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Computational Fluid Dynamics Simulation of a Fluid Catalytic Cracking Regenerator

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Abstract: The aim of this study is to simulate a Fluid Catalytic Cracking (FCC) Regenerator, of a local refinery, using the Fluent Ansys.13 program and subsequently to investigate the impact of the change in geometry on the unit's performance. Three different geometrical models of FCC Regenerator were simulated. The Solid Works program was used to build up the computational domain and the commercial CFD code Ansys-Fluent 13 was used for meshing, models setup and solving. Three cases were examined: base case with a single air inlet, case one with five air inlets, and case two with five air inlets, however with the catalyst inlet axis raised by 100%. The results showed that the carbon solid mass content (used to represent the coke) decreases from 0.39 to 0.23 in the base case and to 0.12 in case one and to 0.19 in case two for the regenerated catalyst. Case one resulted in a decrease in carbon content by 100%, with a carbon monoxide emission of 10ppm (the base case at a value of 200ppm) which increased in case two to 100ppm. Furthermore the impact of air mass flow rate in case one (best case) was investigated starting with a mass flow rate of 29.5kg/s. The flow rate was further increased by 100% and 200% which resulted in a carbon mass content of 0.092 and 0.08 respectively.

Keywords: *Fluid catalytic cracking (FCC); Regenerator; Computational Fluid Dynamics (CFD).*

1. INTRODUCTION

Petroleum refineries are large, capital-intensive manufacturing facilities with extremely complex processing schemes. They convert crude oils and other input streams into dozens of refined (co-)products, including: liquefied petroleum gases (LPG), gasoline, jet fuel, kerosene, diesel fuel, petrochemicals feed stocks, lubricant oils and waxes, fuel oil and asphalt. Each refinery has a unique physical configuration, as well as unique operating characteristics and economics. A refinery's configuration and performance characteristics are determined primarily by the refinery's location, availability of funds for capital investment, available crude oils, product demand (from local and/or export markets), product quality requirements, environmental regulations and standards. There are several processes included in refineries distillation, cracking, upgrading, treating, separation, blending and utilities.

Cracking processes carry out chemical reactions that fracture large high-boiling hydrocarbon molecules (of low economic value) into smaller, lighter molecules suitable, after further processing, for blending to gasoline, jet fuel, diesel fuel, petrochemical feed stocks, and other high-value light products. Cracking units form the essential core of modern refining operations as they enable the refinery to achieve high yields of transportation fuels and other valuable light products, provide operating flexibility for maintaining light product output in the face of normal fluctuations in crude oil quality, and permit the economic use of heavy, sour crude oils.

The cracking processes of primary interest are fluid catalytic cracking (FCC), hydro-cracking, and coking. The most important process is the FCC which is the single most important refining process downstream of crude distillation, in terms of both industry-wide throughput capacity and its overall effect on refining economics and operations. The process operates at high temperature and low pressure and employs a catalyst to convert heavy gas oil from crude distillation (and other heavy streams as well) to light gases, petrochemical feed stocks, gasoline blend stock (FCC naphtha), and diesel fuel blend stock (light cycle oil). FCC offers high yields of gasoline and distillate material, high reliability and low operating costs, and operating flexibility to adapt to changes in crude oil quality and refined product requirements. In a large, transportation fuels oriented refinery, the FCC unit accounts for more than about 45% of all gasoline comes from FCC and ancillary units, such as the alkylation unit [1]. The FCC unit is composed of several pieces of equipment however in this research our prime focus is on regenerator.

Fluid flows are governed by partial differential equations which represent conservation laws for the mass, momentum, and energy. Computational Fluid Dynamics (CFD) software is widely used to solve those equations. CFD provides a qualitative and quantitative prediction of fluid flows by means of mathematical modelling, numerical methods and software tools. CFD enables chemical engineers to maximize the yield from their equipment and petroleum engineers to devise optimal oil recovery strategies. Important work has been published in the area of CFD simulation of FCC units. Muhamed Ahsan [2] has focused on the FCC riser and used commercial CFD software to predict the mass faction profiles of gas oil, gasoline, light gas and coke. Sheng Chen *et al*. [3] focused on the feedstock injection zone in a FCC riser. Their prediction showed good agreement with data and they captured secondary flow phenomena. Other work in the area of FCC riser is presented by [4]-[8]. However, CFD simulations of FCC regenerators have not been extensively studied which is the prime focus of this paper.

2. MATERIALS AND METHODS

2.1 Tools

A local FCC Regenerator is simulated using the Fluent Ansys.13 package. Furthermore, investigation of the impact of change in the geometry will be evaluated upon the unit's performance. An FCC was simulated without a cyclone or air distributer. At the regenerator, the oxygen in the air reacts with coke (assumed as solid carbon) separately with an inflow of matrix which is represented by pure solid silicon and aluminium. The profiles for the velocity, pressure, temperature were evaluated to access the performance of the regenerator. The simulation was performed based on a base case which is composed of a single air inlet (at the side of the regenerator). Subsequently, two other cases were evaluated; case one has multiple air inlets (at the bottom of the regenerator) and case two has multiple air inlets with the axis' of the catalyst inlet raised by 100%.

For the geometrical and computational domain, Solid Work is used as shown in **Fig. 1**. The dimensions shown in Table 1 are the actual dimensions of a local FCC regenerator.

Table 1. Dimensions of the FCC regenerator

Parameters	
Length of the regenerator (m)	26.19
Length of the top section (m)	12.69
Length of the middle section (m)	3.89
Length of the bottom section (m)	9.61
Diameter of the top section (m)	9.6
Diameter of the bottom section (m)	8
Diameter of air inlet (m)	1.95
Diameter of catalyst inlet (m)	1.1
Diameter of outlet(m)	3.51

Due to the symmetry of the regenerator, it has been divided symmetrically as in **Fig 2** (i.e. less meshing elements will be generated).

2.2 Methodology

The CFD simulation was preceded by four simple steps. First the geometry, secondly the mesh for the regenerator symmetry, thirdly the setup for the data and finally the solution setup before results are generated (see **Fig. 3**).

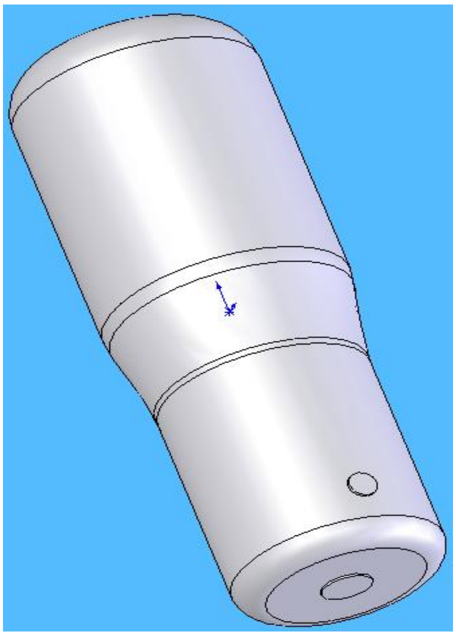

Fig.1. Complete geometry of the Regenerator

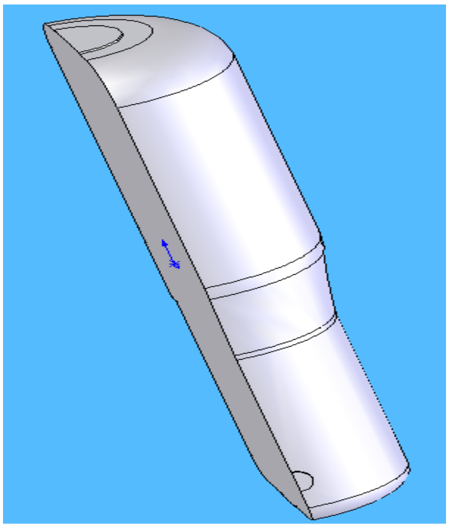

Fig. 2. Regenerator symmetry

Fig. 3. Block diagram for the simulation

2.2.1 Geometry

The three cases geometries are as follows:

a. Base case has single air inlet 1.95 m diameter (**Fig. 4**).
b. Case (1) has multiple air inlets 0.78 m diameter each (**Fig. 5**).
c. Case (2) has multiple air inlets 0.78 m diameter each with axis's of the catalyst inlet raised by 100% 2.5m (**Fig. 6**).

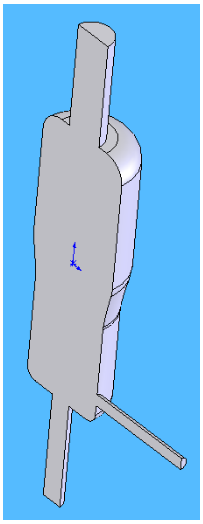

Fig. 4. Base case: single air inlet 1.95m, one catalyst inlet 1.1m, one outlet 3.51m

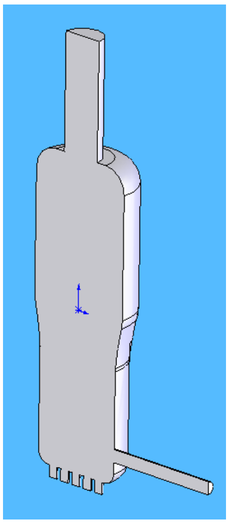

Fig. 5. Case (1): multiple air inlets (5 air inlets) ϕ0.78m, one catalyst inlet 1.1m, one outlet 3.51m

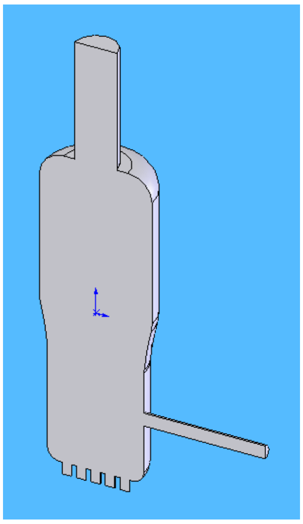

Fig. 6. Case (2): multiple air inlets (5 air inlets) ϕ0.78m, one catalyst inlet 1.1m its axis's raised by 100% 2.5m, outlet catalyst 3.51m

2.2.2 Mesh

After the geometry (IGES file) has been imported into the program, the mesh was generated and the boundaries have been labelled as shown in **Figs 7 to 9**.

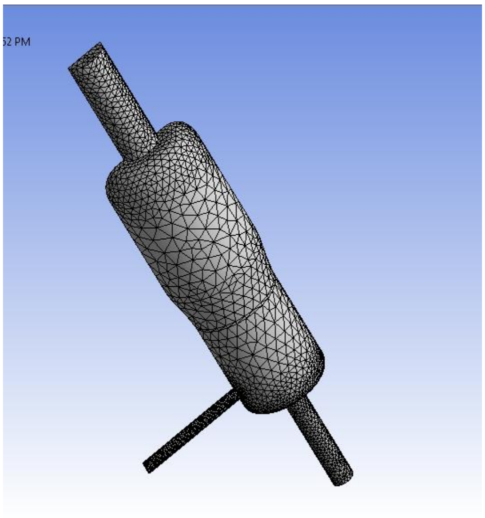

Fig. 7. Mesh of base case regenerator single air inlet

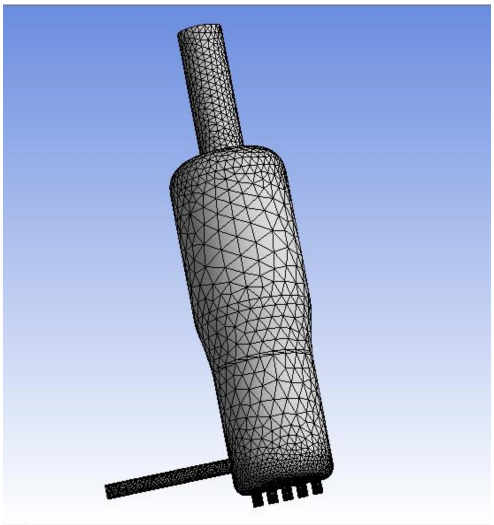

Fig. 8. Mesh for case (1) regenerator multiple air inlets

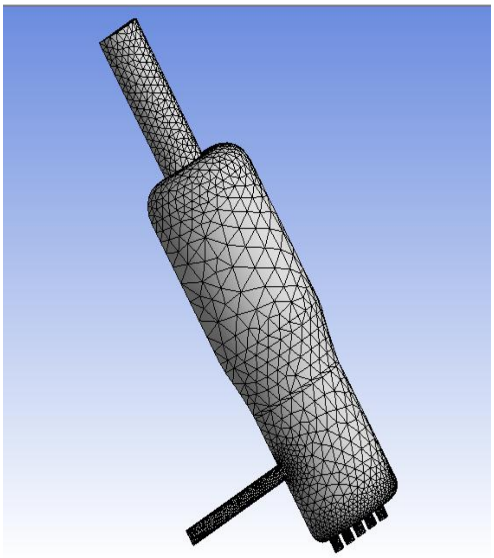

Fig. 9. Mesh for case (2) regenerator multiple air inlets with catalyst inlet axis's raised by 100%

2.2.3 Setup

The following sequence was followed during setup of the CFD software: general, models, materials, cell zone conditions and finally boundary conditions. When the setup appears choose from the problem setup choices general. Press scale to make sure the dimensions are all in meters, press check, the suitable solver type for our case is pressure-based, velocity formulation is absolute, the process operates in the steady state, check gravity because the flow runs from the bottom to the top in the Y direction which is opposite to the acceleration gravity which is equal to -9.81m/s^2.

At the models window, choose energy and then edit tick the box, choose viscous model press edit a window will appear. Choose the type of flow k-epsilon which is suitable for the flow because it have two types of flows one solid and the other one gas then press OK to close the window. Choose species from the model window press edit a window will appear.

Choose species transport model, choose volumetric for the reactions and choose finite-rate/eddy-dissipation for the turbulence-chemistry interaction this type is suitable for any packed or fluidized beds reactors which has catalyst and different kind of reactions can happen. Press OK to close the window another message will appear which tells that the mixture is available press OK also.

Choose material from the problem setup list a window will appear there are three types of materials liquid, solid and mixture. Press creates or edit in the materials window and a window will appear. Choose mixture for the material type which is the catalyst then Press fluent database a window will appear

Choose from the drop down list material type fluid; choose from the fluent fluid materials aluminum-solid (Al<s>) press COPY. Repeat this procedure to choose these materials carbon-dioxide (CO_2), carbon-monoxide (CO), carbon-solid (C<s>) and silicon-solid (Si<s>). The materials were chosen since there was no available option for the catalyst available and thus the nearest elemental and compound composition was chosen.

Return to the material window press edit in the mixture species a window will appear. The materials where in the available materials list when you click at each material and press add it will move to the selected species after that press OK to close this window.

Return to the material window press edit in the reactions and a window will appear. Fill in the data for your reactions there are three reactions:

Reaction (1): $C\langle s\rangle + 0.5O_2 \rightarrow CO$
Reaction (2): $CO + 0.5\,O_2 \rightarrow CO_2$
Reaction (3): $C\langle s\rangle + O_2 \rightarrow CO_2$

Press OK to close this window and then press change/create in the material window and then press CLOSE.

Choose cell zone condition from the problem setup list a window will appear. Choose the type fluid because it's a fluidized bed regenerator and press edit fill the data of the porous media internal resistance 0.042 and viscous resistance 0.016 for an average catalyst size of 150μm.

Select the boundary conditions from the problem setup list a window will appear. Select air inlets from the boundary conditions zone choose the type mass-flow-inlet then press EDIT a window will appear. Fill in the data for the air inlet as shown in the **Table 2**.

The air flows in the regenerator in the Y direction press 1, the turbulent intensity (10%) and the species mass fraction is 0.23 for O_2 press OK to close this window. Repeat this for all the air inlets in cases (1) and (2).

Select catalyst inlet from the zone choose the type mass flow inlet press edit the same window will appear fill the data as shown in the **Table 3** for all the cases.

The catalyst flows in the regenerator in the opposite X direction press -1, the turbulent intensity (10%) and the species mass fraction is 0.39 for C<s> press OK to close this window. Select the interior-solid from the zone type interior , select outlet from the zone type pressure-outlet press edit write 3.51 m in the Hydraulic diameter for all the cases the outlet is the same, select symmetry from the zone type symmetry and select wall solid from the zone type wall .

2.2.4 Solution

Select solution initialization from the problem setup a window will appear. Choose all-zones in the dropdown list in compute from and then press initialize this means the program is ready to calculate.

Select run calculation and a window will appear. Write the number of iterations that you expect the solution will be converged in and then press calculate. For each case, the solution converged differently. Iterations scaled residuals for each case are shown in **Figs 10 to 12.**

Table 2. The data for the regenerator air inlets the for the three cases

	Base Case	Case (1)&(2)
Mass flow rate (kg/s)	147.5	29.5
Pressure (kPa)	300	300
Hydraulic diameter (m)	1.95	0.78
Temperature (K)	473	473

Table 3. The data for the regenerator catalyst inlet for the three cases

Mass flow rate (kg/s)	288.89
Pressure (kPa)	240
Hydraulic diameter(m)	1.1
Temperature (K)	973

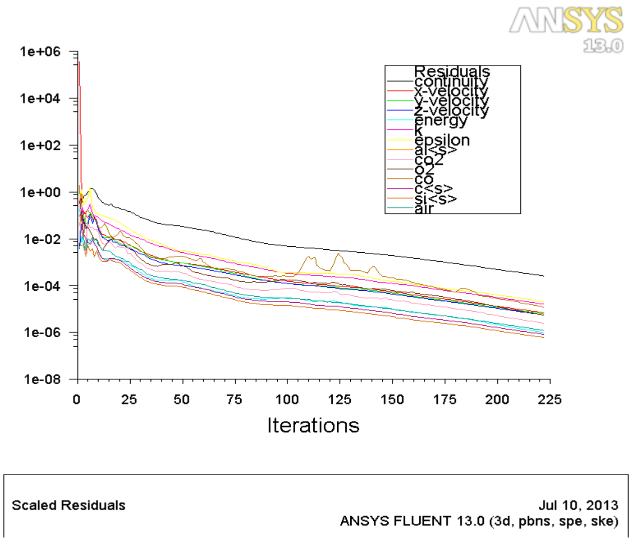

Fig.10. Iterations scaled residuals for base case(solution is converged in 222)

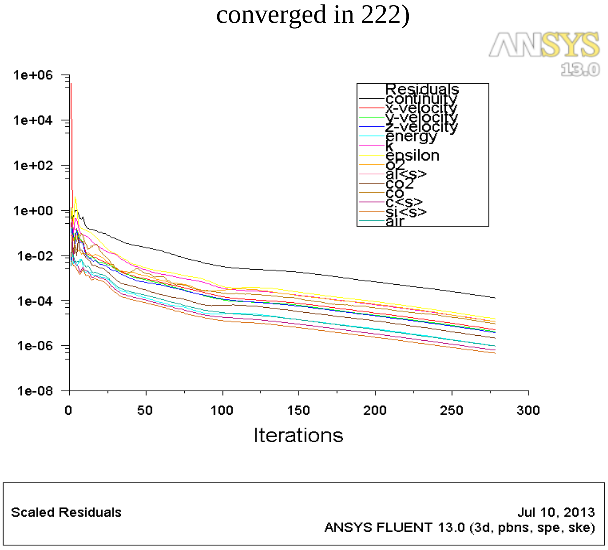

Fig.11. Iterations scaled residuals for case (1) (solution is converged in 278)

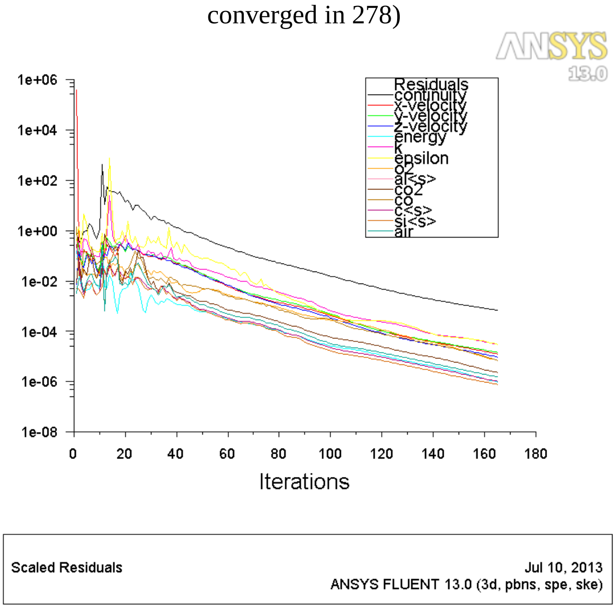

Fig.12. Iterations scaled residuals for case (2),(solution is converged in 165)

3. RESULTS AND DISCUSSION

3.1 Velocity Distribution

The velocity contours are shown in **Fig. 13** for the three cases. It is clear that the velocity in the catalyst inlet is high and in the air inlet is low in all cases. In the outlet the velocity increases in case (1) and (2) relative to the base case due to the multiple air inlets.

3.2 Temperature Distribution

Temperature contours are shown in **Fig. 14** for the three cases. The temperature in case (1) is the highest than in the base case and case (3). This is because in case (2) the reaction between the carbon and air (oxygen) is more and it's a complete reaction. In the base case, the distribution of the air is not enough compared to cases (1) and (2).

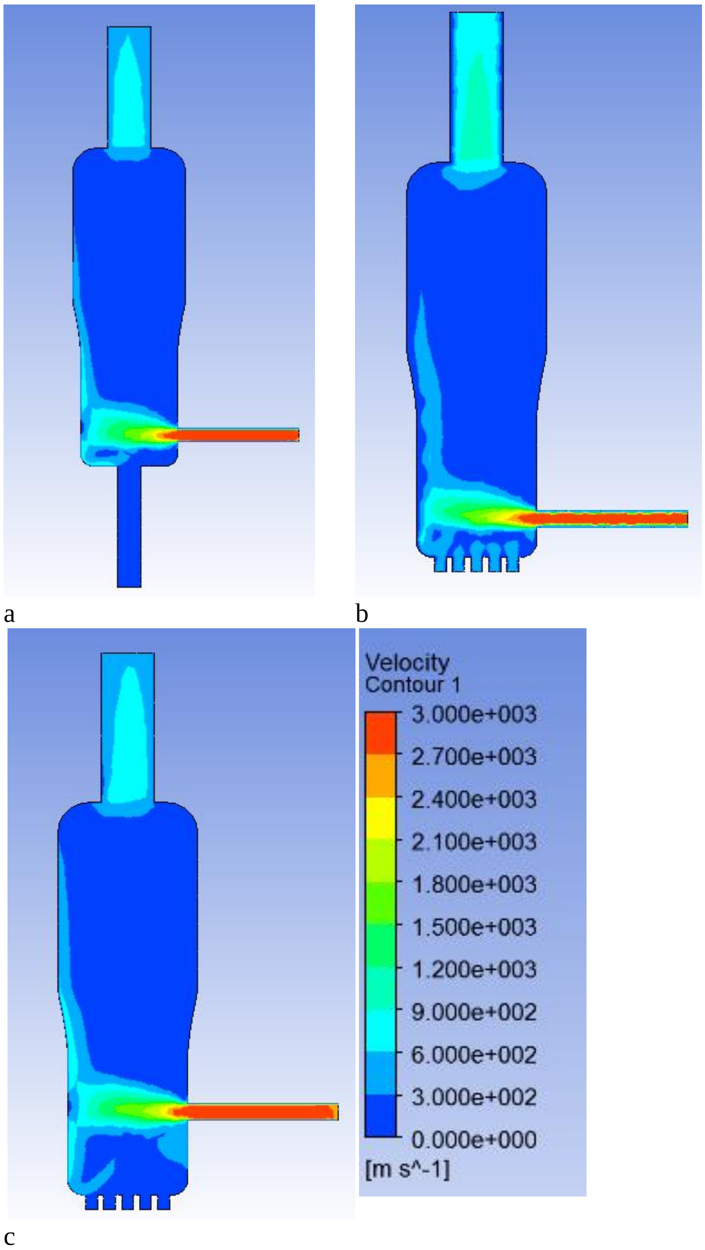

Fig. 13. Velocity contour for a) the base case, b) case one and c) case two

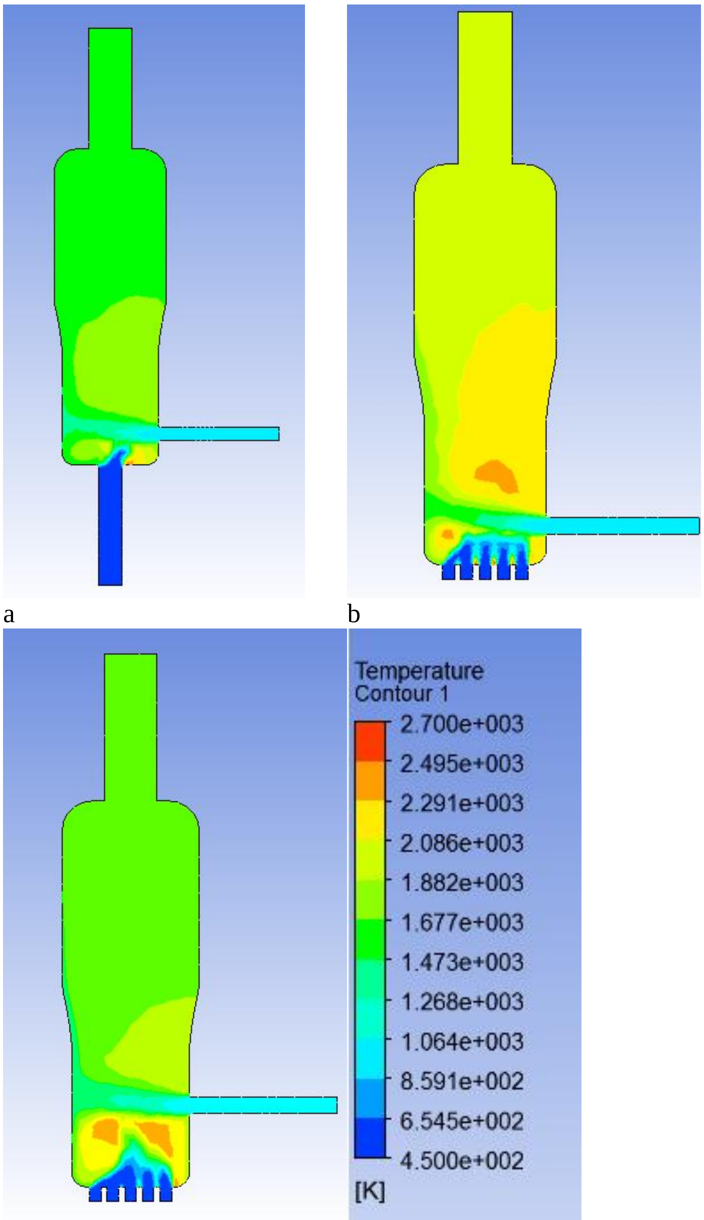

Fig. 14. Temperature contour for a) the base case, b) case one and c) case two

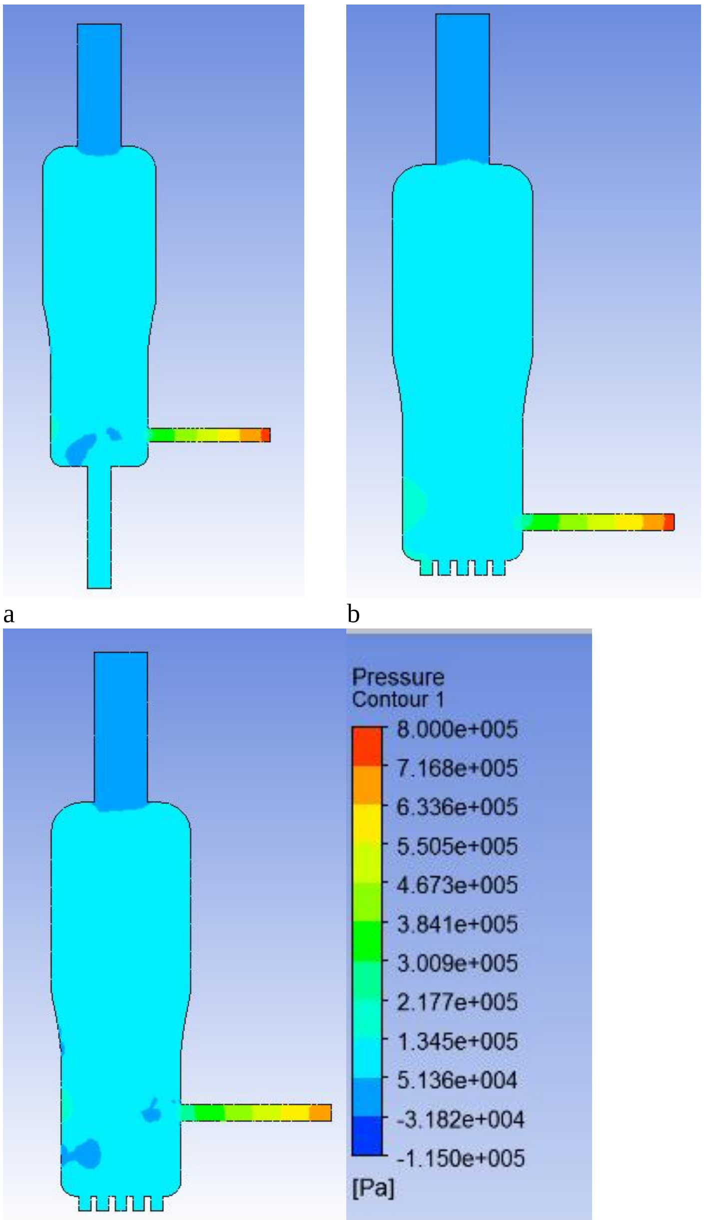

Fig. 15. Pressure contour for a) the base case, b) case one and c) case two

3.3 Pressure Distribution

The pressure contours are shown in Figure 15 for the three cases. The pressure profile is higher in the catalyst inlet because the flow rate is high and the diameter is small, inside the regenerator the pressure decreases with the larger volume and correctional area.

3.4 Carbon Mass Fraction

The carbon solid mass fraction contours is shown in **Fig. 16**. The contours show the carbon mass fraction decreases from 0.39 to 0.23 in the base case, to 0.12 in case (1) and to 0.19 in case (2). The increase in case (2) is due to the smaller residence time.

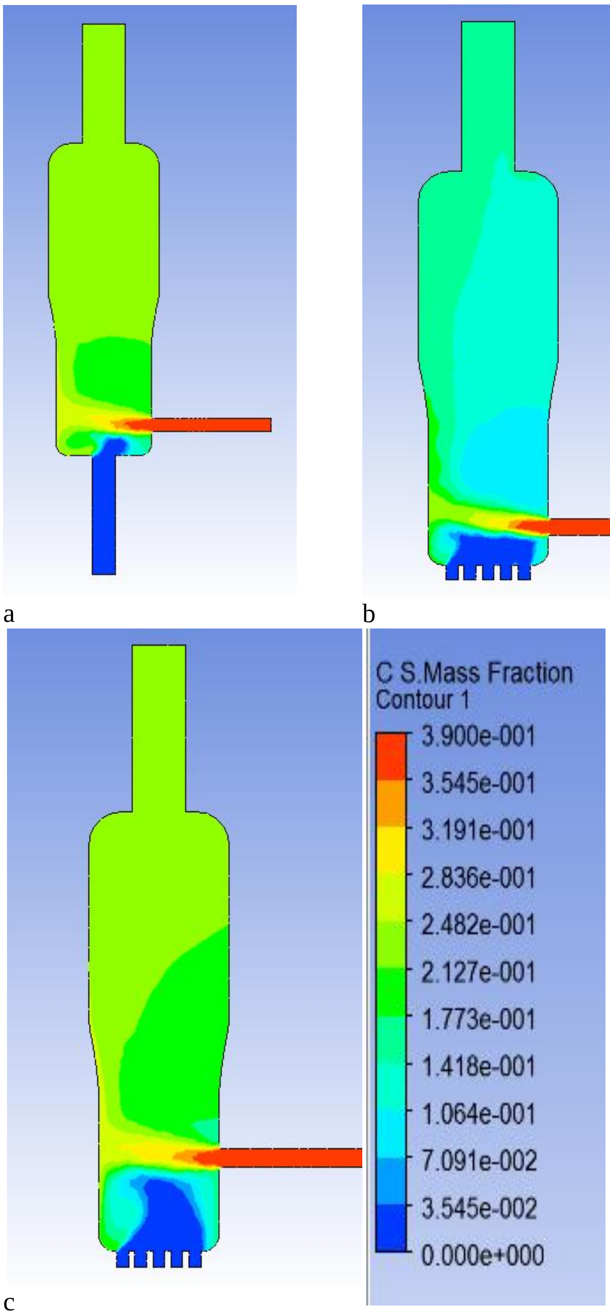

Fig. 16. Carbon solid mass fraction contour for a) the base case, b) case one and c) case two

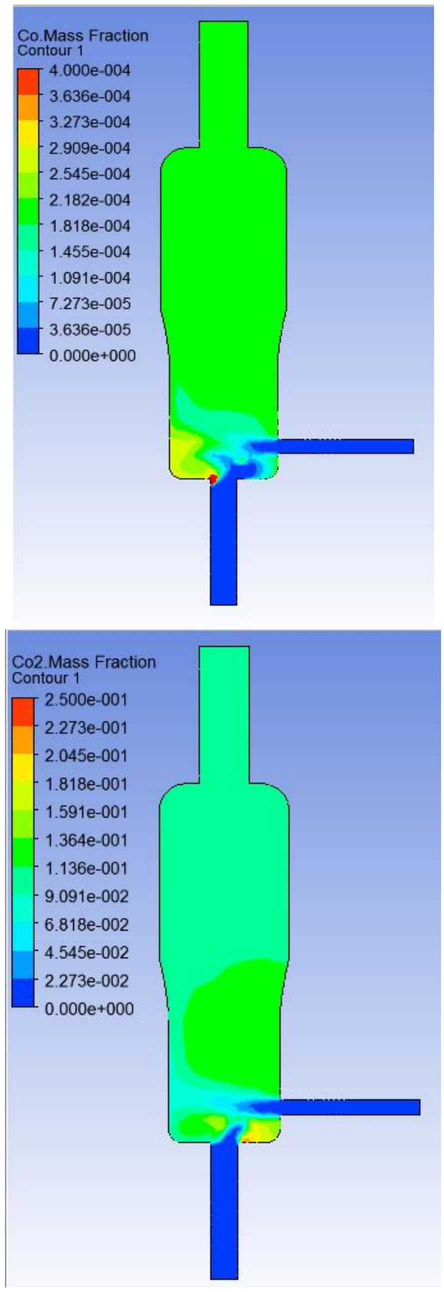

Fig. 17a. CO and CO_2 mass fraction contour for base case regenerator single air inlet

3.5 CO and CO_2 Mass Fraction

The CO and CO_2 mass fraction contours are shown in **Fig. 17 a, b and c**. In **Fig. 17a**, the air distribution is not enough to turn the entire CO into CO_2.In Figure 17b, air distribution is enough to convert most of the CO to CO_2 and also the reaction has more time to turn most of the CO to CO_2. In Fig. 17c, more CO is produced due to the shorter residence time.

3.6 Aluminium and Silicon Mass Fraction

The aluminium and silicon solid contours are shown in **Fig. 18 a, b and c.** The contours show the distribution of the aluminium solid and silicon solid. It is clear that it is high in the inlet prior to its distribution in the regenerator and subsequent exit. The properties of the outlet are shown in Table 4.

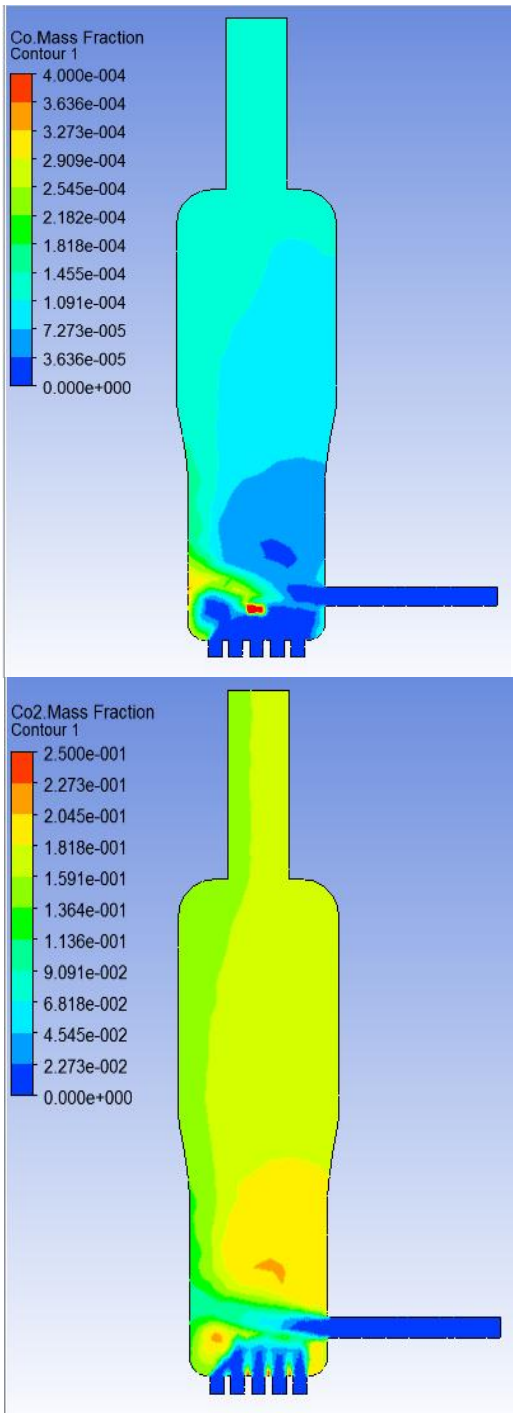

Fig. 17b. CO and CO_2 mass fraction contour for case (1) regenerator multiple air inlets

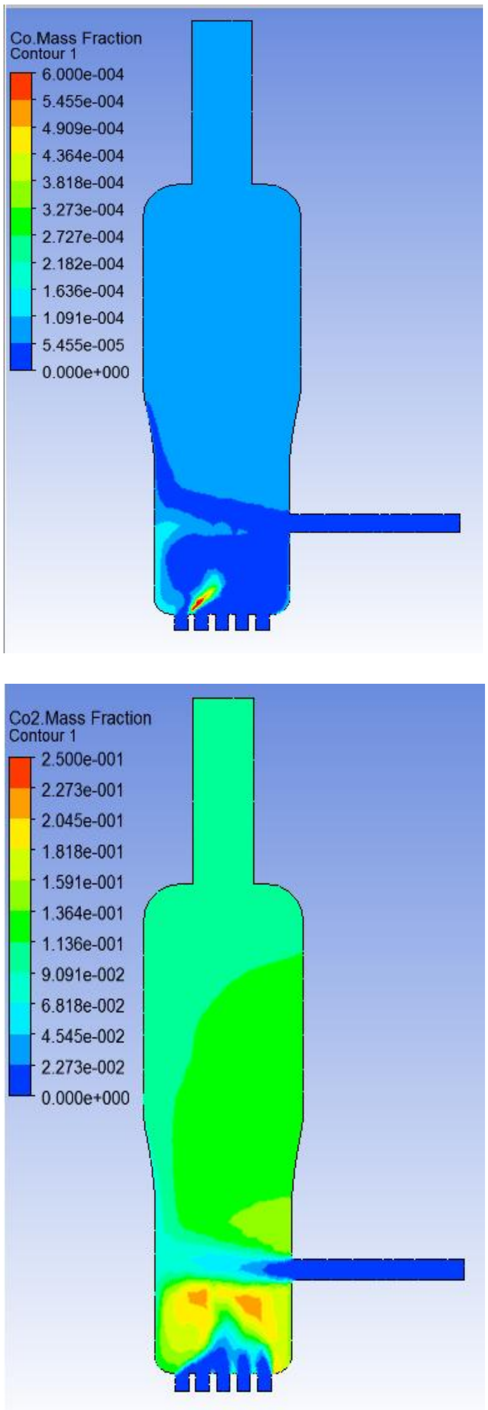

Fig. 17c. CO and CO_2 mass fraction contour for case (2) regenerator multiple air inlets with catalyst inlet axis's raised by 100%

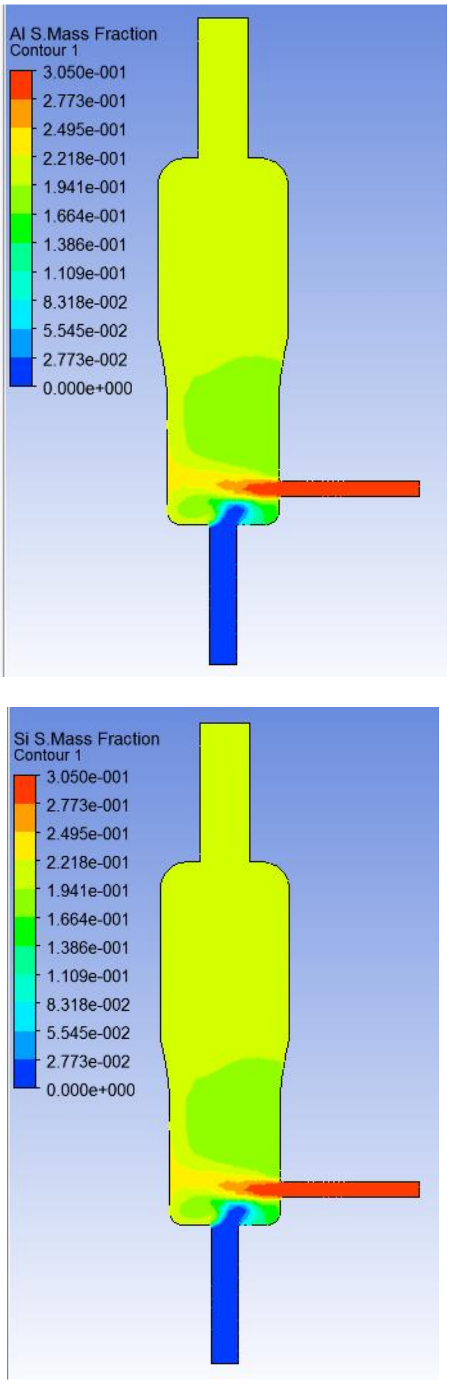

Fig. 18a. Al solid and Si solid mass fraction contour for base case regenerator single air inlet

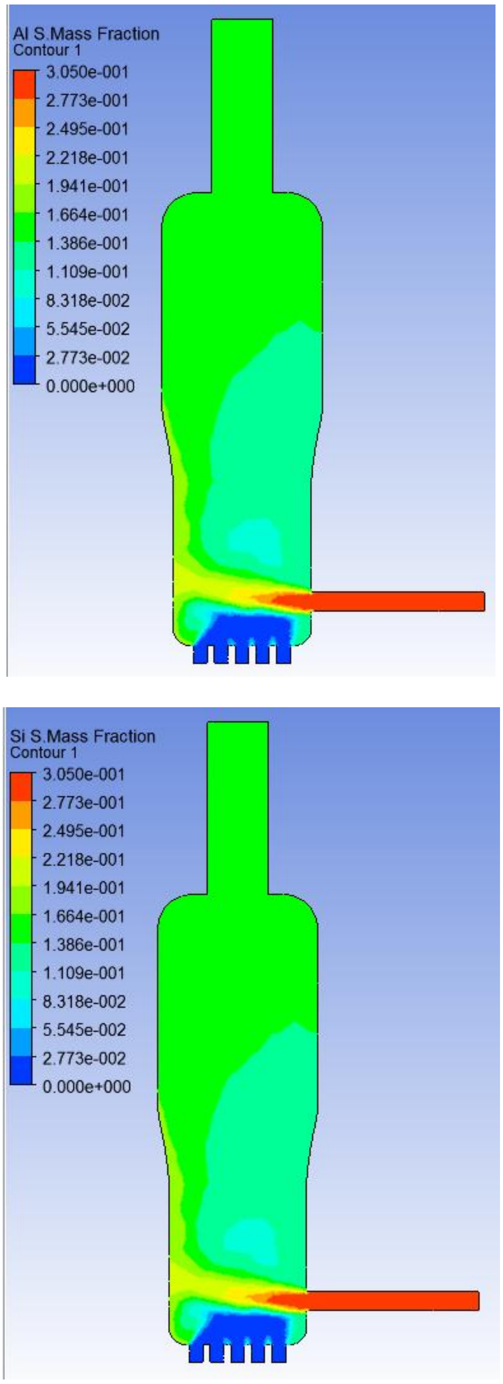

Fig. 18b. Al solid and Si solid mass fraction contour for case (1) regenerator multiple air inlets

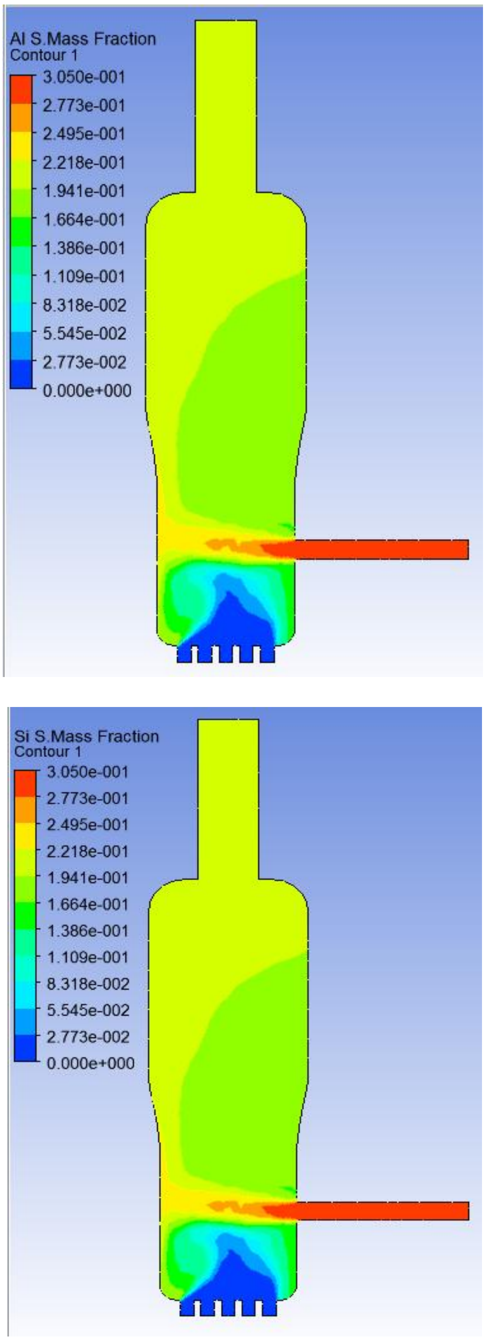

Fig. 18c. Al solid and Si solid mass fraction contour for case (2) regenerator multiple air inlets with catalyst inlet raised by 100%

From all of these results it can see that case (2) is the nearest to reality that's why it tried to increase the flow rate of the air to see if more carbon can be removed when we increase the air flow rate from 29.5kg/s to 59kg/s and then to 88.5kg/s the carbon mass fraction decreased from 0.12 to 0.093 and then to 0.082 consequently and this is the same results as the Khartoum refinery. It realized that the more it increase the air flow rate the carbon content decrease but also the temperature and pressure rises we have to pay attention to the temperature and pressure because it affects the equipment and may cause rupture to the equipment that's why it have to choose the optimum conditions for the regenerator to operate in.

Table 4. The properties of the regenerator outlet in each case

Properties	Base Case	Case (1)	Case (2)
Velocity (m/s)	295.7	575.2	576.5
Temperature (K)	1479	1782	1583
Pressure (Pa)	557.149	428.5	399.29
Carbon solid mass fraction	0.23	0.12	0.19
Carbon monoxide mass fraction	0.0002	0.00001	0.0001
Carbon dioxide mass fraction	0.13	0.24	0.15
Aluminium solid mass fraction	0.21	0.21	0.21
Silicon solid mass fraction	0.21	0.21	0.21

4. CONCLUSIONS

The CFD simulation for the fluid catalytic cracking regenerator has been done for three types of configurations: the base case has single air inlet case one has multiple air inlets and case two has multiple air inlets with the catalyst inlet axis's raised by 100% using the data obtained from the Khartoum Refinery Company. The program used for the simulation is a CFD program called Fluent Ansys.13. The result shows that the carbon solid (used instead of the coke) decreases from 0.39 to 0.23 in the base case and to 0.12 in case one and to 0.19 in case two.

Case one resulted in a decrease in carbon content by 100%, with a carbon monoxide emission of 10ppm whereas it increased in case two to 100ppm and the base case to 200ppm which makes case one the best case. Furthermore the impact of air mass flow rate on the best case (case one) was investigated starting with a mass flow rate of 29.5kg/s, the flow rate was increased by 100% and 200% which resulted in a carbon content of 0.092 and 0.08 respectively. Which is what we want but the temperature increases and this may cause damage to the equipment that is why we need to choose the optimal operating conditions and the optimal geometry that give us the best results which is what the CFD offers.

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