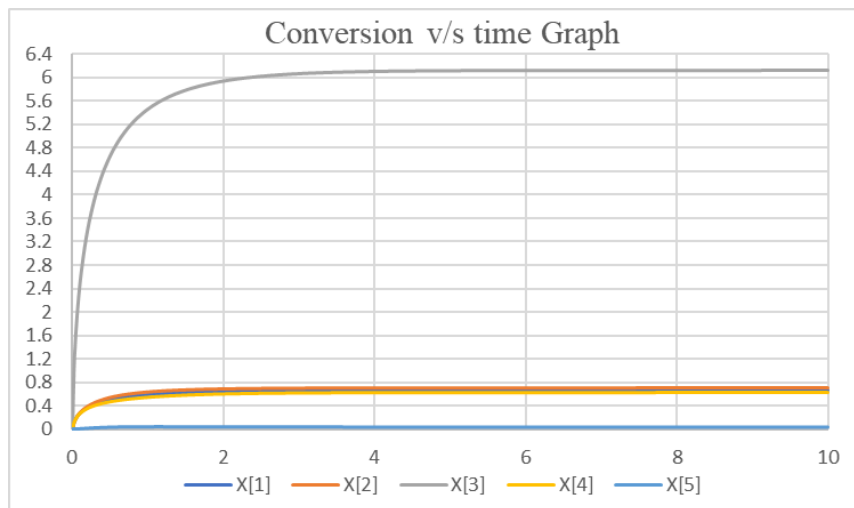
Figure 2: "Conversion Values of Methane, Water, Hydrogen, Carbon Monoxide, and Carbon Dioxide over Time"
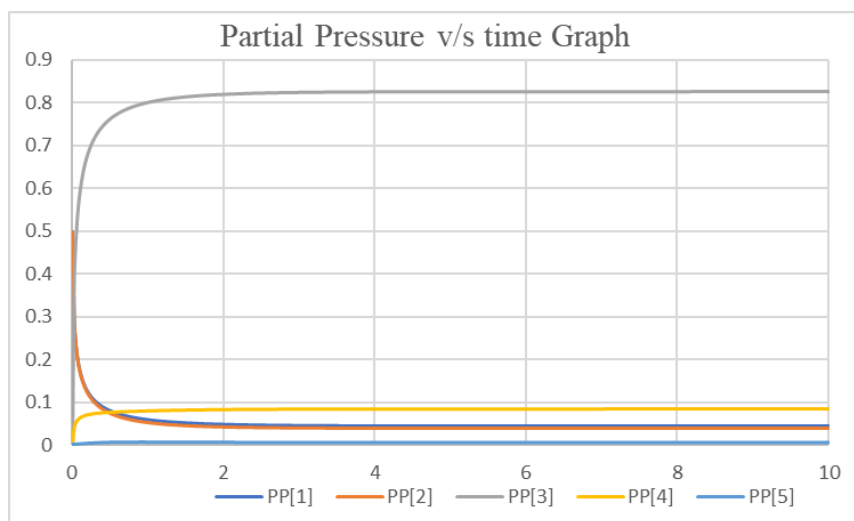

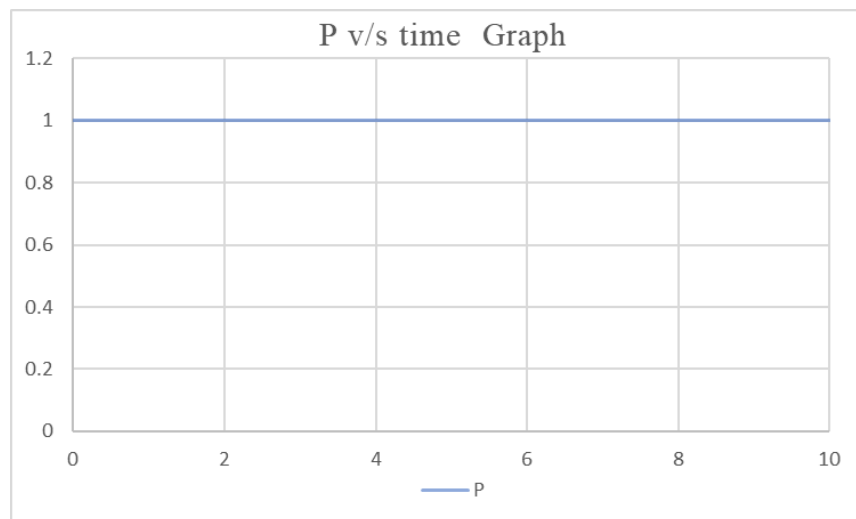Figure 3: Partial Pressure Dynamics of Methane, Water, Hydrogen, Carbon Monoxide, and Carbon Dioxide throughout the Simulation

Figure 4: Total Pressure Dynamics throughout the Simulation