"Heat And Fluid Flow Analysis Of Argon- Ferrocene Mixture In A High Temperature Reactor Used For Producing Carbon Nanotubes"

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ABSTRACT
3D-Single Phase multi species heat and fluid flow analysis of argon ferrocene mixture has been carried out by using CFD tools, GAMBIT for modeling & meshing and FLUENT for analysis. Basically this problem is multi phase problem as at high temperature ferrocene is splits into Carbon, Ferrous and Hydrogen, so chemical reaction of thermal decomposition of ferrocene is incorporated with FLUENT. Different cases, based on plasma torch power and mass inflow of ferrocene are considered and data is generated for the same. Data thus generated is analysed for calculation of cooling rate of the gases inside chamber and estimation of mass fraction of fe is carried out.

Keywords: 3D-multi species, Carbon Nanotubes, CFD, Ferrocene, Gambit, Fluent,

I. INTRODUCTION

In this system, a plasma beam is expanded supersonically while passing through a converging nozzle into a low-pressure chamber. A segmented plasma torch with total nine rings will be used for producing a high power, constricted and stable plasma torch beam. The torch will be connected to the vacuum chamber through an injection-port/ converging nozzle section. The water-cooled double walled vacuum chamber will be pumped down with a roots pump, rotary pump and throttle valve combination.

Hydro-carbon gasses will be injected directly into the plasma as precursor for carbon Nanotubes. Ferrocene will be evaporated in a tubular furnace and then injected into the reactor as swept by hot argon gases.

Inside the chamber, just after the nozzle, a graphite tube will be placed concentric with the chamber.

A substrate will be placed beyond the graphite tube on which the carbon nanostructures are expected to be deposited. This will be 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.

Ferrocene is in the form of powder and cannot flow, therefore the Argon gas is used with ferrocene to flow it.

The data is generated by considering the mass flow rate of 0.000744 kg/s (25 Lpm) for argon and 0.00001488 kg/s (5 Lpm) for ferrocene + argon is considered for further analysis. UDFs for temperature profile at inlet of argon and different properties of argon at different temperatures are attached.

II. SPECIFICATION OF THE SYSTEM COMPONENTS

The system may be divided in to the following subsystems:

1. The double walled stainless steel vacuum chamber
2. The segmented plasma torch
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
8. The Tubular Furnace

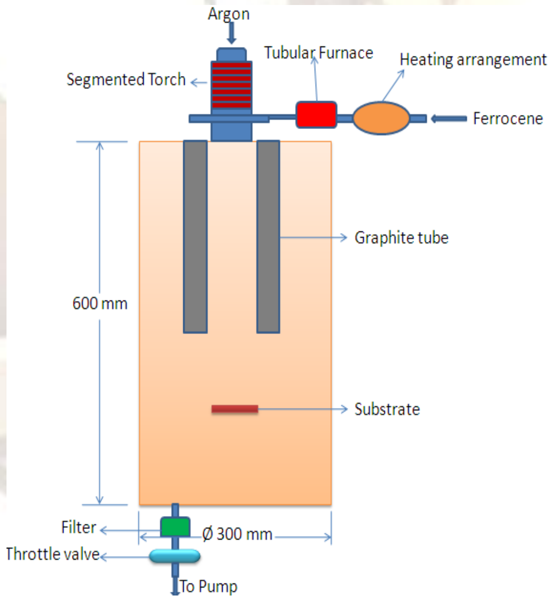


Fig.1: System Components

1. Double walled stainless-steel vacuum chamber

It is a cylindrical vertical chamber fabricated out of non-magnetic stainless steel 300 mm in diameter and 600 mm long. It is a double walled water cooled enclosure with individual wall thickness to be chosen from the lowest achievable pressure. Wall separation should be decided from consideration of 10 Lpm water flow between them.

The bottom of the chamber has a central hole for connection of a substrate holder rod. There is another port on the bottom of chamber for connection of the vacuum pumping line. The pumping line also has to be water cooled. Pulleys and suitable stands are to be provided for easy handling/manipulation of the torch and lifting upper flange of the chamber. All the inside surface shall be cleaned as per the required for high vacuum application and all sharp edges shall be ground smooth. Internal attachments which may lead to entrapment of gases should be avoided. All nuts and bolts used should be made of Stainless steel only.

2. Segmented plasma Torch

It is a cascaded plasma torch, with total nine numbers of ring segments, including the cathode, the anode, the auxiliary anode and six numbers of floating rings.

3. Mating flanges and nozzle injection section

The torch anode is screw joint (3 holes, M6 × 10 mm deep) to a mating flange (145 mm diameter, 20 mm thick) through Teflon gaskets (45 mm diameter), which is then coupled to the copper holder section housing the injection section and the conversion nozzle, the mating flange has Viton O-ring (98/109 mm diameter) at its lower face.

4. Vacuum system

This is for producing minimum base pressure of less than 10^{-3} mbar in the experimental system, with the torch, open tubular furnace, gas-line etc. connected and the graphite tube magnets placed inside the chamber. It is also expected to handle the degassing from the material kept inside.

5. Water circulating system

It is a closed loop water circulating system comprising water headers, water lines, valves flow switches, rotameters and water temperature measurement system.

Water flow at a rate of more than 10 Lpm should be demonstrated through each of the individual water lines connected to the respective module.

6. Graphite tube

Inside the chamber, graphite tube is positioned concentrically just below the nozzle.

A graphite tube (99.99% pure glassy graphite) of length 200 mm (inside diameter 25 mm and outside diameter 60 mm) will be positioned along the axis of the chamber.

7. Substrate Holder

The substrate at 1000 K temperature is placed on a hollow substrate holder rod at 200 mm from bottom of the chamber, through which water flows so that the lower part of the rod does not get heated up. The substrate is a graphite disk (50 mm diameter 5 mm thick) and it shall be arranged to fix it firmly to the holder, so that the incoming plasma/gas streams do not displace it.

8. Tubular Furnace

This is for producing the injecting vapor of ferocene into the injection section of the reactor. It is the stainless steel tube (250 mm length & 50 mm diameter), with end flanges with gaskets. The material to be evaporated is placed on a crucible inside the cylinder.

Before entering the furnace, the gas is first heated up by simple resistive heating. The fabricator is required to prepare the final engineering design.

III. MODELING THE GEOMETRY

For modeling 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.

1. Creating the geometry

The dimensions of initial model which were given are shown in fig.2 and fig.3. By using these dimensions the geometry is created.

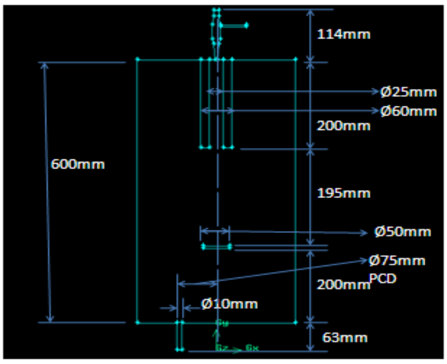


Fig.2: Dimension of model

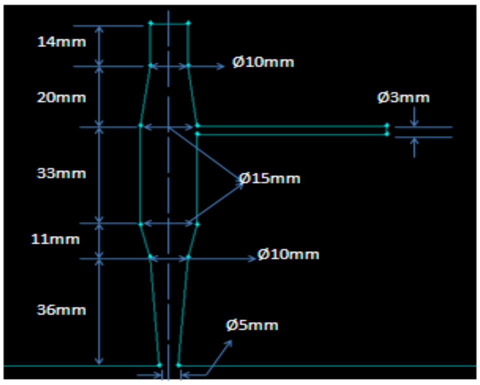


Fig.3: Dimension of Nozzle

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 and other commands are used to compete the modeling. The complete view of the modeled geometry is as shown in the fig.4.

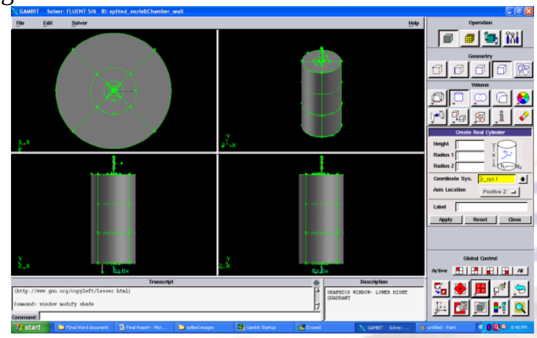


Fig.4: 3D solid model

2. Meshing the model

Meshing, also known as grid generation, is discretization of model into smaller regions called as grids or elements.

In meshing the geometry three meshing schemes are used.

a) **Hex: -** Mesh include only hexahedral elements.

b) **Hex/Wedge: -** The mesh is composed primarily of hexahedral elements but includes wedge elements where appropriate.

c) **Tet/Hybrid: -** The mesh is composed primarily of tetrahedral elements but may include hexahedral, pyramidal, and wedge elements where appropriate.

The main task in meshing was to create a complete hexahedral structural grid. To make it a complete structural grid the geometry has divided into 154 numbers of volumes. The sub parts are shown in the below fig 5.

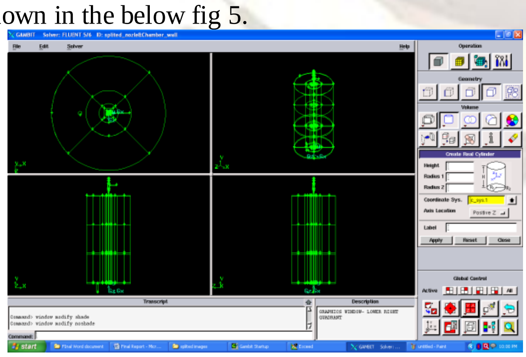


Fig.5: Wireframe model in Gambit

The complete meshed model is as shown in the figure 6.

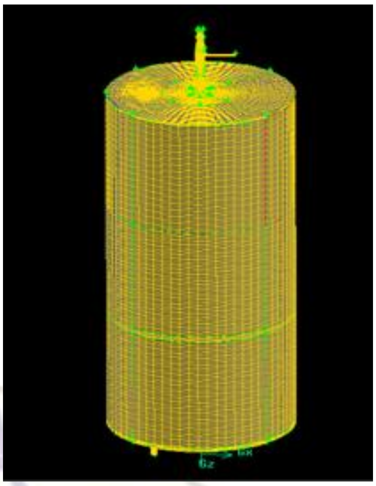


Fig.6: Complete 3D view of Meshed model

Examine mesh

- Total number of volumes = 154
- Total number of elements = 7,75,885
- Worst element equisize skewness = 0.690053

Table.1: 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%

3. 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 type specifications of the model

The inlet and outlet boundary conditions as shown in table 2, fig.7 & fig.8.

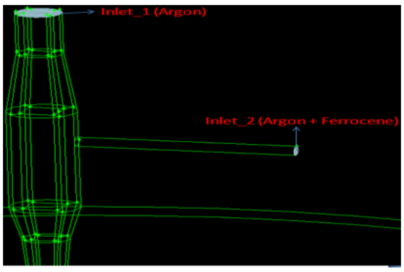


Fig.7: Boundary conditions

Table 2: 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

Continuum type

There are two continuum types, each of which is associated with a set of fundamental transport equations. They are as follows:

- FLUID
- SOLID

The continuum of geometry is defined as shown in fig.8.

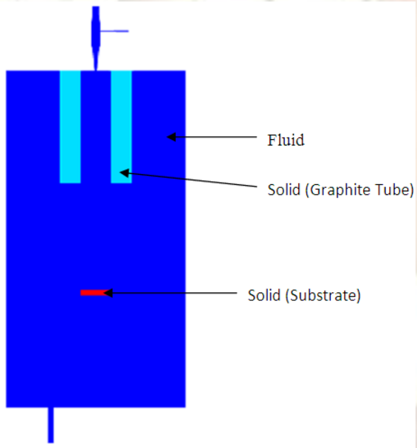


Fig.8: Cross section of model Showing various Domain

FLUENT SETTING

Pressure based solver and standard k-ϵ model selected for analysis purpose.

User Defined Functions

1. UDF for temperature profile at inlet_1

```
#include "udf.h"

#include "sg_pb.h"

double pi=3.14,Bk=1.38E-23,Avg=6.02*1.e23;

double Mono_R=1.82E-10,SrfceTen=.948,atomWeight=56,CCS=.000000001,liqden=2719;

DEFINE_PROFILE(TEMPERATURE, thread, position)
{
double x[ND_ND],R;
double Rad=.005,T0=12000;
face_t f;
begin_f_loop(f, thread)
{
 F_CENTROID(x,f,thread);
F_PROFILE(f, thread, position) = 0. ;
 R=sqrt(x[0]*x[0]+x[2]*x[2]);
if(R<=Rad)
{
F_PROFILE(f, thread, position) = 500+T0*(1-((R*R)/( Rad*Rad)));
}
 }
end_f_loop(f, thread)
}
```

IV. CALCULATION FOR MASS FRACTION

Mass fraction of ferrocene which is entering the system from inlet_ferrocene is calculated for 100mg of ferrocene per minute and 500mg of ferrocene per minute
The chemical formula for ferrocene is Fe (C5 H5)2
We know that the molecular Weight of ferrous, carbon and hydrogen are
Fe=56, C=12, H=5 (g/mol)
Therefore the molecular weight of the ferrocene can be calculated as follows
Molecular weight of the ferrocene = 56+ (12×5+1×5) ×2 = 186 g / mole
i.e. Fe (C5 H5)2 =186 g/mol
Considering volume flow rate = 5 LPM at inlet_ferrocene (ferrocene + Argon)
We know that 22.4 Litre argon = 40 g argon,
Hence, 5 litres per minute = 8.92 g/ min
MAr = 8.92 g / min
For 100 mg/min:
Mass of ferrocene: 100 mg / min, Mass of Argon: 8.92 g / min
Mass Fraction of ferrocene = 0.01008
For 500 mg/min:
Mass of ferrocene: 500 mg / min, Mass of Argon: 8.92 g / min
Mass Fraction of ferrocene = 0.0530

COMPARISON OF THE RESULTS FOR DIFFERENT CASES

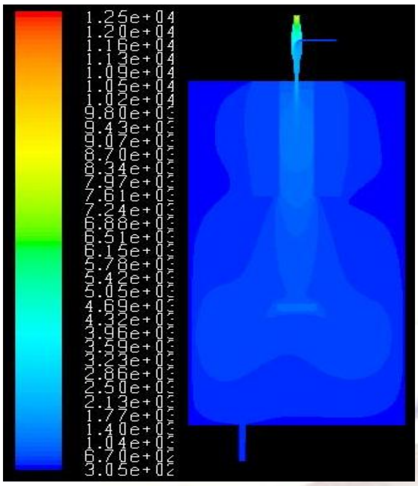


Fig 9: Temperature contour with graphite tube

As shown in fig.9 & fig.10 the above 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.

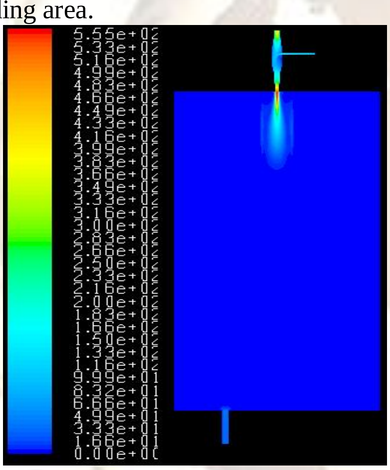
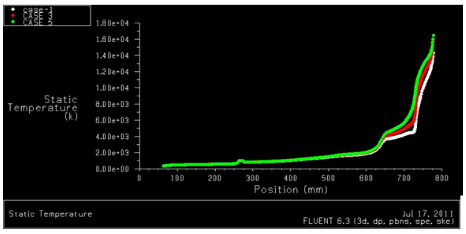


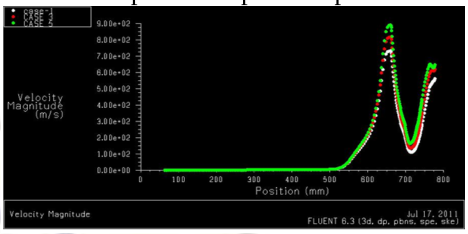
Fig.11: Velocity contour with graphite tube

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.

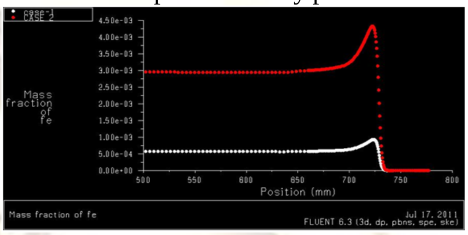
Following all the graphs for temperature "Graph.1", velocity "Graph.2", mass fraction of Carbon "Graph.3", mass fraction of Argon "Graph.4", mass fraction of Ferrous "Graph.5" and mass fraction of Hydrogen "Graph.6" are plotted on the axis of the chamber and nozzle. These all graphs are plotted for both the cases of with graphite tube and without graphite tube.



Graph.1: Temperature plot



Graph.2: Velocity plot



Graph.3: Mass fraction of fe

In the following table the Cooling Rates are shown for all Cases:

Case 1: 10 kW with 100 gm/min of ferrocene
Case 2: 10 kW with 500 gm/min of ferrocene
Case 3: 15 kW with 100 gm/min of ferrocene
Case 4: 15 kW with gm/min of ferrocene
Case 5: 20 kW with 100 gm/min of ferrocene
Case 6: 20 kW with 500 gm/min of ferrocene
Range I: 3500k to 1600k
Range II: 1600k to 1000k
Range III: 1000k to 800k

Case	COOLING RATES (dT / dt): K/sec		
	Range I	Range II	Range III
Case 1	**2.23e6**	**1.34e4**	**2.93e3**
Case 2	**2.6e6**	**1.53e4**	**3.313e3**
Case 3	**8.95e5**	**1.29e4**	**2.55e3**
Case 4	**1.12e6**	**1.47e4**	**2.84e3**

Case 5	**7.71e5**	**1.35e4**	**2.77e3**
Case 6	**5.86e5**	**1.46e4**	**2.50e3**

V. CONCLUSION

Table shows that the cooling rate of gases for different cases stated. With the analysis the mass fraction of fe is estimated for different ferrocene mass flow rate and torch powers and it is in compliance with theoretical value of fe mass fraction. Results shows that there is not much difference in temperature and velocity contours for different cases.

VI. Acknowledgement

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