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Design, Implementation and Simulation of Solar Thermo Chemical Reactor With Multiple Length and Porosity Using CFD

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***Abstract*—Thermo chemical hydrogen production is important because it has the potential to reduce dependence on fossil fuels as an energy source. In a solar power plant, a solar receiver is a device in which solar energy is absorbed by liquids and/or materials and converted into thermal energy. When solar energy is used to drive a reaction, the receiver also acts as a reactor. The diversity of thermo chemical processes, the variety of operations and requirements for connecting receivers to concentration systems have led to the development of a wide variety of reactor configurations. The aim of this project is to determine general rules for solar reactor/receiver design. For this purpose, a first presentation of a solar receiver/generator produced in a paper for different applications is given. The main problems encountered in modeling these systems are described. Finally, selected examples are discussed in more detail to illustrate ways to improve solar reactor design. The study found that the most common constraints used to describe the operation of reactors are (i) energy conversion, (ii) energy losses associated with irreversible processes and (iii) thermo-mechanical stress. The overall choice of reactor design depends on the type of reaction. The optimization process can be performed by acting on (i) the shape and size of the acceptor, (ii) the reactant feeding method, and (iii) the particle morphology of the reactants.**

Keywords— Solar thermal energy, porosity, thermo chemical fuel, syngas, meshing, boundary condition, renewable energy sources

I. Introduction

While a suitable alternative is electrification of cars which is thought to get the ability to improve the internal combustion engine, for air transport, analyses show that long-range transport is quite dependent on renewable resources too in the future because specific energy of its batteries is constrained. To get the pushy goals predefined by the aviation industry the uses of alternative fuels is thus imperative. Various options occur, like the electrochemical mechanism that integrates solar energy with electrolysis, or the photochemical mechanism that generates hydrogen using biomass or synthetic leaves. By the use of complete solar radiation the thermo-chemical fuel offers high conversion efficiencies and it has recorded major performance advances in the past decades. The mechanism transforms CO2 and water into CO and H2 (syngas) utilizing concentrated sun's radiation as a fount of heat through a redox cycle controlled at high temperature, metal oxide is a substance that decreases partial pressure at low oxygen and high temperature, and oxidizes at lower temperatures with water and carbon di oxide. The produced syngas then converted attentively liquid hydrocarbons in the Fischer-Tropsch synthesis (FT), whereas a low-temperature synthesis gives longer-chained hydrocarbons, which then converted into chains of crave length in the jet fuel range by hydro- cracking and distillation. Benefit of solar thermo-chemical process is that the hydrogen and carbon mono oxide feed streams could be generated in independent reactors and thus easily taken to the needed around two in the FT reactor ratio of H2 / CO.

1.1 Thermodynamics of Solar Thermo-chemical conversion

Because thermodynamics is the science that describes the conversion of one form of energy into another form, it is germane to the area of Solar Thermo chemistry. Solar thermo chemical processes convert radiant energy into chemical energy. The two fundamental thermodynamic laws that give practical information with regard to any solar thermo chemical process are the 1st and 2nd laws. Using the 1st law, one establishes the minimum quantity of solar energy needs to produce a particular fuel or chemical species. The 2nd law indicates, among other things, whether or not the chosen path for producing the fuel is physically possible. Both types of information are required for a process designer (Steinfeld and Palumbo, 2003).

1.2 Principles of Solar Energy Concentration

The conventional method of concentrating solar energy, i.e. collection of solar energy over some large area and delivering it to a smaller one, is by parabolic shaped mirrors. Parabolic centres in its focal point the rays parallel to its axis. Sun rays aren't identical though. For a well approximation it can be assumed that they originate on a disc that subtends the radian angle = 0.0093. When a perfectly specular reflective paraboloid of focal length f and rim angle Φ rim is aligned to the sun, reflection of the rays at the focal plane forms a circular image centred.

1.3 Thermo chemical heat storage material

THS systems often classified as reversible chemical reactions and action processes. in a auction process, heat is hold on by disturbing the binding force between the material and also the frappe in the terms of the chemical potential. For the heat energy sorption process, the process is only occurs while the dried materials are uncovered to working sorbent (dried) materials area unit exposed to the operating fluid or material. Thus, in essence, as long because the materials area unit hermitically sealed, and the storage is loss-free.

1.4 Types of Solar energy

It is clear from the stated facts about the sun that there is an enormous energy potential in sunlight. Why is solar energy not being used for the majority of our energy needs? Primarily it is cost and conversion capacity that stands in the way of solar energy. Fossil fuels are much more cost effective because they are rich concentrated sources of energy, but the sunlight is a widely spread resource with a much lower energy density.

II. LITERATURE REVIEW

Zhang *et al.*, 2018) explains that thermal transfer and fluid flow characteristics have important impacts on the performance of hydrogen output as a primary technological parameter for porous media solar thermo-chemical reactor. The implementation of computational fluid dynamics (CFD) could solve these problems more effectively and at a lower cost. Additionally, the option of various models of thermal transport may cause results to vary.

(Falter and Pitz-Paal, 2018) explained in his paper that the solar thermo-chemical fuel processing pathway is being explored as an appealing alternative for transport sector decarburization. Usage of cerium as a reactive material and the new published literature data on inert gases demand and energy need for the vacuum pumping, Analyzes the energy output of the thermo-chemical reactor for vacuum pumping and gas mixture sweeping, and describes the process parameters needed to achieve high efficiency.

(Huang et al., 2018) introduces a heavily biased and robust iron-based $La_{0.6}Sr_{0.4}Fe_{0.8}Al_{0.2}O_{3-\delta}$ oxygen carrier for syngas processing via a thermo chemical process powered by solar energy. It is observed that during redox cycling a complex structural transition occurs between the perovskite layer and a core – shell composite of Fe0@oxides.

(Zsembinszki et al., 2018) analysed that to conduct a summary of the state-of-the-art reactors found in the literature that are used for solid gas reactions or thermal decomposition processes around 1000 C, which could be further applied for thermo-chemical energy storage in CSP (concentrated solar power) plants, specifically for SPT (solar power tower) technology. Direct and indirect mechanisms can be applied, and the most studied are direct and closed mechanisms.

Kodama et al., 2017) said that by using solar thermal power for the production of high temperature fuel has the potential to significantly reduce the dependence on fossil fuel in our current economy. Over the last two decades, remarkable progress has been made in the development of solar-driven thermo-chemical reactors for hydrogen and syngas production, as they are promising transport energy carriers, domestic and industrial applications.

(Guene Lougou *et al.*, 2017a) in his paper investigated thermal overall performance evaluation of solar thermo-chemical reactor for syngas production. P1 radiation model was once used to observe the reactor thermal performance. It used to be determined that the temperature distribution resulted in the incident radiation depth distribution during the reactor internal cavity. However, the greater temperature used to be attributed to a awesome absorption of incident radiation heat flux intensity.

(Rao and Dey, 2017) discussed that Solar photochemical potential of splitting water (artificial photosynthesis) to generate hydrogen is rising as a workable process. The photo voltaic thermo-chemical route additionally guarantees to be an attractive capability of accomplishing this objective. These encompass the low-temperature multistep system as nicely as the high-temperature two-step process. It is noteworthy that multistep manner primarily based on the Mn(II)/Mn(III) oxide machine can be carried out at 700 °C or 750 °C. The two-step technique has been finished at 1,300°C/900°C by way of the usage of yttrium-based uncommon earth manganites. It appears viable to render this high temperature method as an isothermal process.

(Falter and Pitz-Paal, 2017) explained that for non-stoichiometric redox reactions that produce CO and H_2 from CO_2 and water, heat recuperation from the solid phase is a promising mechanism to improve the cycle efficiency. In solar thermo-chemical reactor principles several various approaches to heat recovery and the gas separation have recently been proposed. To describe many possible degrees of freedom in the reactor design, a generic reactor model is described for two-step redox reactions of solid pieces of reactant moving in counter flow between reduction and oxidation chamber.

Villafán-Vidales et al., 2017) said in his paper that Hydrogen is an exciting means of transport, household, and industrial energy carrier. Nowadays the chemical industry basically consumes hydrogen, but its demand is expected to grow significantly in the long term due to emerging market. Hence hydrogen production with sustainable method is a relevant issue. This research provides a description of the different thermo-chemical processes aided by CSP for the production of hydrogen and syngas. Some relevant prototypes of solar proven reactor are characterized for each process.

III. METHODOLOGY AND ANALYSIS

3.1 Steps of working

1. Design and modeling of porous media solar thermo-chemical reactor in NX 11 according to the selected base paper.
2. Further converting the NX 11 File in .STEP format for importing it in ANSYS Fluent work bench.
3. Assigning the name selection to the different parts of thermo chemical reactor model.
4. Meshing of thermo chemical reactor model for performing the simulation process.
5. Providing the suitable boundary condition according to the selected base paper.
6. Assigning the material properties to the model.
7. Setting the proper setup for CFD analysis procedure.
8. Evaluating the results after the finish of simulation work.

3.2 Case design

To increase the length of porous media in a chemical reactor, seven cases are taken which are shown in table below. In first three cases, the porosity will increase gradually while the velocity and length of porous media will remain constant. The best result from three cases will be taken for case 4 and 5, in this velocity will be changed. After that the best resulted porosity and best result of velocity will be taken for the next two cases; case 6 and 7. The results of last two cases will show the changes in length of porous media.

3.3 Software used for study

NX 11

In the present study NX11 software is used for CAD modelling. NX11 offer the various stages of the product development which include computer aided design (CAD), computer aided engineering (CAE) computer aided manufacturing (CAM). It also provide the platform for performing various design modules such as wireframe and surface and shape design, mechanical and electrical system design etc.

ANSYS

It is the software used for modelling as well as for testing the products durability, temperature distribution in product and the movement of fluid under various boundary conditions. It make possible to analyse the condition of the model under various operating environment and also helped to simulate the effect on model of an object. The basic module of the ANSYS software is FEA, CFD.

3.4 Mathematical model

Figure 3.1 displays SiC porous media solar thermo-chemical reactor that is used for computational simulation. The absorbed solar energy is transferred through the clear quartz glass window mounted at the reactor's front surface through the reactor's inner cavity. As indicated in Figure 3.1, the angle of the front cavity wall is designed to 45° to the axis in order to effectively collect incident solar energy. Two opposite inlets in the (y) direction lead the reactant gas into reactor inner cavity. Because of the influence of carrier gas flow the quartz window is swept and kept clear from solid deposition. At the reactor exit the water-cooled system is mounted to lower the exhaust gas temperature. In addition, the entire reactor is covered with strong thermal insulation to secure the reactor and reducing heat loss during the progress of thermo chemical reactions.

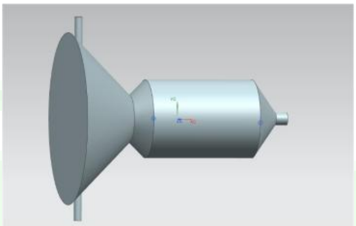


Figure 3.1 Schematic sketches of solar thermo-chemical reactor in NX 11

3.5 Meshing

Meshing is an integral a part of the CAE simulation method. The mesh affects the accuracy, convergence and speed of the solution. Furthermore, the time it takes to create and mesh a version is often a good sized part of the time it takes to get consequences from a CAE solution. Therefore, the higher and extra automated the meshing equipment, the better the solution.

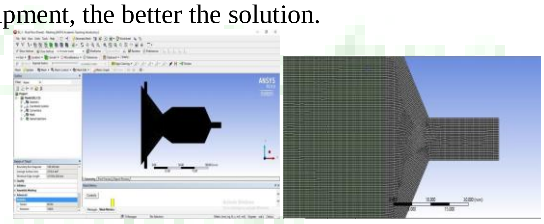
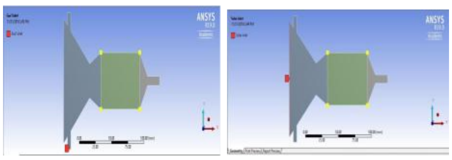


Figure 3.2 Mesh with enlarged image

3.6 Name Selection and Boundary Conditions

Assigning the name selection to the of tube, providing the suitable boundary condition according to the selected base paper, materials properties are assigned, the material property is shown in below table. There are two material is used which are Silicon carbide and air. The solar thermochemical reactor contained silicon carbide porous medium and air is used as heat transfer fluid.



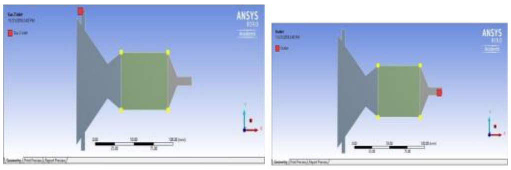


Figure 3.3 Name selection

3.7 Mathematical model

3.7.1 Continuity equation

The continuity conversation equation, momentum conservation equation and energy conservation equation for the solar thermo chemical reactor.

IV. SIMULATION AND RESULTS

4.1 Result for selecting porosity

The solar thermo chemical reactor consists of a chemical reactor for which three case are taken to select the porosity of the material. Three cases with constant velocity and same length of porous media are taken in which the porosity is increased by 10% in every case is shown in table.

4.1.1 Temperature

To select the porosity of the material, temperature is one of the main parameter to be considered. Following are the results of three cases temperature contour.

Case 1- The temperature contour for case 1 is shown in figure 4.1. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

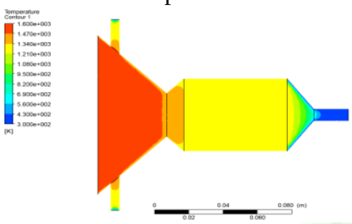


Figure 4.1 Temperature contour for Case 1

Case 2- The temperature contour for case 2 is shown in figure 4.2. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

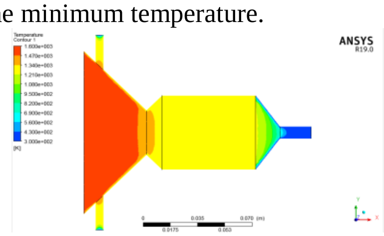


Figure 4.2 Temperature contour for Case 2

Case 3- The temperature contour for case 3 is shown in figure 4.3. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

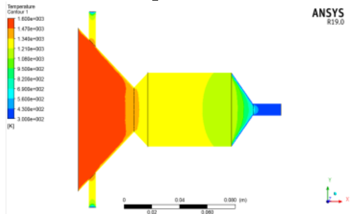
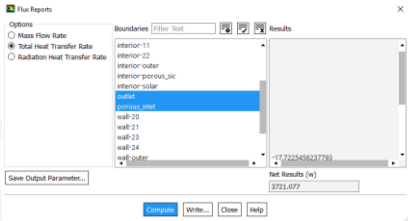


Figure 4.3 Temperature contour for Case 3

4.1.2 Heat transfer rate

Case 1- The heat transfer rate of Case1 is shown in figure 4.4 .The result of total heat transfer rate is 3721.077.



Case 2- The heat transfer rate of Case2 is shown in figure 4.5 .The result of total heat transfer rate is 4327.929.

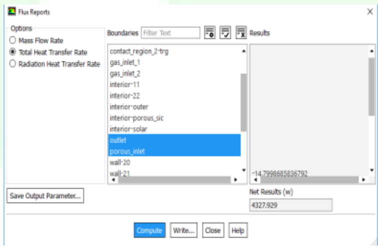


Figure 4.5 Heat transfer rate of Case 2

Case 3- The heat transfer rate of Case3 is shown in figure 4.6 .The result of total heat transfer rate is 4818.513.

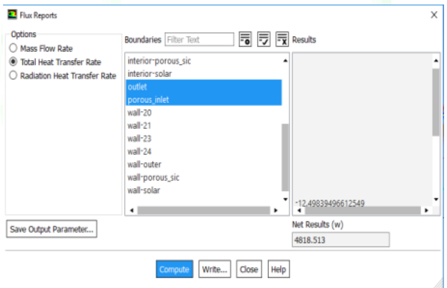


Figure 4.6 Heat transfer rate of Case 3

4.1.3 Temperature comparisons

The graph show that while increasing the porosity the temperature decreases. The porous medium at a length of 0.05 to 0.1 meter remained quite stable. This change in temperature is produced because high porous material of alloy has to move gas in large quantity in porous contact zone. Case 3 will be ideal for the chemical reactor as its temperature is lowest when the length is increased.

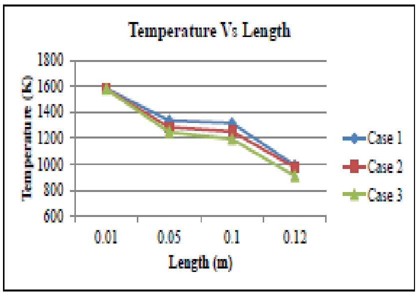


Figure 4.7 Graph representing variations in temperature when length changed

Figure 4.8 shows the same results like the above graph. Case 3 is decreasing rapidly when length of porous media is increased.

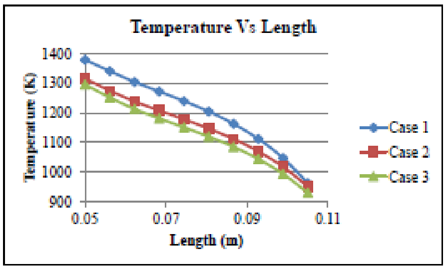


Figure 4.8 Graph representing Temperature v/s Length

4.1.4 Pressure comparisons

When length of the porous media is increased, the pressure decreases. In the table given below, it is clear that in each case the pressure is decreasing as the length of porous mode is increasing.

Table 4.2 Pressure comparison with length

	Case 1	Case 2	Case 3
0.01	0.0243	0.0246	0.0246
0.05	0.0208	0.0210	0.0210
0.1	0.0024	0.0026	0.0026
0.12	0.0014	0.0016	0.0015

With the increase of length of material the pressure decreases, shown by a graph in figure 4.9.

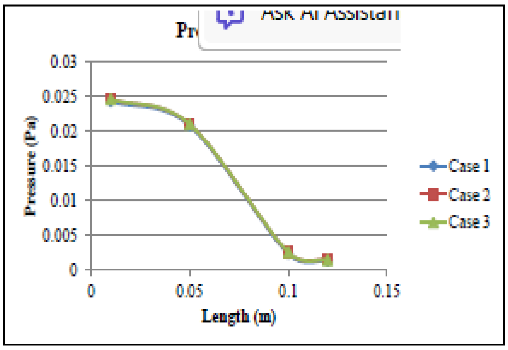


Figure 4.9 Graph represents Pressure v/s Length

4.1.5 Velocity Comparison

The velocity graph is divided in three section A is inlet, B is Porous Region and C is Outlet. The graph showed porous zone in decrease the velocity of gas. At this region higher heat transfer is achieved.

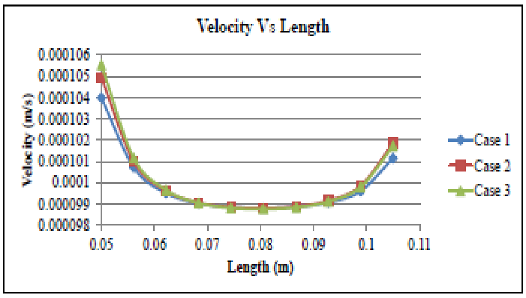


Figure 4.10 Velocity comparison graph

4.2 Result for selecting Velocity

The solar thermochemical reactor consists of a chemical reactor for which earlier three cases were taken to select the porosity. Now two cases will be taken to select the velocity. Best result porosity will be taken as porosity in case 4 and 5. The length of the porous media will also remain constant. To select the velocity, velocity will be varied as shown in table 4.3.

Table 4.3 Cases for selecting velocity

	Porosity	Velocity (m/s)	Length of porous Media (mm)
Case 4	0.9	0.09	60
Case 5	0.9	0.002	60

4.2.1 Temperature

To select the velocity of the material, temperature is one of the main parameter to be considered. And while increasing the material the temperature should decrease maximum. Following are the results of two cases; Case 4 and 5 temperature contour.

Case 4- The temperature contour for case 4 is shown in figure 4.10. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

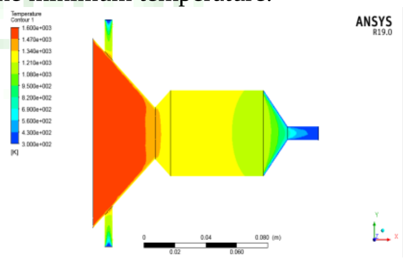


Figure 4.11 Temperature contour of Case 4

Case 5- The temperature contour for case 5 is shown in the figure 4.11. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

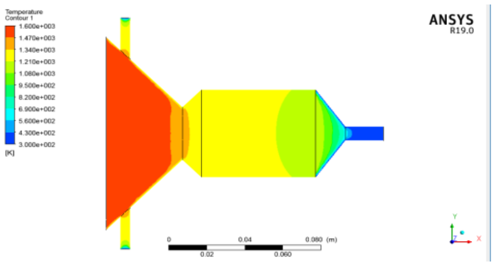


Figure 4.12 Temperature Contour of Case 5

4.2.2 Heat transfer rate

To select the velocity, the heat transfer rate of Case 4 and 5 are shown in figure 4.12. It is clear from the figure that heat transfer of Case 4 is 4818.583 and heat transfer rate of Case 5 is 4818.388. Heat transfer rate of Case 4 is higher than Case 5 from the results shown in the graph.

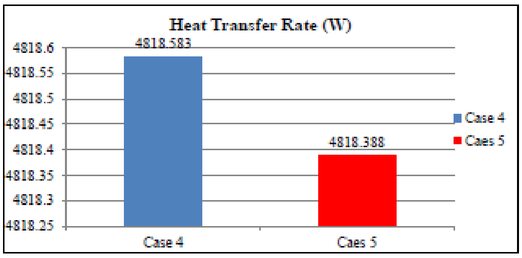


Figure 4.13 Graph representing Heat Transfer Rate

4.2.3 Temperature comparisons

The graph show that when length of the material is increased, the temperature decreased. The temperature decrease is same in both the cases.

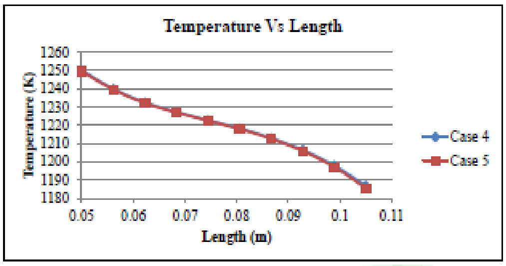


Figure 4.14 representing temperature comparison

4.3 Result for selecting Length

The solar thermochemical reactor consists of a chemical reactor for which five cases were taken earlier. Now two cases, Case 6 and 7 will be taken to select the length of the material. The cases with constant velocity and porosity are taken in which the length of porous material is different for both cases as shown in the table:

	Porosity	Velocity (m/s)	Length of poro Media (mm)
Case 6	0.9	0.002	70
Case 7	0.9	0.002	50

4.3.1 Temperature

To select the length of the material, temperature is one of the main parameter to be considered. Following are the results of temperature contour of two cases.

Case 6- The temperature contour for case 6 is shown in figure 4.14. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

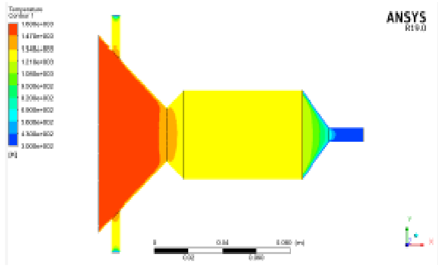


Figure 4.15 Temperature contour for Case 6

Case 7- The temperature contour for case 7 is shown in figure 4.15. Various colours in the figure shows different temperature range such as orange colour indicates the maximum temperature and blue colour shows the minimum temperature.

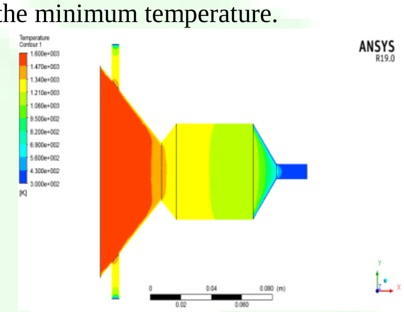


Figure 4.16 Temperature contour for Case 7

4.3.2 Heat transfer rate comparisons

To select the length, the heat transfer rate of Case 6 and 7 are shown in figure 4.12. It is clear from the figure that heat transfer of Case 6 is 4410.123 and heat transfer rate of Case 7 is4901.343. Heat transfer rate of Case 7 is higher than Case 6 from the results shown in the graph:

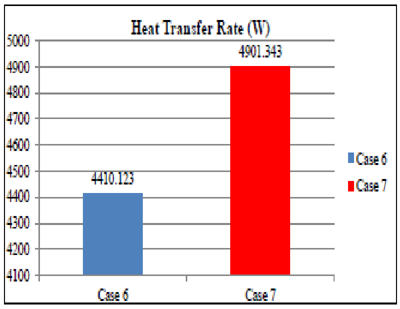
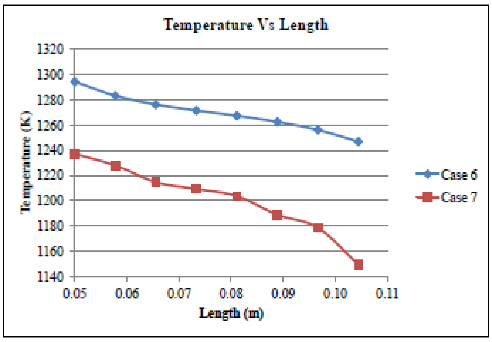


Figure 4.17 graph showing heat transfer rate

4.3.3 Temperature comparison

The graph show that when length of the material is increased, the temperature decreased. The temperature decrease is different in both the cases. The maximum temperature decrease is done by Case 7 in comparison to Case 6.



4.4 Overall Heat Transfer Comparisons

The heat transfer rate of all the cases is shown in figure 4.17 given below. It is the comparison of all the parameters such as porosity, velocity and length of the porous media with respect to heat transfer comparison. Case 1 shows the least heat transfer rate, its value is 3721.077W. While Case 7 shows the highest Heat Transfer Rate which is 4901.343W.

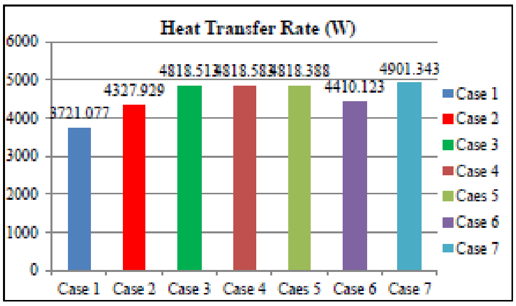


Figure 4.18 Graph showing Overall Heat Transfer Rate

4.5 Overall Temperature Comparisons

The temperature comparison of all the cases is shown in figure 4.18 given below. It is the comparison of all the parameters such as porosity, velocity and length of the porous media with respect to temperature. Case 3 shows the least value of temperature when the length increased which is required by the chemical reactor.

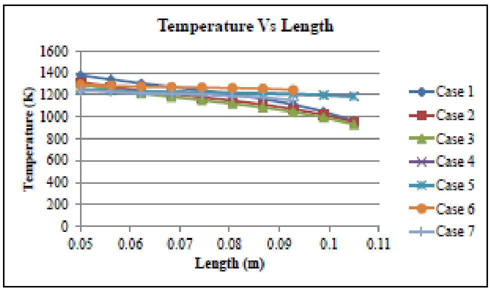


Figure 4.19 Graph showing overall Temperature Comparison

4.6 Average Temperature Comparisons

The graph given below shows the different temperatures. Here the average of each case is given, from which it can be concluded that Case 1 and Case 4 are showing the maximum average temperature which is also same i.e. 1327.64K. And case 6 shows the least value 1205.23K of average temperature.

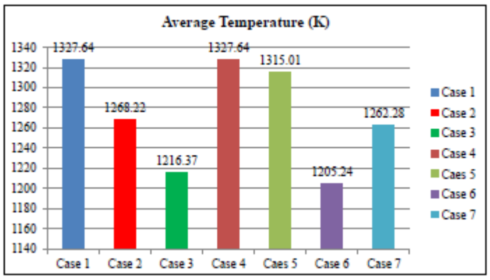


Figure 4.20 Average temperature comparision graph waveform

V.CONCLUSION AND FUTURE SCOPE

5.1 Conclusion

Thermodynamics shows us, in quite simplistic words, that at higher temperature we transmit solar energy to our process, more innovative we could be about what gets out like an end product. The same experiment was performed in the above case. To increase the length of porous media in a chemical reactor, seven cases were taken. The conclusions obtained from these cases are discussed below:

- From the table 4.1, case 1 to 3 is considered first. While increasing the porosity, the temperature decreases and Case 3 will be ideal for the chemical reactor as its temperature is lowest when the length is increased. The porosity of 0.9 shows the best results and other parameters remained constant.

From the table 4.2, case 4 and 5 are considered then. While varying the velocity in two cases, it can be concluded that less velocity gives better results.

From the table 4.4, case 6 and 7 are considered last. Here the length of the material varied and as a result it was observed that when length of the material is increased, the temperature decreased. The temperature decrease is different in both the cases. The maximum temperature decrease is observed in Case 7.

The overall comparison of heat transfer, temperature and average temperature are also calculated. Case 7 shows the highest Heat Transfer Rate i.e. 4901.343W, Case 3 shows the least value of temperature when the length increased i.e. 900K; Case 1 and Case 4 are showing the maximum average temperature i.e. 1327.64K.

5.2 Future scope

In the above experiment Silicon Carbide (SiC) is used for enhancing the working of the reactor. In future, other materials like zinc oxide can be used.

This experiment is performed on software NX11 and ANSYS; experimental analysis can be further performed. Parameters like heat transfer rate, pressure, velocity and temperature are observed in it. Efficiency, heat flux and many other parameters can be considered in further studies.

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