CFD Analysis Of Laser Ablation For Nanotube Production – A Review

Bhautik R. Pabani[1], Dr. Kedar A. Pathak[2]
1 P.G Student, U.V Patel College of Engineering, Kherva, Mehsana
2 Associate Prof., U.V Patel College of Engineering, Kherva, Mehsana

ABSTRACT

Laser ablation process is important for production of nanotube with 70-90% purity. Now a day use of nanotube is very wide because of its extraordinary properties. And so production of nanotube in mass quantity is also important. This paper reviews the experimental work as well as computational analysis for the production of nanotube. Computationally so many work done for the analysis of furnace geometry for the laser ablation process. Now some new suggestion also made through this review and till now 2D analysis of laser ablation furnace is done by various researcher so now some scope for 3D analysis of furnace in which laser ablation occur and nanotube produce. This kind of analysis is done by computational fluid dynamic with use of software tool and then compares the analysis data with experimental data for validation.

Keywords – Computational fluid dynamics, laser ablation process, nanotube.

1. Introduction

Laser Ablation Process For Nanotube Production

Laser ablation is the process of removing material from the solid surface by evaporating. In laser ablation process material is heated at low flux by getting energy from the laser and converted in to plasma state at high flux.

In 1995 smally's group at Rice University reported the synthesis of carbon nanotube by laser vaporization. A pulsed or continuous laser is used to vaporize the graphite target in oven at 1200°C. The main difference between continuous and pulsed laser, is that the pulsed laser demands a much higher light intensity (100 kW/cm2 compared with 12 kW/cm2). The oven is filled with helium or argon gas in order to keep the pressure at 500 Torr. A very hot vapour plume forms, then expands and cools rapidly. As the vaporized species cool, small carbon molecules and atoms quickly condense to form

larger clusters, possibly including fullerenes. The catalysts also begin to condense, but more slowly at first, and attach to carbon clusters and prevent their closing into cage structures.

From these initial clusters, tubular molecules grow into single-wall carbon nanotubes until the catalyst particles become too large, or until conditions have cooled sufficiently that carbon no longer can diffuse through or over the surface of the catalyst particles.

2. Computational Fluid Dynamics

CFD implies that prediction of fluid flow with the complication of simultaneous flow of heat, mass transfer, phase change, chemical reaction etc using computer. History of the CFD starts early 1970. It is the combination of physics, numerical and mathematics and computer science employed to analysis fluid flow. First application of the CFD method was the simulation of transonic flow based on the solution of the nonlinear potential equation.

With the beginning of 1980 the solution for first two dimensional and then also three dimensional Euler Equation become feasible. With the mid 1980 the focus started to shift significantly more demanding simulation of viscous flow govern by the Navier-Stockes equation. CFD method are concern with the solution of equation of motion of the fluid as well as with the inviscid fluid(Euler Equation) and of viscous fluid(Navier Stokes Equation) so called governing equation.

The ultimate goal of the computational fluid dynamics is to understand the physical events that occur in the flow of fluid around and within designed objects these events are related to the action and interaction of phenomena such as dissipation, diffusion, convection, shock waves, slip surface, boundary layer and turbulence.

There are several advantages of CFD include:

- With use of CFD analysis time and cost are reduce of new design. And it will affect the total production cost positively.
- CFD enables where so many modifications is required and also help. And also find optimum solution.
- CFD provides the environment to study systems under hazardous conditions and beyond their normal performance limits.

- CFD facilitates practically unlimited level of details of results.

Steps for CFD analysis process:
(1) Pre-processing
• Represent objects in the flow domain, e.g. Furnace geometry, using CAD tools (Shown in fig1.) made in CFDexpert4.5
• split the flow domain into sub-volumes to create a mesh(fig2.)
(2) Obtaining a Flow-Solution
• run a flow-solver using the mesh for flow conditions specified by the user
(3) Post-processing
• extract and visualize the flow data from the results of the flow-solver.

3. Literature Survey

3.1. Introduction

In recent year, the improvements in computer power have increased the interest of engineers and researchers to simulate their problems with computational methods. A lot of computational tools and methods have been developed in the last decades to analyses fluid dynamics, combustion, and different modes of heat transfer, which can be used in two- and three-dimensional configurations. Among other practical problems, one of the most important practical problems having highlighted role in fluid mechanics , and fluid flow analysis has received considerable attention. In this section the experimental and computational investigations on the laser ablation process for nanotube production is reviewed. Here, as far as experimental investigations are concerned, the emphasis is put on general trends and not on details. It is intended to give an overall idea about experiments in laser ablation and review the most of computational work are available. Numerical methods that make the basis for theoretical studies are also discussed.

3.2. Literature

2.1 Computational Work In Production Of carbon Nanotube By Laser Ablation

Greendyke et al [1] studied the CFD simulation of laser ablation carbon nanotube production. They get the result computationally. They summaries that simulation of the plume resulting from single 10ns laser pulse are used for the analysis of flow field dynamics and chemical concentrations using C6 as an indicator species for fullerene production.

They observe the experimental set-up at NASA JSC in which two concentric quartz tubes of 1.5 mm thickness from the inner and outer tubes with inside diameter of 2.2 and 5.08 cm respectively at one of the end of inner tube are located two 10Hz pulsed laser operating at 1064nm and 532nm wavelength with the longitudinal axis of the inner quartz tube. For standard production runs a 10ns 532 nm pulse is followed 50 ns later by a 10 ns 1064 nm pulse. Each pulse is of 300 mj energy. In this study they use VULCAN code also they use TECHPLOT Graphics software for

Generation of grid With computational experiment they observe that the initial temperature of the injected carbon ablation product is 4950K however the temperature of the plume rapidly rise after injection to the recombination of simpler carbon molecules releasing more energy in to the flow. They also examine the plume production , plume dynamics also get the result related to the mass fraction for the entire simulated flow field regime.

"Modeling of dynamics with shielding in laser ablation of carbon " by Dr.pathak et al [2]

The plume dynamics in laser ablation is important to study for many reason including temperature of plume particles and shielding of target by previously ablated plumes. Shielding leads directly to the change in energy deposition of incident laser pulse at the target surface and in turn influences the ablation dynamics and amount of material removed. For effectively model highly nonlinear plume dynamics a scheme is developed by Dr.pathak et al. This scheme is the combination of two other, Godunov method and ENO-Roe method. This paper describes physical setup, the mathematical model of plume dynamics and the model of shielding of laser beam. Here also vorticity based model of plume dynamic is introduced to interpret the accuracy of numerical method and their combination.

The vaporized material ejected from the target is modeled as a compressible, viscous ideal gas. Therefor there dynamical state is described by compressible Navier-stokes equation. The combination of nonlinear Godunov and linearized Roe method for discretization of plume gas dynamic equation is suitable for modeling plume dynamic in laser ablation. They conclude from the cfd simulation that the ablation rate is non-monotonic with the decrease of time interval between the successive laser pulses. This results from the two reason (1) plume pressure and temperature which are larger for shorter time between pulse and (2) The path length that laser beam has to travel through the plume before it reaches the target, which increase with time interval between pulses.

2.2 Experimental Work In Production Of Carbon Nanotube By Laser Ablation

Growth mechanism for single wall carbon nanotubes in a laser ablation process by C.D.scott et al. [3]

They investigate the mechanisms of single-wall carbon Nano tube formation in the pulsed laser ablation process. Time and space dependent emission spectroscopic and laser induced florescence measurements are obtained during production of SWNTS within a double tube reactor in a 1200C oven. The condition for their experiment to producing SWNTs is one in which argon at about 67KPa flow slowly (about 3mm/s)down a 25mm inner tube . A 12mm diameter graphite target containing 1at percent each of cobalt and nickel is located at the end of the tube. The tube and target are enclosed in a 56 mm tube all of which are placed in a tube furnace heated to 1473 K. Two Nd: YAG pulsed laser are flared along the axis of the tube to ablate the end of the target.

Y. Zhang et al. [4] investigated the production of SWNTs in a nitrogen atmosphere, comparing the product with that produced in argon in similar conditions. Their findings indicated that the nanotubes were created in the high-temperature zone close to the target in a region where nitrogen was essentially excluded by the ablation products. Later, after mixing of the plume with background nitrogen, amorphous carbons were formed that had nitrogen inclusions.

A continuous-wave (CW) carbon dioxide laser was used to produce SWNTs by Maser et al [5]

They heated a graphite rod containing Ni/Y and Ni/Co catalysts in an argon atmosphere. They found that Ni/Y (4.2/1 at.percent) yielded the most nanotubes, followed by the Ni/Y (2/0.5 at.percent) mixture, then Ni/Co (2/2 at.percent). TheNi/Y (4.2/1 at.percent) catalyst mix is the same as that found to be best in the arc method by C. Journet et al [7]. Because they found that the SWNTs were deposited very close to the target, they concluded that SWNTs must be formed very rapidly in the gas phase, either17 in the hot plasma plume or very close to it, where the temperature is still high enoughto support their growth. They suggest that the temperature of the hot region around thelaser-ablation spot on the target is high enough to assure SWNT growth without an external oven. Since external gas ow rates are very low around the target, the time scale could be rather long for nanotube formation. It is interesting to note that the CW laser ablation is similar to arc ablation in that the background gas and catalyst mix found to be best is the same as in the arc process. This may imply that heat transfer and di_usion dominate continuous processes as compared with pulsed proesses.

In a **single pulsed Nd:YAG laser-beam experiment Yudasaka et al. [6]** found that for pulses with only 0.1-s intervals(10 Hz) the nanotube production was superior to longer intervals and that the amount produced was greater. However, the size of tubes was not by pulse intervals from 0.1 to 120 s.

They concluded that the surface temperature that is influenced by average energy flux affects the rate of production. Using a 20-ms-duration pulsed CO2 laser in single-pulse mode to ablate graphite containing 0.6 at .percent Co/Ni catalysts, **Kokai et al[6]** investigated the effect of oven temperature on nanotube growth. They found that larger diameter nanotubes are produced at higher temperatures, which is consistent with the results of Bandow et al [8].

Kokai et al [6] reported a yield greater than 60 percent for an oven temperature of 1473 K. Using high-speed video and emission spectroscopy, they found that carbonaceous materials with SWNTs were visible about 3 ms after the beginning of the laser pulse. Blackbody emission from clusters was observed for more than one second. They suggested that SWNTs grow from molten carbon metal particles via super saturation at ablation temperatures, followed by segregation at about 1593 K. This model is based on C-Ni and C-Co eutectics. A continuous supply of hot carbon clusters and the maintenance of a hot SWNT growth zone during the 20-ms laser pulse are important. They also suggest that the temperature of the SWNT growth zone may be higher than 1473 K.

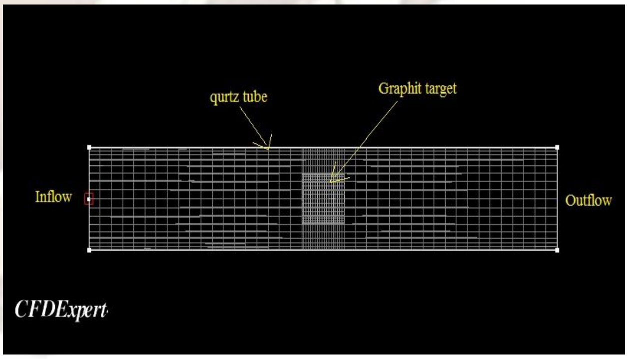

Fig1. Furnace Geometry

4. Conclusion and Discussion

For the production of nanotube with maximum yield some of the parameter is very important. And more affective thing is plume dynamic so it's important to understand the temperature and pressure profile of produce plume during laser ablation process. From the literature we can conclude that till now experimental work as well as 2d analysis of laser ablation furnace with the help of CFD tool is done by various author so there is scope for 3D CFDanalysis of furnace that we can understand the phenomena very nearly and increase chance for pure nanotube production. After that data getting from the analysis is compared with the experimental data for validation of analysis.

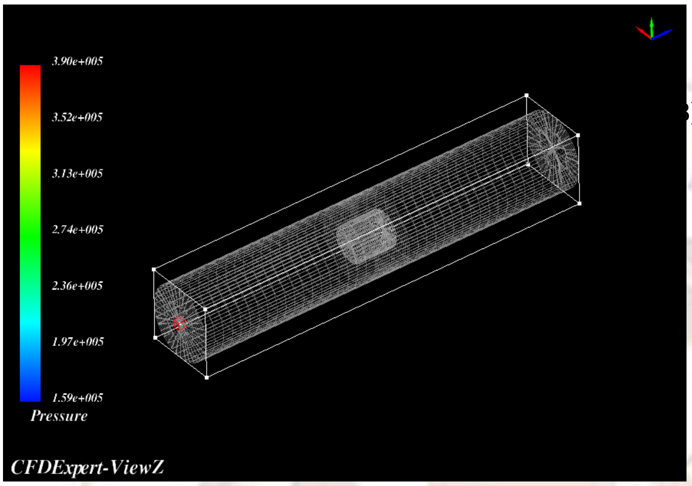

Fig2. Flow domain in sub volume

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