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Research Article

CFD Analysis for Production of Carbon Nanotubes

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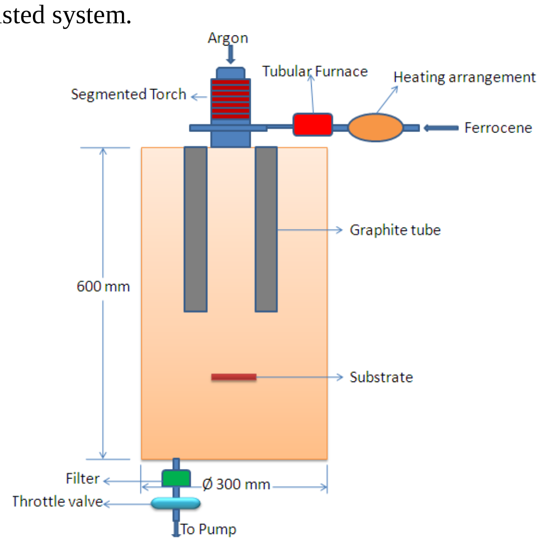
Abstract

Carbon nanotubes are cylindrical molecules with a diameter of as little as 1 nanometer and length up to many micrometers. It consist of only carbon atoms. By using CFD tools, GAMBIT and FLUENT heat and fluid flow analysis of argon ferrocene mixture has been carried out. At high temperature ferrocene is splits into Carbon, Ferrous and Hydrogen. So to reduce the analysis time, instead of entering ferrocene in the form of powder, the species of carbon, ferrous and hydrogen are entered. Analysis is done and data is generated for the reactor with graphite tube & without graphite tube. Velocity of all the species in without graphite tube reactor is high & temperature in with graphite tube reactor is high.

Keywords: *Carbon Nanotubes, Ferrocene, Fluent, Gambit, Multi species.*

1. Introduction

This is plasma chemical reactor system for synthesis of novel carbon nanostructures in a segmented plasma torch assisted system.



The system is divided in to the following components:

1. The segmented plasma torch
2. The double walled stainless steel vacuum chamber
3. The mating flange and nozzle- injection section
4. The pumping system
5. The water cooling system
6. The Graphite tube.
7. The substrate Holder and substrate
8. The Tubular Furnace

A plasma beam is expanded supersonically and passing into a low-pressure chamber through a converging nozzle. A segmented plasma torch with nine rings is used for producing a high temperature. The torch is connected to the vacuum chamber with the help of converging nozzle section. The double walled water-cooled vacuum chamber will be pumped down with a rotary pump, roots pump and throttle valve combination.

Hydro-carbon gasses will be injected directly into the plasma as precursor for carbon Nanotubes. In tubular furnace ferrocene is evaporated and then injected into the reactor as swept by hot argon gases coming from plasma torch. Just after the nozzle, inside the chamber a graphite tube will be placed concentric with the chamber. carbon nanostructures are expected to be deposited on a substrate which is placed beyond the graphite tube. The substrate is designed to be heated up to 1000 K with an electrical heater. Also, it has to be arranged to bias the substrate up to ± 1 KV adjustable continuously.

2. Ferrocene

Fig. 2: Ferrocene powder

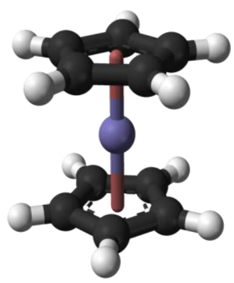


Fig.3: Ferrocene compound

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Ferrocene with the formula Fe(C5H5)2 is an organometallic compound. The properties of ferrocene are shown in table 1, and image of the ferrocene powder and ferrocene chemical structure is as shown in figure 2 and figure 3 respectively.

Table 1 Properties of Ferrocene

Properties	
Molecular formula	$FeC_{10}H_{10}$
Molar mass	186.04 g/mol
Appearance	Light orange powder
Density	1.107 g/cm^3 (0^0 C), 1.490 g/cm^3 (20^0 C)
Melting point	174 ^{0}C
Boiling point	249 ^{0}C
Solubility in water	Insoluble in water, soluble in most organic solvents

3. Modeling

For modelling and meshing GAMBIT is used which is the default modeling & meshing tool for fluent. Because of its higher compatibility with fluent it's always better to model and mesh in Gambit for CFD simulation using Fluent. Though model & mesh generated using other CAD packages can be imported through gambit but they have to be checked for distortion & geometry clean up is also required.

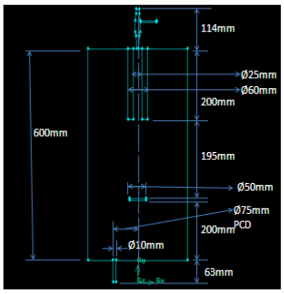


Fig.4: Dimension of model

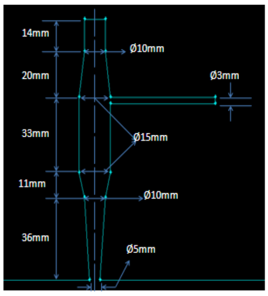


Fig.5: Dimension of Nozzle

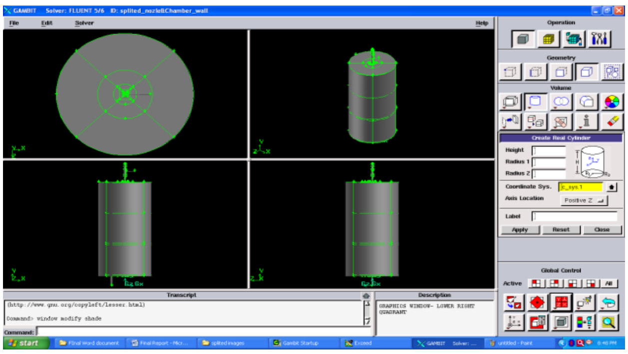


Fig.6: 3D solid model

The dimensions of model are given in figure 4 and figure 5. By using these dimensions the geometry is created. By using standard command like create real cylinder the different cylinders are created, then by using different Boolean operations like unite, subtract and intersect the geometry is created. The complete view of the modeled geometry is as shown in the figure 6.

4. Meshing the model

Meshing, also known as grid generation, is discretization of model into smaller regions called as grids or elements. Generated grid has a significant effect on rate of convergence (or even lack of convergence), accuracy and computation time. So it is important to select appropriate elements type, meshing scheme and grid density.

The main task in meshing is to create a complete hexahedral structural grid. It is very difficult to make complete hexahedral mesh without broking the model into number of volume. Because the model is having the reactor, graphite tube, substrate, nozzle, two different inlets and one offset outlet. Due to these different components the geometry is difficult to mesh with structured meshing scheme. To make it a complete structural grid the geometry has divided into number of volumes. The sub parts are shown in the below figure7.

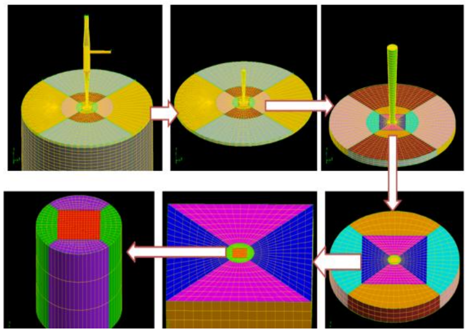


Fig.7: Exploded view of upper part of the Chamber

Table 2 Mesh examine table

Equisize skewness	No of elements	Percentage
0 to 0.1	5,31,033	70.30%
0.1 to 0.2	98,524	12.70%
0.2 to 0.3	52,253	6.73%
0.3 to 0.4	57,538	7.42%
0.4 to 0.5	21,779	2.81%
0.5 to 0.6	5,928	0.79%
0.6 to 0.7	1,850	0.04%

5. Specifying zone and Boundary types

Zone-type specifications define the physical and operational characteristics of the model at its boundaries and within specific regions of its domain. There are two classes of zone-type specifications:

- Boundary types
- Continuum types

Boundary Conditions are specifications of properties or conditions on the surfaces of Domains and are required to fully define the flow simulation. The type of Boundary Condition that can be set depends upon what sort of boundary or interface the Boundary Condition is placed on.

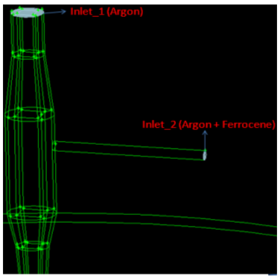
Boundary type specifications of the model

The inlet and outlet boundary conditions as shown in table 3.2 and figure 3.12.

Table 3 Boundary conditions

Boundary	Colour code in Gambit	Type
Inlet_1 Argon	Gray	Mass Flow inlet
Inlet_2 (Argon + Ferrocene)	Gray	Mass Flow inlet
Substrate	White	Wall
Outlet Type	Red	Pressure Outlet

Following figure 8 shows the boundary conditions for the model.



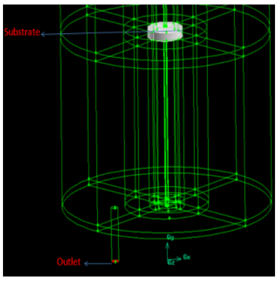


Fig.8 Boundary conditions

Data is generated by considering different case and different boundary condition as shown below in table 4, table 5 and table 6. In all the cases the Operating pressure remain same and is equal to 1 atmospheric pressure = 101325 Pa

For inlet_1 (Argon) – Mass flow inlet

Table 4 Inlet Boundary condition

Inlet mass flow rate (kg/s)	0.000744 (25 Lpm)
Inlet Temperature (K)	3000
Turbulence Intensity (%)	10
Turbulent Length Scale	10

For inlet_2 (Argon + Ferrocene) – Mass flow inlet

Table 5 Inlet Boundary condition

Inlet mass flow rate (LPM)	0.0001488 (5 Lpm)
Inlet Temperature (K)	400
Turbulence Intensity (%)	3
Turbulent Length Scale	10

For outlet- Pressure outlet

Table 6 Outlet Boundary condition

Gauge pressure (Pa)	-50662.5
Back Flow Turbulent Intensity (%)	10
Back Flow Hydraulic Diameter (m)	10
Outlet temperature (K)	300

Boundary-type specifications define the characteristics of the model at its external or internal boundaries. Continuum-type specifications define the characteristics of the model within specified regions of its domain.

6. Continuum type

Continuum-type specifications define the physical characteristics of the model within specified regions of its domain. For example, if we assign a FLUID continuum-type specification to a volume entity, the model is defined such that equations of momentum, continuity, and species transport apply at mesh nodes or cells that exist within the volume. Conversely, if we assign a SOLID continuum-type specification to a volume entity, only the energy and species transport equations (without convection) apply at the mesh nodes or cells that exist within the volume.
figure 9 shows the continuum of geometry.

- Gas -Fluid
- Graphite tube - Solid
- Substrate - Solid

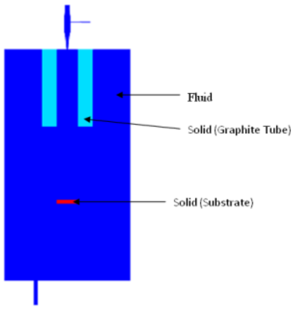


Fig.9: Cross section of model Showing various Domain

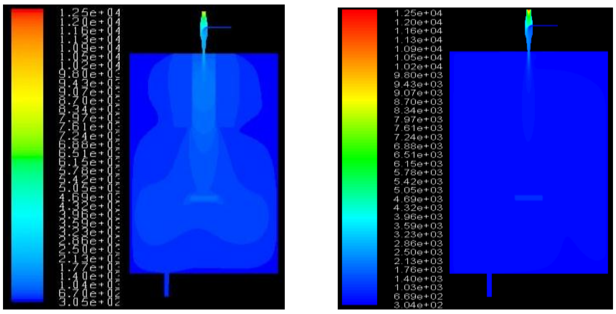
7. Results and discussion

The requirement is to get the temperature of near about 2000K at inlet of the chamber. The input power from the plasma torch is 10 to 15 KW. Therefore we have to set the temperature of inlet_1 such that we get the input power of 10 to 15 KW.

By considering the volume flow rate for inlet_1 as 25 LPM (liter per minute) and for inlet_2 as 5 LPM the result have generated for following two cases

1) With graphite tube
2) Without graphite tube

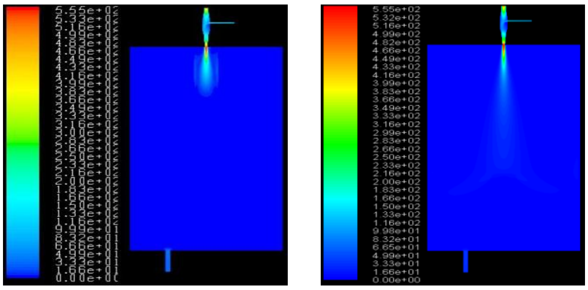
As shown in figure 10 (a) & (b) the contours for the cases of with graphite tube & without graphite tube. In case of with graphite tube model, the graphite tube is heated and heating up the surrounding area.



(a) With graphite tube (b) without graphite tube

Fig.10: Temperature contour

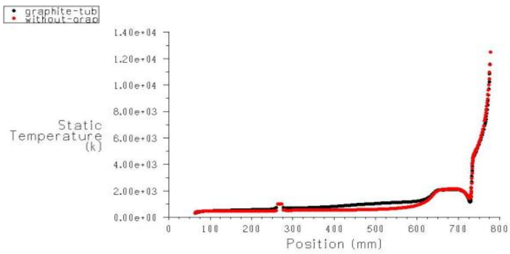
The highest velocity at inlet of the chamber for both the cases is same and is equal to 555 m/s. The effect of the highest velocity in case of without graphite tube is longer than that of the second case of with graphite tube.



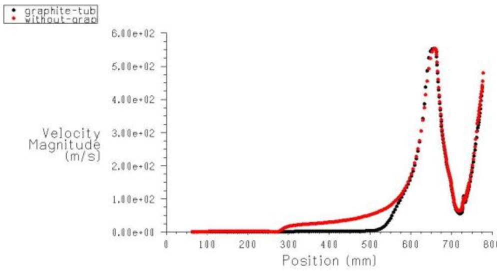
a) With graphite tube (b) without graphite tube

Fig. 11: Velocity contour

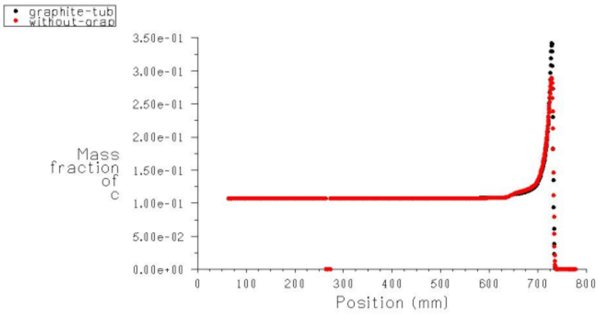
Following all the graphs for temperature, velocity, mass fraction of argon and mass fraction of carbon are plotted on the axis of the chamber and nozzle. These all graphs are plotted for both the cases of with graphite tube and without graphite tube.



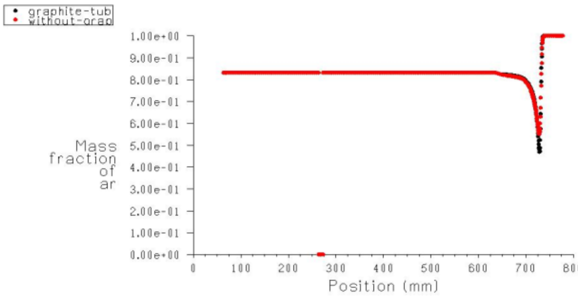
Graph 1: Temperature plot



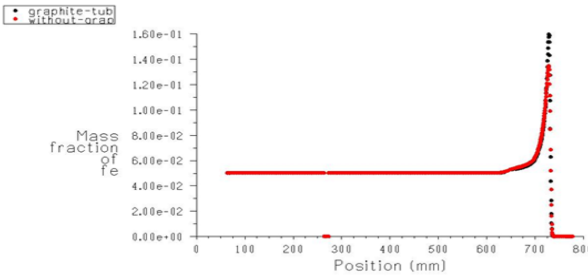
Graph 2: Velocity plot



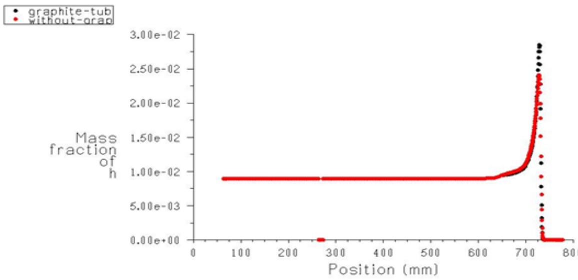
Graph 3: Mass fraction of Carbon



Graph 4: Mass fraction of Argon



Graph 5: Mass fraction of Fe



Graph 6: Mass fraction of hydrogen

Table 7 Comparison of maximum velocities at different planes

Sr. No.	Position from top in mm	Maximum Velocity in m/s	
		With graphite	Without
1	0	495	495
2	113	550	550
3	164	255	255
4	264	7.5	65
5	364	2.5	32.5
6	464	1.5	21
7	664	0.35	2

Table 8 Comparison of maximum temperatures at different planes

Sr. No.	Position from top in mm	Maximum Temperature in K	
		With graphite tube	Without graphite tube
1	0	12500	12500
2	113	2160	2160
3	164	1350	1080
4	264	1080	650
5	364	850	550
6	464	750	550
7	664	650	490

Conclusion

Table.7 shows that the velocity is same up to 164 mm from top for both the cases of with graphite tube and without graphite tube. Then after 164 mm the velocity in case of with graphite tube reduces very fast as compare to the case of without graphite tube.

Table.8 shows that the temperature is higher in the case of with graphite tube than the case of without graphite tube at all positions. As the graphite tube heated and carries heat in it due to this heat carried by the graphite tube the surrounding area always have high temperature.

Mass fraction of ferrous, hydrogen, carbon, and argon are not much affected by graphite tube.

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