

Sabatier Reactor for conversion of CO₂ into CH₄

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Abstract

This Report discusses about the **Sabatier Reaction**. A brief understanding of the reaction and its various applications. The various optimal conditions **depending on the situation** for the reaction to take place. The main purpose of the paper however is to address the issue of how **computationally costly** it is, to simulate such a reaction using a software¹. We try to solve this issue in this report.

1 Introduction

The **Sabatier reaction** mainly is the production of methane and water from a reaction of hydrogen and carbon dioxide at elevated temperatures (optimally 300-400 °C) and pressures (about 30 bar [□]) in the presence of nickel catalyst. It was discovered by the French Chemists **Paul Sabatier and Jean - Baptiste** in 1897. Alternatively, aluminium oxide makes a more efficient catalyst. Different metal catalyst like Ru and Rh for methanation reaction have been investigated (including Ni) for the purpose of producing CH₄ from **syngas** and other power to gas initiatives . Nickel however, is more widely used. Sabatier is an exothermic reaction. [□]

The Reaction has various applications:

- Creation of synthetic natural gas.
- Ammonia synthesis
- International Space Station Life support
- Manufacturing propellant on Mars

Take note that this is not an exhaustive list. There are more applications to this reaction which even may not have been discovered yet!

There are various simulating softwares² which help industrial engineers to predict the output of the reaction which they are concerned with (in this case the sabatier reacton). They do this to ensure if the reaction or any mechanism for that matter is feasible at all in the first place before they develop the **infrastructure**³ to accommodate the reaction ⁴. This way they don't have to construct the plant before they know the outcome of their plans. These software not only tells the user of the output their intended simulations, but provide all the intricacies, erroneous sections of their input etc in their simulation. It provides them with a pictorial representation, contours etc. all additional information which might be useless to a manager/industrial manager at the initial stages of the plant.⁵.

At first glance it may seem that this is fine, however to run such simulations an expensive equipment is needed and takes a significant amount of time is required to run such simulations. For some start-ups this is an arduous task to come by.

¹ Expensive hardware like RAM, graphics processor (GPU) etc is needed to simulate complex reactions in software like COMSOL, DWSIM etc.

² Ansys, Simulink, COMSOL etc.

³ Reactor, pipe, valve locations, distillation column etc

⁴ It is also a means to ensure the structure is able to withstand the conditions it is being imposed to.

⁵ The plant still hasn't been installed and is tentative whether to go with the plan. The engineers only want to have a rough/crude idea

This is the **trade-off** : For the convenience of using such softwares (**user-friendly**) , which will give additional information which may not be required ⁶ you need to have exceptional equipment to run these simulations as they are not as efficient as running some code in the terminal of your computer.

2 Background

Several authors designed reactive systems for the production of Synthetic Natural Gas(SNG) from CO₂ . A classical solution to perform the Sabatier reaction is the use of several adiabatic stages with intermediate cooling. De Saint Jean et al. presented a system composed of four adiabatic steps with intermediate cooling and a condensation step. Schaaf et al. analyzed the Sabatier reaction in two different systems, one consisting of two reactors with intermediate condensation and one composed of six reactors combined with four gas inter-cooling units.

Moioli et al. did a parametric study of the thermal properties of the reaction to determine the minimal feed temperature for the normal operation of a reactor and proposed a reactor configuration that adjusts the thermodynamic limitations and respects the minimal requirements for reaction ignition, allowing a more stable operation and avoiding the functioning at excessive temperature.

Koytsoompaa et al. presented equilibrium based simulations performed for both CO and CO₂ methanation in order to define the optimum process parameters. Three kinetic models for CO₂ methanation at 10atm, 17atm and 20atm from the literature are compared. They evaluated quality of SNG produced depending on the different operating pressure and temperature of CO₂ derived SNG process.

Fabio et al. provided a quantitative description of the performance of a representative Ru-based catalyst with a low metal loading, under process conditions of interest for intensified Power-to-Gas processes.

The Chemical reactions taking place in the reactor include, strongly exothermic Sabatier Reaction, Eq.(1), accompanied by the mildly endothermic reverse water gas shift reaction, Eq.(2), and the exothermic CO methanation, Eq.(3).



Sabatier Reaction is Exothermic and thermodynamically favorable at low room temperature with a $\Delta H_{298}^\circ = -164.9 \text{ kJ/mol}$ and a $\Delta G_{298}^\circ = -113.59 \text{ kJ/mol}$. The Gibbs free energy increases rapidly with temperature and, at about 500 degree C, it becomes positive and causes the spontaneous reaction to the opposite.

The Sabatier reactor shown in fig. is a heat-exchanger type packed bed internally cooled by molten salt flowing in multiple cooling tubes.

We studied one-dimensional mathematical model. The reactor dimensions are selected in a way that the radial dimension is as small as possible. In order to minimize the heat transfer distance, the minimum number of cooling tubes is set to $N_c=12$. The maximum no of tubes

⁶These software are not open source, so usually a significant amount of fee has to be paid to obtain licence of such softwares as well

are taken as $N_c=22$, to allow enough space for catalytic pellets between the cooling tubes. Molten salt has high thermal conductivity, due to which, in the cooling tubes, significant radial gradients are not expected to develop. For the suggested dimensions, the reactor volume is approximately 30 L.

A transient, one-dimensional, pseudo-homogeneous mathematical model is used to simulate the reactor. The model accounts for the temperature variation in the heat transfer fluid and temperature dependence of thermo-physical properties. It also includes the axial mass and heat dispersion.

Component mass balance and component energy balance for the packed bed compartment is given by Eqs.(4) and (5) respectively. The temperature distribution in a single molten salt tube is given by Eq.(6). The initial conditions and boundary conditions are listed in Eqs.(7) and (8). To calculate the average gas density, ideal gas behavior is assumed. Ergun equation is used to calculate pressure drop, Eq.(9). The variations in the gas velocity due to the change in number of moles are considered by Eq.(10). Eq.(11) is used to define the heat capacity used in Eq.(5).

This is the component mass balance equation

$$\varepsilon \frac{\partial C_i}{\partial t} = D_{ae} \frac{\partial^2 C_i}{\partial z^2} - \varepsilon v_g \frac{\partial C_i}{\partial z} + \rho_s (1 - \varepsilon) \sum_j \eta_j R_{ij} \quad (4)$$

This is the component energy balance equation

$$(\rho C_p)_{eff} \frac{\partial T}{\partial t} = k_{ae} \frac{\partial^2 T}{\partial z^2} - \varepsilon \rho_g C_{pg} v_g \frac{\partial T}{\partial z} + \rho_s (1 - \varepsilon) \sum_j (-\Delta H_j) \eta_j R_j - N_c U_{w,HE} a_{r,HE} (T - T_c) - U_{w,HL} a_{r,HL} (T - T_c) \quad (5)$$

This is the energy distribution of the molten salt

$$\rho_c C_{pc} \frac{\partial T_c}{\partial t} = \lambda_c \frac{\partial^2 T_c}{\partial z^2} - \rho_c C_{pc} v_c \frac{\partial T_c}{\partial z} - U_{w,HE} a_{c,HE} (T - T_c) \quad (6)$$

$$\begin{aligned} z=0 \quad \varepsilon v_{gf} (C_{i,f} - C_i) &= -D_{ae} \frac{\partial C_i}{\partial z} & z=L \quad \frac{\partial C_i}{\partial z} &= 0 \\ \varepsilon \rho_g v_{gf} C_{pg} (T_f - T) &= -k_{ae} \frac{\partial T}{\partial z} & \frac{\partial T}{\partial z} &= 0 \\ \rho_c v_{cf} C_c (T_{c,f} - T_c) &= -k_c \frac{\partial T_c}{\partial z} & \frac{\partial T_c}{\partial z} &= 0 \end{aligned} \quad (7)$$

$$\begin{aligned} \text{at } t=0: \quad C_i(0,z) &= C_{i,int} \\ T(0,z) &= T_{int} \\ T_c(0,z) &= T_{c,int} \end{aligned} \quad (8)$$

This is the Ergun equation

$$\frac{dP}{dz} = -150 \frac{(1-\varepsilon)^2 \mu_g}{d_p^2 \varepsilon^3} v_g - 1.75 \frac{(1-\varepsilon) \rho_g}{d_p \varepsilon^3} v_g^2 P(0) = P_{tf} \quad (9)$$

$$v_g(z) = v_{gf} \frac{\sum_i C_i(z)}{\sum_i C_{i,f}} \quad (10)$$

$$(\rho C_p)_{eff} = \varepsilon \rho_g C_{pg} + (1 - \varepsilon) \rho_s C_{ps} \quad (11)$$

Reactions rates are calculated using the commonly used kinetics for methane reforming over the Ni/Al₂O₃ catalyst, Eqs.(12a)-(12c).

$$R_1 = \frac{k_1}{P_{H_2}^{2.5}} (P_{CH_4} P_{H_2O} - \frac{P_{H_2}^3 P_{CO}}{K_{1,eq}}) \frac{1}{den^2} \quad (12a)$$

$$R_2 = \frac{k_2}{P_{H_2}} (P_{CO} P_{H_2O} - \frac{P_{H_2} P_{CO_2}}{K_{2,eq}}) \frac{1}{den^2} \quad -(12b)$$

$$R_3 = \frac{k_3}{P_{H_2}^{3.5}} (P_{CH_4} P_{H_2O}^2 - \frac{P_{H_2} P_{CO_2}}{K_{3,eq}}) \frac{1}{den^2} \quad -(12c)$$

$$den = 1 + K_{CO} P_{CO} + K_{H_2} P_{H_2} + K_{CH_4} P_{CH_4} + \frac{K_{H_2O} P_{H_2O}}{P_{H_2}}$$

$$k_j = A_j \exp\left(\frac{-E_j}{R_g T}\right)$$

$$K_i = B_i \exp\left(\frac{-\Delta H_i}{R_g T}\right)$$

To calculate the internal effectiveness factor, standard expression for spherical pellet is used, Eq.(13). The Thiele modulus is defined for each reaction with the corresponding reaction rate constant (k_j in Eq.(12)):

$$\eta_j = \frac{3}{\phi_j} \left(\frac{1}{\tanh \phi_j} - \frac{1}{\phi_j} \right); \quad \phi_j = \sqrt{\frac{\hat{k}_j d_p^2}{4D_m}} \quad -(13)$$

$$\hat{k}_1 = \frac{k_1 \rho_s (1-\varepsilon)}{\sqrt{P_{if} \rho_g \varepsilon}}; \quad \hat{k}_2 = \frac{k_2 \rho_s (1-\varepsilon) P_{if}}{\rho_g \varepsilon}; \quad \hat{k}_3 = \frac{k_3 \rho_s (1-\varepsilon)}{\sqrt{P_{if} \rho_g \varepsilon}}$$

To calculate the effective axial mass dispersion coefficient, correlation in Eq.(14) is used.

$$D_{ae} = \varepsilon \left(\frac{D_m}{\tau_b} + 0.5 d_p v_g \right); \quad \tau_b = \frac{1}{\varepsilon^{0.5}} \quad -(14)$$

$$k_{ae} = \lambda_g (8 + 0.05 Re_p^{1.09}); \quad Re_p = \frac{v_g \rho_g d_p}{\mu_g} \quad -(15)$$

$$U_{w,HE} = \left(\frac{1}{h_{wr}} + \frac{d_w}{\lambda_w} + \frac{1}{h_{wc}} \right)^{-1} \quad -(16a)$$

$$U_{w,HL} = \left(\frac{1}{h_{wr}} + \frac{d_w}{k_w} + \frac{d_{iw}}{k_{iw}} + \frac{1}{h_{nc}} \right)^{-1} \quad -(16b)$$

$$U_{w,HL} = \left(\frac{1}{h_{wr}} + \frac{d_w}{k_w} + \frac{d_{iw}}{k_{iw}} + \frac{1}{h_{nc}} \right)^{-1} \quad -(16b)$$

$$Nu_p = \frac{h_{wr} d_p}{\lambda_g} = 24 + 0.34 Re_p^{0.77}; \quad Re_p = \frac{v_g \rho_g d_p}{\mu_g} \quad -(17)$$

$$\text{for } Re_c < 2030: \quad Nu_c = 3.66 + \frac{0.065 Re_c Pr_c (D_c/L)}{1 + 0.04 [Re_c Pr_c (D_c/L)]^{2/3}} \quad -(18a)$$

$$\text{for } 2030 < Re_c < 4000: \quad Nu_{wc} = 0.012 (Re_c^{0.87} - 280) Pr_c^{0.4} [1 + (D_c/L)^{2/3}] \quad -(18b)$$

$$\text{for } Re_c > 4000: \quad Nu_c = 0.027 Re_c^{0.8} Pr_c^{1/3} \quad -(18c)$$

$$Nu_c = \frac{h_{wc} D_c}{\lambda_c}; \quad Re_c = \frac{v_c \rho_c D_c}{\mu_c}; \quad Pr_c = \frac{C_{pc} \mu_c}{\lambda_c}$$

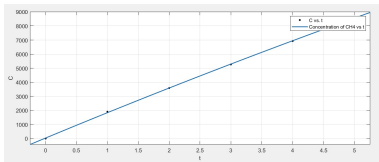
3 Problem Statement

As discussed briefly in the introduction, simulation is costly. They are normally not **Open Source**⁷ and a significant fee needs to be paid to obtain the license⁸. In addition to this, to run simulations in such softwares is computationally heavy and costly. The softwares have inbuilt **GUI**⁹ and other such features which make it more user-friendly which in turns makes them less efficient than **CLI**¹⁰ (running on a terminal). Such softwares when running the simulation, solves thousands of equations each time it is executed (depending on the granularity of the mesh size). It gives us the pressure, heat contours and all such intricacies of the simulation which is not always useful. The system required for such simulations is also quite expensive.

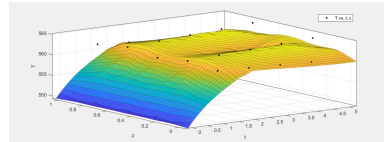
We are trying to develop a solver using **MATLAB** and a Neural Network using **Python/Jupyter Notebook** which will greatly diminish the hardware requirement for such a task and will give the user an insight to the output of the reaction. In our case the **Sabatier reaction**. (The estimate will be crude however compared to the actual simulation)

4 Result and Discussion

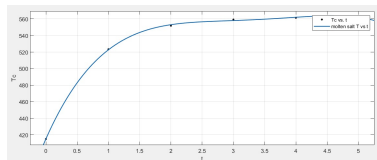
From the Matlab model of Sabatier reactor and with the help of cftool, we plotted the Concentration of CO₂ vs time, shown in Fig.1(a), Reaction Temperature vs time and space(z), shown in Fig.1(b) and Temperature of Molten salt vs time, shown in Fig.1(c).



(a) C vs t



(b) T vs t,z



(c) Tc vs t

Figure 1: Results obtained in cftool

For the Simulations, we used time step of 1 second due to high computational costs. The Concentration of CH₄ reaches to 9000 mole/cubic metres in 5 seconds. Molten Salt temper-

⁷Free and publicly available

⁸Sometimes these licences can't be shared amongst multiple users

⁹Graphical user interface

¹⁰Command line input

ature profile shows the change of temperature from 400 K to 560 K in the span of 5 seconds. The plots obtained are similar to the literature followed.

5 Conclusion

Our method is still crude compared to the simulating softwares. The software solves the **governing equations** in each grid/mesh of the simulation and so will get a more accurate result as compared to our method. However we get a "ball-park" estimate in a shorter duration of time using our method. Due to the pre-defined weights in our network and CLI we don't need an expensive system. Care should be taken that these are just weights and some activation functions in our networks which don't provide any insight to the computer of the complex turbulent system and the exact mechanism taking place. With a large and growing data-set we can progressively get a better and better estimate. (The weights can keep being refined)

6 Future Scope

MARS's has >95 percent CO₂ in it's atmosphere. Methane, Water and Energy from the Sabatier reaction is everything needed for a MARS colony. The energy produced through this reaction could be turned into electricity or heat or could be used to keep the Sabatier process going. The methane could be used directly as rocket fuel when combined with liquid oxygen. The water produced could be used for drinking, farming or rehydrating stored foods or can be used for other reactions.

Multiple reactors can also be used in series combination. There is also a possibility of splitting the feed of CO₂ into several parts, so as to improve the heat management.

This is an open source code and will be beneficial to all start-up which are reluctant to invest money before they have a concrete plan¹¹. They wont be as confused, due to the information given by the solver is concise and brief as opposed to the abundant information given by simulating softwares. No license or an expensive hardware is required.

But due to the **observed trend of computer technology**[9]. The way more efficient hardware is becoming less and less expensive. This in time may no longer be useful to **save computation cost** perhaps. Entrepreneurs could potentially buy a supercomputer and easily tackle the problem of such softwares being less efficient. However if such simulating softwares require a license still, this method is still viable¹².

References

- [1] Jens; Matthischke Steffi; Schlüter Michael; Götz Manuel; Lefebvre Jonathan; Prabhakaran Praseeth; Bajohr Siegfried Rönsch, Stefan; Schneider. Review on methanation. *fundamentals to current projects, Fuel*, 166(1):276–296, 2016.
- [2] Methanation Unit. Helmeth project. *Retrieved 2020-11-13*.

¹¹Initially they don't know whether to even go with their plans as they don't know if its feasible or not

¹²Multi-time sharing softwares like the SAP license is worth Crores of Rupees, so it is not an understatement that our Solver is still viable

- [3] Kim Ann Zimmermann. History of computers: A brief timeline. *Live Science Contributor*, 7 September 2017.

7 Appendices

The solver was made from the Authentic Mathwork website . <https://www.mathworks.com/help/releases/R2019b/matlab/math/solve-system-of-pdes.html>

Appendix-1

solver.m

```
clc;
clear;
m=1;
z = linspace(0,1,5);
t = 0:1:5;
sol=abs(pdepe(m,@pdefun,@pdeic,@pdebc,z,t));
```

Appendix-2

pdefun.m

```
function [c,f,s] = pdefun(z,t,u,dudz)
Ci=(u(1));
T=(u(2));
Tc=(u(3));
epsilon=0.5;
GHSV=10000;
L=10; % m
rhog=1; % Assumption of molar density 1mol/m3
c1=0.333e+5;
c2=0.7993e+5;
c3=2.87e+3;
c4=0.416e+5;
c5=991.96;
Cpg=c1+c2*((c3/T)/sinh(c3/T))^2+c4*((c5/T)/cosh(c5/T))^2;%at550K%https://gyazo.com/c
//gyazo.com/3c4f07b55f723d88a9cd04ad4435cc02
Cpg = (Cpg/1000000);%kJ/molK
rhos = 3460;
Cps = 0.836;%atNi/Al2O3catalyst10%Ni%kJ/kgK
rhoc = 2200;%moltensaltcoolantkg/m3
Cpc = 1.53;%moltensalteutecticmixture0.6sodiumnitrate0.4
potassiumnitrate%kJ/kgK
rhocp = epsilon*rhog*Cpg + (1-epsilon)*rhos*Cps;%equation11Fornickelaluminacatalyst
rhocpc = rhoc*Cpc;%heatcapacitydensity
c = [epsilon;rhocp;rhocpc];%Solvingeqn4,5,6simultaneously
Dae = 0.00009;%Diffusivityat400K(Dispersionataxialcoefficient)
dp = 0.003;
sumCi = 2;
sumCif = 5;
```



```

vgf = GHSV * L/epsilon;
%vg = vgf * Ci/sumCif; %vgf = 200000m/sGHSV = 10000
vg = vgf;
mug = 2.333e - 5;
Rep = vg * rhog * dp/mug; %gasreynold'snumber,eq17/15
lambdag = 0.00007857; %0.00007857;
kae = lambdag * (8 + 0.05 * Rep1.09); %eq15
lambdac = 0.000536; %0.000536;
f = [Dae;kae;lambdac]; %.*dudz;
dCidz = (dudz(1));
k1 = 3.66 * 1014 * exp(-240.1/(T * 8.314 * 10-3)); %rateconstants
k2 = 5.41 * 10-3 * exp(-67.1/(T * 8.314 * 10-3));
k3 = 8.83 * 1013 * exp(243.9/(T * 8.314 * 10-3));
delta1 = -164.9; % (kJ/mol)enthalpychangeat25C
delta2 = 41.2;
delta3 = -206.1;
KCO = 8.23 * 10-10 * exp(70.7/(T * 8.314 * 10-3)); %Adsorbtionconstants
KH2 = 6.12 * 10-14 * exp(82.9/(T * 8.314 * 10-3));
KCH4 = 6.65 * 10-9 * exp(38.3/(T * 8.314 * 10-3));
KH2O = 1.77 * 105 * exp(-88.7/(T * 8.314 * 10-3));
K1eq = 1.026676 * 1010 * exp(-26830/T + 30.11); %equilibriumconstant
K2eq = exp(4400/T - 4.063);
K3eq = K1eq * K2eq; %K1/K2
P0 = 500000; %Pa
Ptf = -150 * (((1 - epsilon)2 * mug)/(dp2 * epsilon3)) * vg - 1.75 * (((1 - epsilon) * rhog)/(dp * epsilon3)) * vg2 * P0; %eq9
kcap1 = k1 * rhos * (1 - epsilon)/(sqrt(Ptf) * rhog * epsilon); %eq13
Dm = (Dae/epsilon - 0.0015 * vg)/(epsilon0.5); %eq14
phi1 = sqrt(kcap1 * dp2/(4 * Dm));
eta1 = (3/phi1) * (inv(tanh(phi1)) - inv(phi1));
pCO = 100000;
%partial pressures
pH2 = 400000;
pCH4 = 0;
pH2O = 0;
den = 1 + KCO * pCO + KH2 * pH2 + KCH4 * pCH4 + (KH2O * pH2O/pH2);
Ri1 = (k1/pH22.5) * (pCH4 * pH2O - (pCO * pH23/K1eq))/den2; %eq12a
kcap2 = k2 * rhos * (1 - epsilon) * Ptf/(rhog * epsilon); %eq13
phi2 = sqrt(kcap2 * dp2/(4 * Dm));
eta2 = 3/phi2 * (inv(tanh(phi2)) - inv(phi2));
Ri2 = (k2/pH2) * (pCO * pH2O - pH2 * pCO/K2eq)/den2; %eq12b
kcap3 = k3 * rhos * (1 - epsilon)/(sqrt(Ptf) * rhog * epsilon); %eq13
phi3 = sqrt(kcap3 * dp2/(4 * Dm));
eta3 = 3/phi3 * (inv(tanh(phi3)) - inv(phi3));
Ri3 = (k3/pH23.5) * (pCH4 * pH2O2 - pH2 * pCO/K2eq)/den2; %eq12b
sumetajRij = eta1 * Ri1 + eta2 * Ri2 + eta3 * Ri3;
%dCidz = dudz(1);
%eq4

```

```

s1 = -epsilon*vg*dCidz + rhos*(1 - epsilon)*sumetajRi j;
dTdz = (dudz(2));
sumdeltaHetajRj = delta1*eta1*Ri1 + delta2*eta2*Ri2 + delta3*eta3*Ri3;
Nc = 20; %minimumnumberofcoolingtubes
hwr = (24 + 0.34*Rep0.77)*lambdag/dp; %eq17
dw = 0.002;
lambdac = 0.00007281; %thermalconductivityofcoolant
lambdaw = 0.045; %Steel
vc = 20000;
Dc = 0.02;
muc = 0.0000936; %at280C
Rec = vc*rhoc*Dc/muc; %coolantreynold'sno.
Prc = Cpc*muc/lambdac; %coolantprandtlno.
if Rec < 2030
    hwc = (3.66 + (0.065*Rec*Prc*(Dc/L))/(1 + 0.04*((Rec*Prc*(Dc/L))(2/3)))) * lambdac/Dc;
elseif 2030 < Rec < 4000
    hwc = (0.012*(Rec0.87 - 280)*Prc0.4*(1 + (Dc/L)(2/3))) * lambdac/Dc; %eq18b
elseif Rec > 4000
    hwc = (0.027*Rec0.8*Prc(1/3))*lambdac/Dc; %eq18c
end
UwHE = inv(1/hwr + dw/lambdaw + 1/hwc); %eq16a
arHE = 2.463;
UwHL = 0.01;
arHL = 20;
Te = 298;
s2 = -epsilon*rhog*Cpg*vg*dTdz + rhos*(1 - epsilon)*sumdeltaHetajRj - Nc*
UwHE*arHE*(T - Tc) - UwHL*arHL*(T - Te); %eq5
dTcdz = (dudz(3));
acHE = 200;
s3 = -rhoc*Cpc*vc*dTcdz - UwHE*acHE*(Tc - T); %eq6
s = [s1;s2;s3];
end

```

Appendix – 3

pdeic.m

```

function u0 = pdeic(z)
Ciint = 1;
Tiint = 550;
Tciint = 415;
u0 = [Ciint;Tiint;Tciint];
end

```

Appendix – 4

pdebc.m

```

function [pl,ql,pr,qr] = pdebc(xl,ul,xr,ur,t)
epsilon = 0.5;
vgf = 200000; %Allvelocity: gasfluid,coolantetc.are200000m/sdespitetheirpositioninthereactor
Cif = 1;
rhog = 1;
T = (ul(2));

```

```

c1 = 0.333e + 5;
c2 = 0.7993e + 5;
c3 = 2.87e + 3;
c4 = 0.416e + 5;
c5 = 991.96;
Cpg = c1 + c2 * ((c3/T)/sinh(c3/T))^2 + c4 * ((c5/T)/cosh(c5/T))^2;
%at550K%https://gyazo.com/c9012c69258e2cb50730de0503c5d1a8%https://gyazo.com/
Cpg = (Cpg/1000000);
dp = 0.003;
mug = 2.333e - 5;
vg = 200000;
Tf = 550;
rhoc = 2200;
vcf = 20000;
Dae = 0.00009;
kc = 5;
lambdac = 0.00007281;
Cc = 1
Tcf = 415;
pl1 = epsilon*vgf*(Cif - (ul(1)));
pl2 = epsilon*rhog*vgf*Cpg*(Tf - (ul(2)));
pl3 = rhoc*vcf*Cc*(Tcf - (ul(3)));%eq7
pl = [pl1;pl2;pl3];%z = 0BC
ql = [1;1;kc/lambdac];
pr = [0;0;0];%z = LBC
qr = [1;1;1];
end

```