COMPUTATIONAL FLUID DYNAMICS ANALYSIS OF CARBON NANOTUBE SYNTHESIS IN A CHEMICAL VAPOUR DEPOSITION REACTOR SYSTEM

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Abstract
Carbon nanotube synthesis requires time, effort and there is a need for a comprehensive and low cost way to characterize the flow in the furnace in order to understand how process parameters may affect CNTs formation. In this research, development of three-dimensional numerical models to elucidate the hydrodynamic behaviour and the percentage deposition of CNTs in a chemical vapour deposition (CVD) reactor was studied. Using computational fluid dynamics, constant and temperature dependent variables (piecewise linear) approximations were adopted for simulation of CNT deposition in a CVD reactor and there after validated with experimental data. Simulation results with temperature dependent variable approximate was observed to be more accurate because it provided less than 5% error when compared with experimental data. Effects of catalyst, carrier gas, and temperature on the simulation of carbon nanotube were also investigated using temperature dependent variables approximation. Catalyst, carrier gas, and temperature were found to have great influence on the velocity flow structures and therefore affect the deposition rate of carbon nanotubes. The optimum conditions obtained were; temperature (1073.15 K), argon velocity (0.002040 m/s), acetylene velocity (0.001099 m/s) and this gives 90.5 % deposition for simulation as compared to experimental yield of 92 %.

Keywords: Carbon nanotubes, Chemical vapour deposit, Numerical analysis, Computational fluid dynamic, Tangential velocity, Axial velocity

Introduction

Carbon nanotubes (CNTs) are tubular structures, produced by manipulation of carbon atoms with diameter in a range of 1 - 100 nm. After the discovery of Iijima in 1991, CNTs have been an area of interest because of its attractive electrical, thermal and mechanical properties. However, one of the most important issues in this field that must be well addressed is challenges with mass production and the high cost of production of CNTs (Liang *et al*., 2004). Thus different method of producing high quality CNTs at low cost have been examined (Oyeyemi *et al.,* 2019). Chemical Vapour Deposition (CVD) method is the most used technique, due to its handling procedure, simplicity and possibility of high production rate and yield with low impurity (Lee *et al*., 2002; Oyeyemi *et al.,* 2019). Flow rate of the carrier gas, and carbon source, reaction/deposition temperature, catalyst types are some of the parameters to be considered for CNTs growth rate in an atmospheric pressure CVD (APCVD) reactor (Zahed *et al*., 2013). Due to the complexity in the production of CNTs via CVD, there is a need for a more systematic approach such as predictive models that can help towards understanding how to avoid reduction and avoidance of complexity involved during the production of CNTs (Aliyu, 2017).

Numerical studies is one of the predictive models that can be used to investigate the effect of various conditions and also to help in understanding the details of processes for interpretation of different parameters such as growth rate, flow rate and reaction mechanisms. Bimetallic catalysts especially Fe-Co for CNT growth has attracted much attention because of the efficiency of these metals and high-quality CNTs that are been produced (Prasek *et al*., 2011; Bankole *et al.,* 2018). In this regard, Endo *et al*., (2004)

predicted carbon nanotubes production rate in a CVD reactor, with respect to ferrocene decomposition, Fe catalyst deposition, Argon with 10% hydrogen (carrier gas) and xylene (carbon source). 3D laminar flow and temperature dependent properties of species were assumed and prediction of uniform velocity and temperature distributions was established inside the furnace and total production rate was successful. By coupling the results with reactions, concentration was calculated and 90% agreement of their data with experimental results was archieved. In addition, Kuwana and Saito (2005) presented a two-equation model that can predict the formation of Fe nanoparticles from ferrocene fed into a CVD reactor. The model predicted that the diameter of a particle will increase with an increase in the reaction temperature. Zahed *et al,* (2013) studied the growth rate and uniformity of CNTs based on CVD technique by using a numerical model where the SIMPLE algorithm was adopted for the pressure-velocity coupling and governing equations were discretized using the finite volume approach. Yashar, (2015) used computational fluid dynamic (CFD) commercial codes to investigate four models which were compared to determine how the presence of the sample boat, composition of the precursor gas, consumption of species at the template surface affect the temperature profiles and velocity fields in the system. In this paper, CVD technique for the production of CNT is modelled numerically and simulation result validated with experimental data.

Methodology

Physical Model & Grid Sensitivity Test

The horizontal CVD reactor as shown in Figure 1 consists of a tube with 1010 mm, internal and external diameter of 52 mm and 62 mm respectively with 4 mm wall thickness. Sections A and C in Figure 1 are the inlet and outlet respectively. B is the furnace zone and has a dimension from 190 mm to 560 mm. The furnace zone of the CVD reactor was selected for modeling in order to reduce the complexity of the geometry and because the reaction occurs at the centre of the reactor where the catalyst is placed. Catalyst was added through the use of source terms to the boat already positioned inside the CVD reactor. The inlet gas is modelled in such a way that carrier gas (argon) was used to purge after which mixture template for carbon source (acetylene) was then after introduced. Reactor processes is modelled with a single reaction which allows for the creation of site for the carbon nanotubes properties (ANSYS Fluent, 2016). The stoichiometry equation of reaction involved in the simulation of CNT deposition in a CVD reactor is given by Equation (1):

$$C_2H_2 \xrightarrow{\text{Fe-Co/Kaolin}} 2C + H_2 + C_2H_2 + \text{Fe-Co/Kaolin} \quad (1)$$

Reaction	PEF	AE	TE
C_2H_2 + C_s	$1.7x10^9$	0.06	0

Puengjinda *et al*., (2009) estimated the reaction parameters and rate of CNTs formation using the general Arrhenius equation. PEF, AE and TE stand for Pre Exponential Factor, Activation Energy and Temperature Exponent.

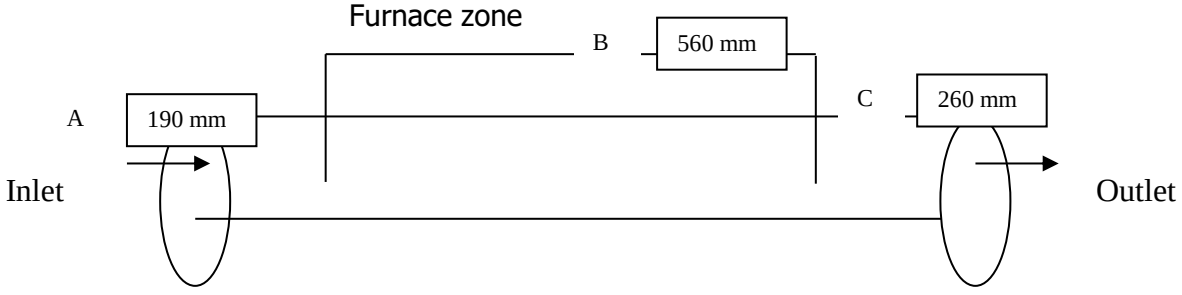


Figure 1: Schematic Diagram of CVD reactor

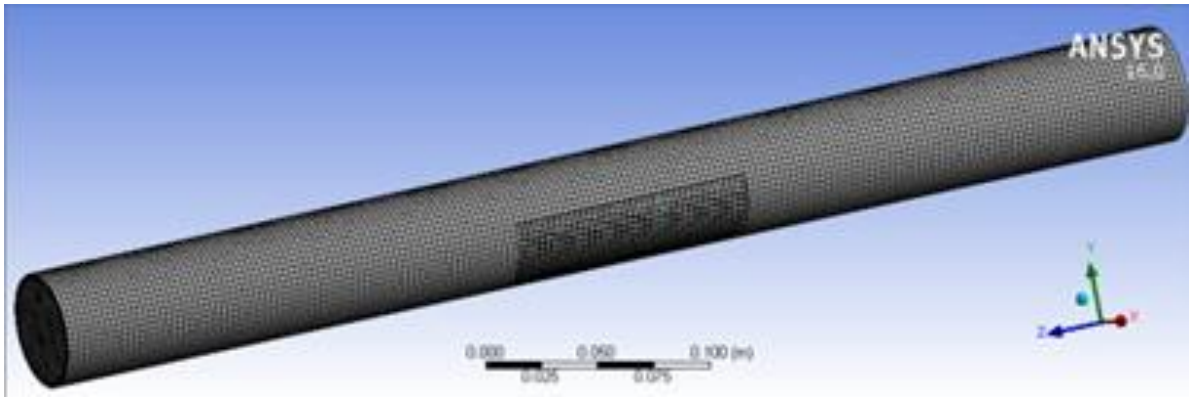


Figure 2: Meshed Geometry for the CVD reactor

Meshing was done using ANSYS Fluent meshing option as shown in Figure 2. A smooth transition in element size is important for achieving maximum accuracy in a simulation (Timothy, 2016). Multizone method was enabled because they are identified by regular connectivity which gives quadrilateral element in 2D and hexahedral in 3D.

Mathematical modeling

Using a 3-dimensional model and steady state process, the governing equations were solved with respect to the following assumptions:

(i) Reactor walls are impermeable and no slip condition is considered for the velocity at walls.
(ii) Constant temperature at the wall of the furnace.
(iii) Laminar flow regime
(iv) Steady state condition
(v) Ideal gas behaviour
(vi) Gas has a continuum behaviour
(vii) Viscous dissipation is neglected

Continuity and Momentum equations that govern the simulation of CNT production by CVD method are presented in Equations 2 and 3 respectively.

$$\frac{d\rho}{dt} = -\nabla.(\rho \underset{V}{\rightarrow}) \quad (2)$$

$$\frac{d\rho\vec{V}}{dt} = -\nabla.\left(\rho \underset{V}{\rightarrow} \underset{V}{\rightarrow}\right) + \nabla.\tau - \nabla p + \rho \vec{g} \quad (3)$$

For Newtonian fluids such as exists in gases for CVD process, viscous stress tensor is as presented by Equation 4.

$$\tau = \mu[(\nabla\vec{V} + (\nabla\vec{V})^{T}) - \frac{2}{3}\nabla.\vec{V}\,I] \quad (4)$$

On rearrangement, Equations 2-4 and coupled with energy equation to obtain Equation 5:

$$Cp\frac{d\rho T}{dt} = -Cp\nabla.(\rho \underset{V}{\rightarrow} T) + \nabla.(\lambda\nabla T) + \nabla.(RT\sum_{i=1}^{n}\frac{D_I^T}{m_i}(\nabla ln fi)) + \sum_{i=1}^{N}\frac{H_i}{m_i}\nabla.j_i - \sum_{i=1}^{N}\sum_{K=1}^{K}H_i V_{ik}(R_k^g - R_{-k}^g). \quad (5)$$

Inter-diffusion and Dufour effect (energy flux due to mass gradients) give rise to very small contributions to the energy flux at normal CVD conditions, and can therefore be excluded.

$$Cp\frac{d\rho T}{dt} = -Cp\nabla.(\rho \underset{V}{\rightarrow} T) + \nabla.(\lambda\nabla T) - \sum_{i=1}^{N}\sum_{K=1}^{K}H_i V_{ik}(R_k^g - R_{-k}^g). \quad (6)$$

Species transport equation is presented in Equation 7:

$\frac{\partial(\rho\omega_i)}{\partial t} = \nabla.\left(\rho \underset{V}{\rightarrow} \omega_i\right) + \nabla.\underset{J}{\rightarrow} + m_i \sum_{K=1}^{K} V_{ik} \ (R_k^g - R_{-k}^g).$ (7)

(Zahed *et al*; 2014; ANSYS Fluent 2016)

Numerical procedure

The governing equations were discretized using the finite volume approach. This approach involves discretizing the spatial domain into finite control volume. SIMPLE (semi implicit for pressure linked equation) algorithm was adopted for the pressure-velocity coupling. In simulating the model, second order upwind was used for mass, momentum and energy equations. Convergence criterion for energy equation was set to 10^{-10}, while that of other equations such as continuity, momentum and species transport etc. was 10^{-6} with net fraction from fluxes report assumed to be less than 0.5 for the species equation (ANSYS Fluent 16). Physical properties such as viscosity, thermal conductivity and specific heat capacity for each species are assumed to be thermal dependent. These properties for the gas mixture were obtained using the Piecewise linear approximation for simulation involving temperature dependent variables. This was done because carbon nanotubes are mainly temperature dependent process which was found to be capable of demonstrating the buoyancy and flow shear effects associated with the CNT process in a CVD reactor. Therefore, the application of temperature dependent variables option will greatly reduce the uncertainty and reversible reaction during numerical simulations.

Results and Discussion

This study is focused on numerical simulation of factors that influence the growth of CNTs in a CVD reactor. To validate the simulated results, CNTs was grown in a CVD reactor with composite of Fe/CO on kaolin support as the catalyst. The effect of catalyst on the production of carbon nanotube was also investigated at optimum condition of 1073.15 K, argon velocity 0.002040 m/s and acetylene velocity of 0.001099 m/s.

Validation of numerical results

Well-structured hexahedral grid, that is refined at the near walls where the gradient of the parameters are important, is selected. Several different grid distributions have been tested to ensure the results are grid independent. The selected grid number was 107441. In addition to show the accuracy of the results, comparisons are made between the obtained numerical results and experimental result. Figure 3 shows the validation of simulated result with experimental result at different acetylene velocity. It can be observed that constant variable have the least yield of 78% and temperature dependent variable has closer yield of 82% to experimental result of 86%. At argon flow rate of 0.00204m/s and acetylene flow rate of 0.001099m/s, 90.5% was obtained for simulated result using temperature dependent Variable and 86.4% for constant variable compared to 92% yield from experimental result. Temperature dependent variable is more reliable and gives closer percent yield to that of experimental results because it manages to demonstrate buoyancy and flow shear effects.

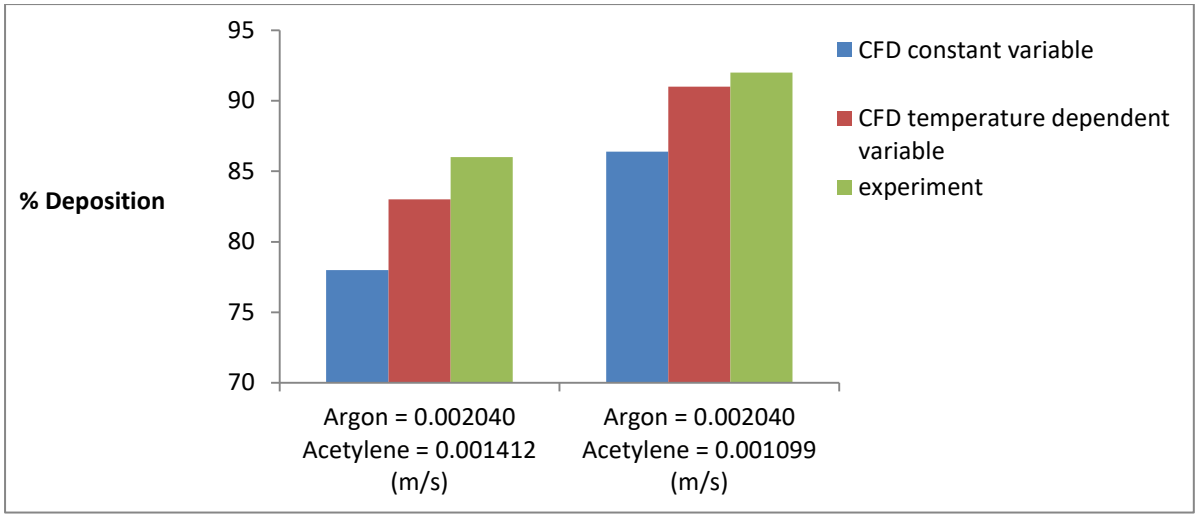


Figure 3: Validation of numerical result with experimental result

Figure 4 shows the validation of simulated result with experimental result at different argon velocity. It can be observed that a yield of 86.3% was obtained for a constant variable and 88.1% for temperature dependent variable. For Argon flow rate of 0.001726m/s and acetylene flow rate of 0.001099m/s, a yield of 86.5% was obtained for simulated result using constant variable and 89.4% was obtained using temperature dependent variable. Temperature dependent variable is more reliable and gives closer yield to that of the experimental results because it manages to account for buoyancy and flow shear effects associated with the CNT deposition in a CVD reactor.

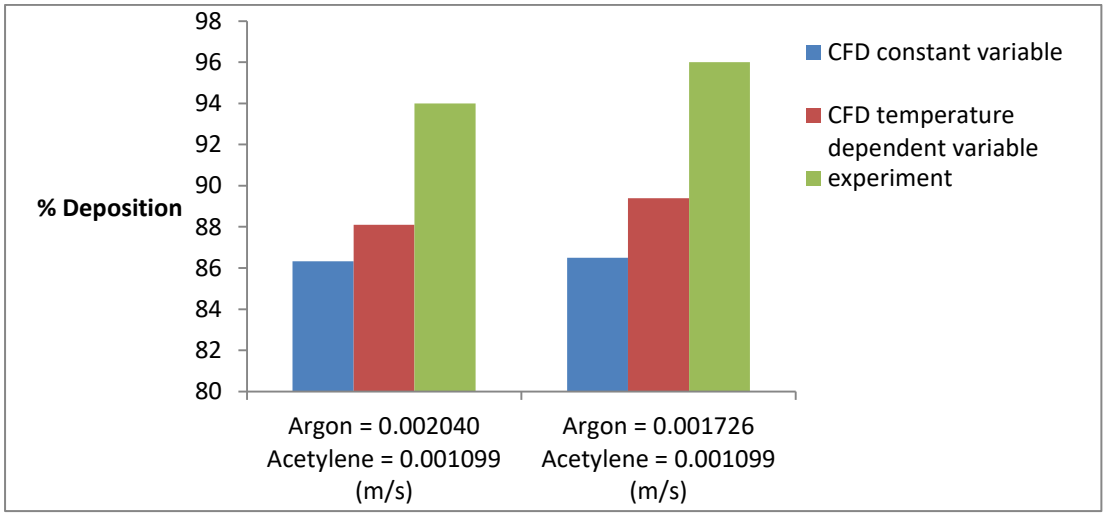


Figure 4: Validation of numerical result with experimental result.

According to Zahed *et al;* (2013), less than 5% error is acceptable between experimental result and simulated result. Hence, temperature dependent variable based simulation results show good agreement with experimental results and was used to investigate the effect of synthesis parameters on the yield of CNTs.

Effect of catalyst on deposition rate of CNTs is shown in Figure 5. The case with catalyst has higher deposition of 90.5% compared with that without catalyst of 65.38%. This is because the presence of catalyst increases the activity of the reaction leading to larger deposition of CNT. Dupius (2005) opined that the main function of a catalyst in CNT formation is to

increase the rate at which the acetylene decompose to form CNT. This explains why the case with catalyst has more deposition than the case without catalyst.

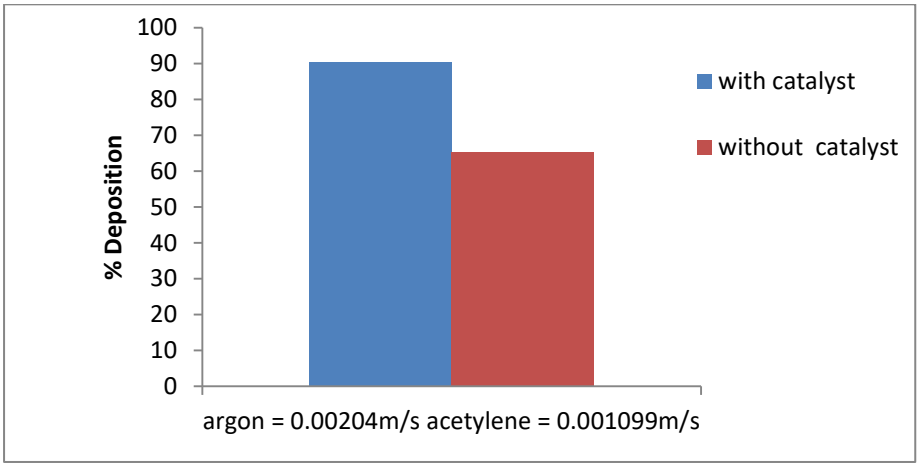
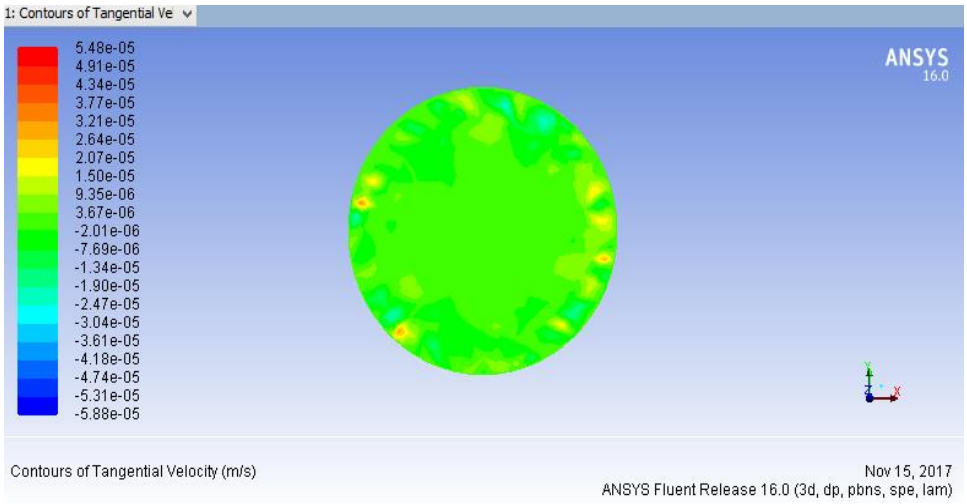
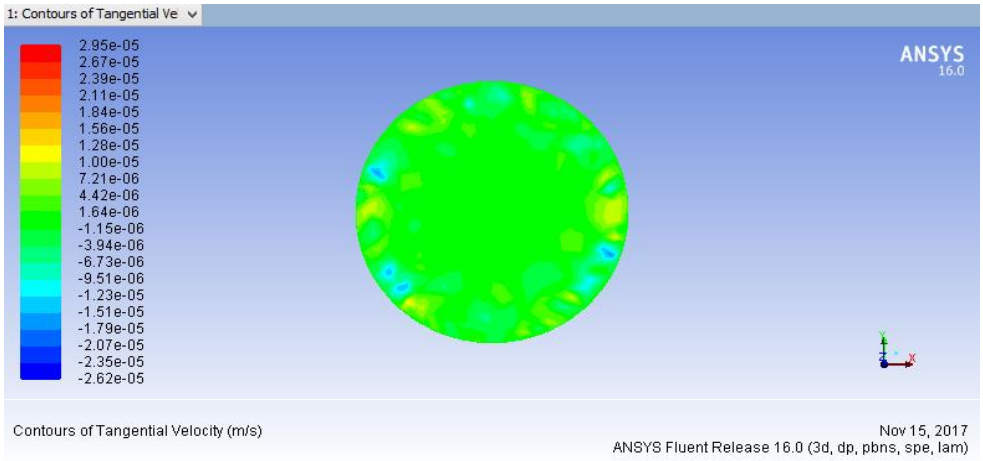


Figure 5: Comparison between cases with catalyst and without catalyst

Figures 6 and 7 show the contours of the tangential velocity at Z = 0 (which is slightly after the inlet) and Z = -270 (at the outlet section) for cases with and without catalyst. It can be observed from the plot for cases without catalyst have more backflows than that with catalyst which is an indication of instability of the simulation. The case with catalyst has greater magnitude in term of tangential velocity and this is attributed to an increase in inlet velocity (addition of catalyst) compared with case without catalyst. Therefore, the absence of catalyst plays vital role on the velocity within the reactor and velocity is a function of the rate of deposition of CNT.

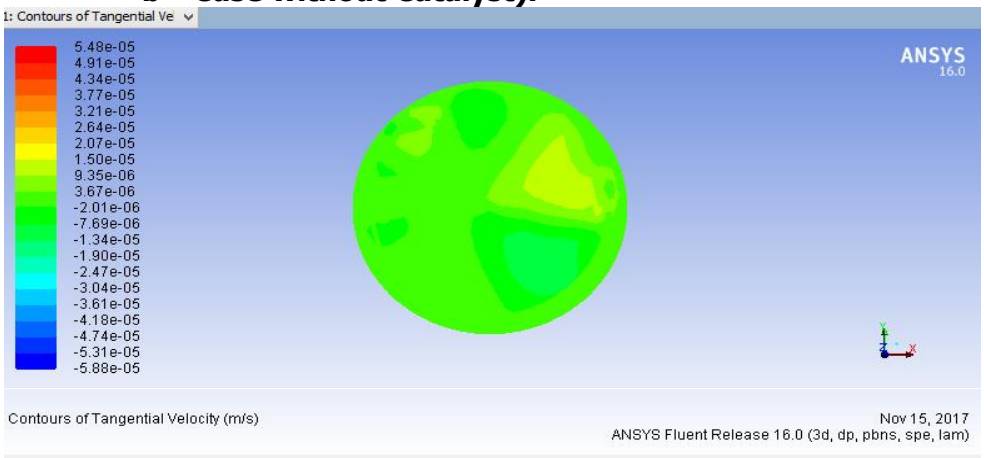


(a)

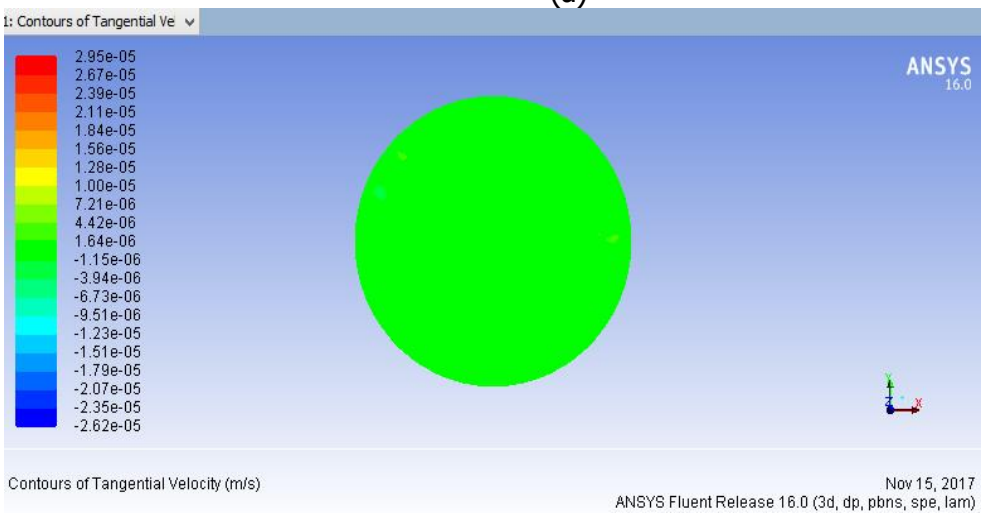


(b)

Figure 6: Contour of Tangential Velocity at z=0. (a= Case with Catalyst and b= Case without Catalyst).



(a)



(b)

Figure 7: Contours of Tangential Velocity at z= -270 (a) with catalyst and (b) without catalyst.

Figures 8 and 9 shows the Axial velocity at Z = -240 and Z = -310 (all at the boat centre) for case with and without catalyst. Generally axial velocity for the case with catalyst has higher magnitude than the case without catalyst. It is observed from the plots that catalyst

plays a vital role in the interaction of reagent with the substrate. Axial velocity increases to a point at which the temperature is higher. (Marcele *et al,* 2015).

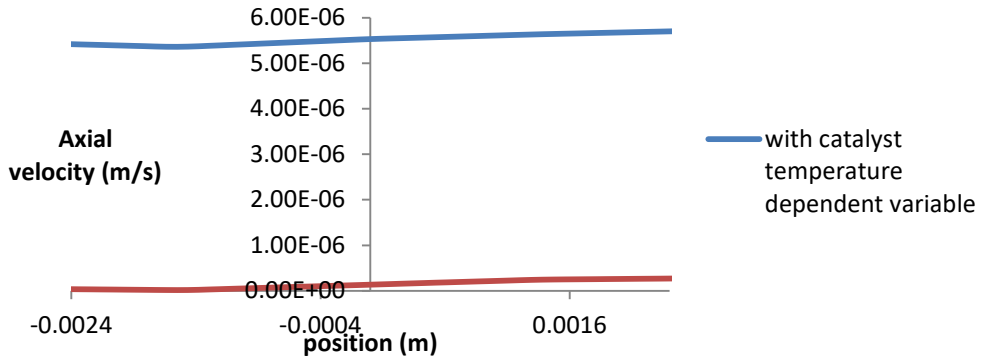


Figure 8: Graph of Axial Velocity at z= -240

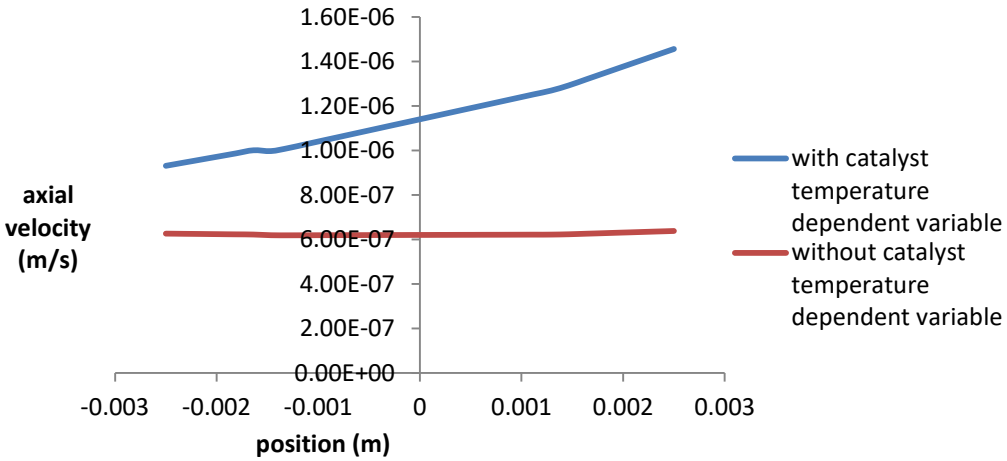


Figure 9: Graph of Axial Velocity at z= -310

Comparison between cases with and without carrier gas is shown in Figure 10**.** 90.5% was obtained for the case with carrier gas and 27.19% was obtained for case without carrier gas. This is because the rate at which carbon source moves into the reactor is increased by the presence of carrier gas (Aguilar *et al.,* 2006). The absence of argon can cause oxidation and less CNT will be deposited. Therefore more deposition can occur if carbon source are made available in the reactor.

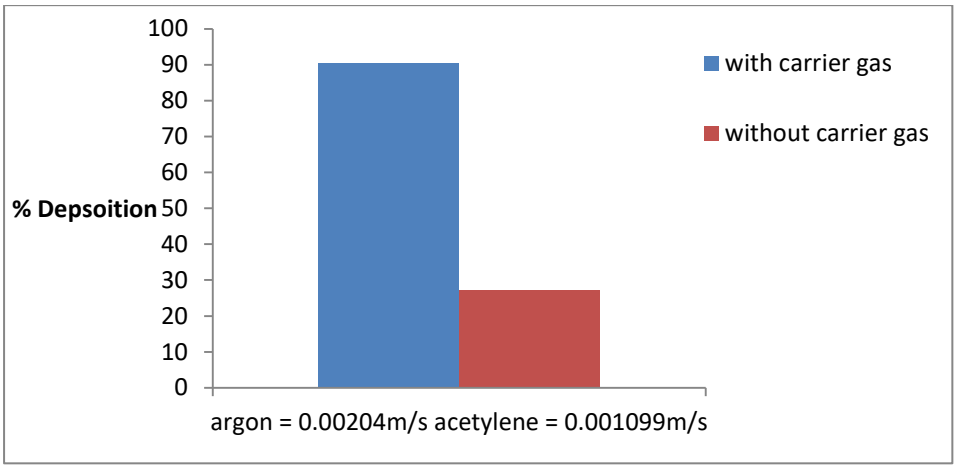
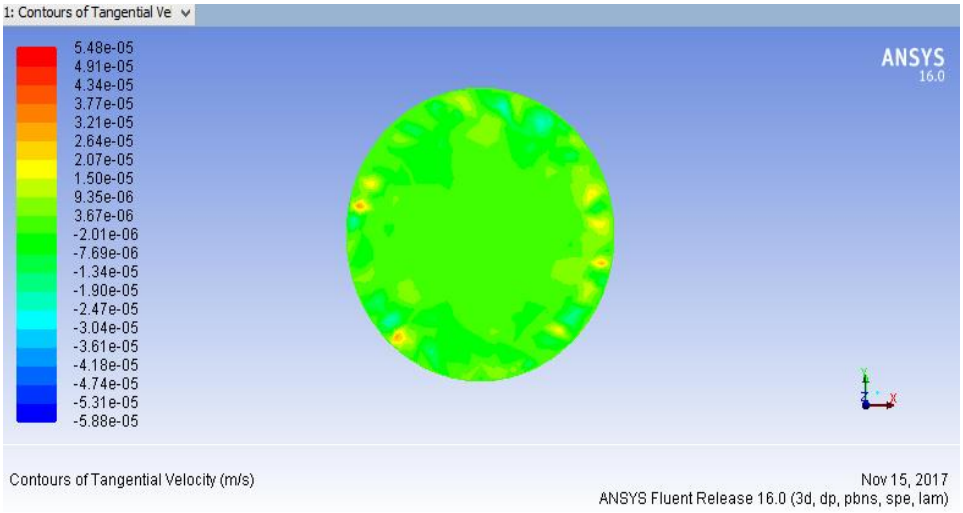
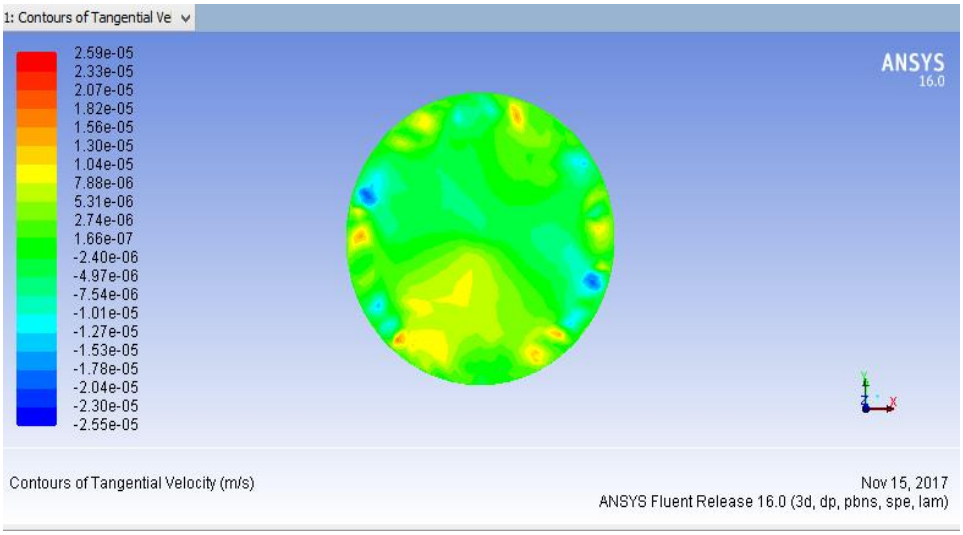


Figure 10: Effect of carrier gas on the deposition of CNT

Figure 11 shows the Tangential velocity for case with and without carrier gas at Z = 0, it can be observed that carrier gas plays a vital role on the velocity distribution and flow structure of carbon nanotube simulation in a CVD reactor. Contours have different magnitude and shape. Mitrovic *et al*; (2007) observed that an increase in flow rate of the carrier gas leads to higher operating pressures and high deposition rate of CNT at the end. The presence of carrier gas increases the velocity within the reactor thereby increases the rate by which acetylene moves into the reactor.



(a)



(b)

Figure 11: Contours of Tangential Velocity at z= 0. a= Case with Carrier Gas and b= Case without Carrier Gas.

Figure 12 shows the graph of axial velocity at -240 (on the boat). It can be observed that the case with carrier gas is more stable and moves from negative to positive. The case without carrier gas can be seen to have more negative value which is an indication of back flows. The case with carrier gas has higher magnitude compare with the case without carrier gas and this justifies the high percentage deposition for the case with carrier gas.

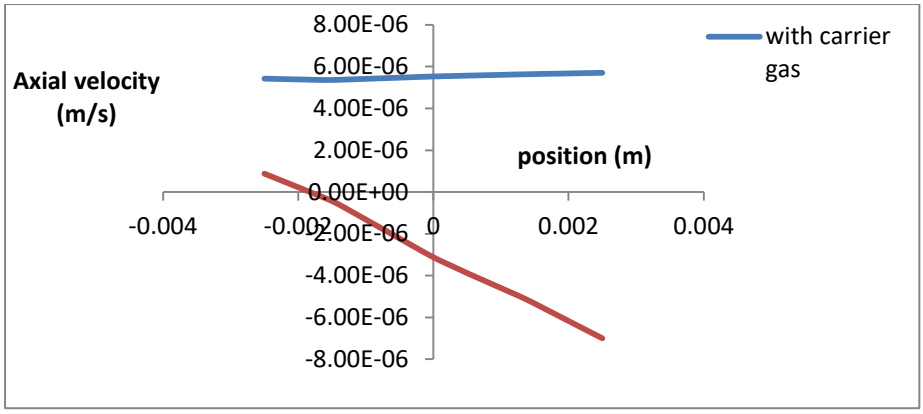


Figure 12: Graph of Axial Velocity at z= -240

Figure 13 shows the axial velocity plot at x = -310. The two cases: with carrier gas and without carrier gas can be seen to be more stable at this position on the boat. This is because no back flows can be seen from the plot at this position. Therefore, more deposition can occur at this position. The case with carrier has higher magnitude compare to the case without carrier gas.

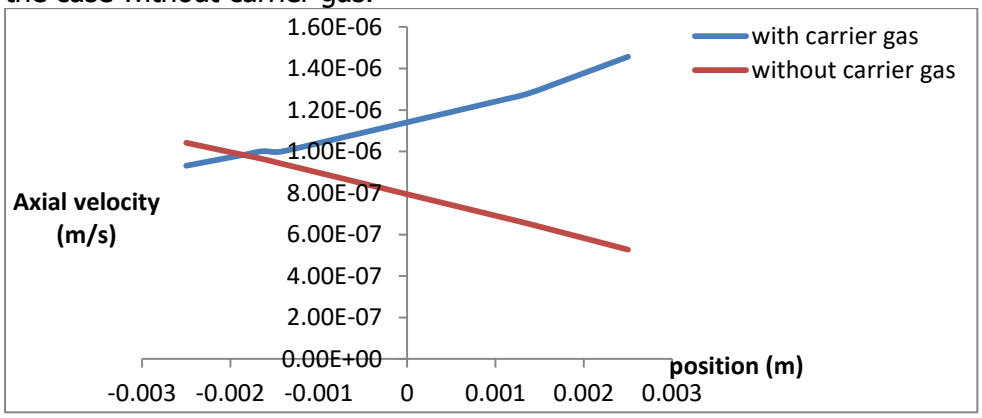


Figure 13: Graph of Axial Velocity at Z= -310

The effect of temperature on CNT yield is shown in Figure 14. Simulation was done using the same boundary condition at different furnace temperature. 92% deposition from experiment is compared with CFD result of 90.5% deposition of CNT obtained for 1073.15K and 85.94% was obtained for 973.15K and 89.7% for 1173.15K. The result is in accordance with Sinha *et al.,* 2000 who reported that lower temperatures result in lower CNTs yield.

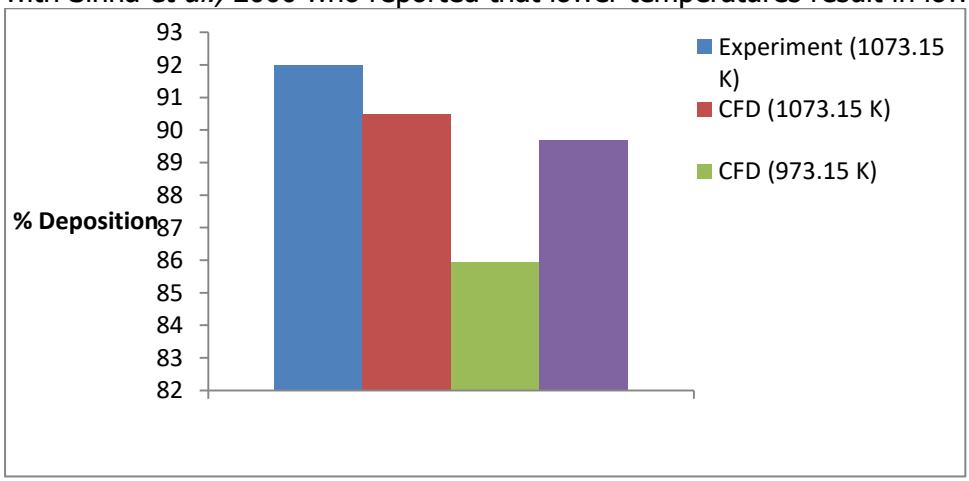
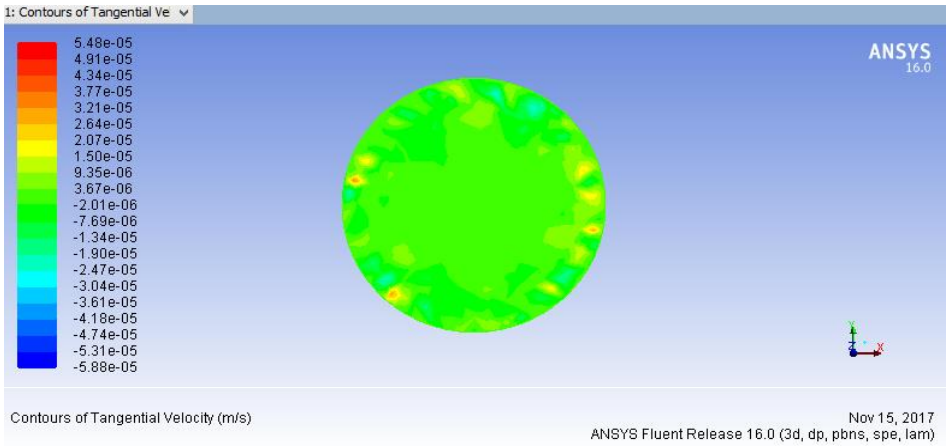
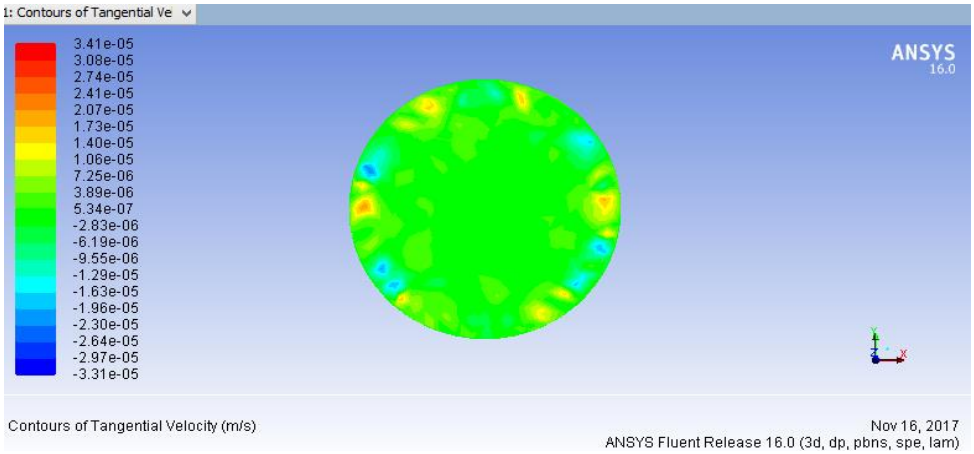


Figure 14: Comparison between experiment and different temperatures

Figure 15 obtained from the simulations allow the evaluation of the impact of temperature on the fluid profile of the CNT deposition in a CVD reactor. It can be observed that contour have almost the same shape but different magnitude. The difference in magnitude is as a result of change in temperature. At Z = 0, more back flows are observed at T = 973.15 and this is because of the reduction of temperature. Generally velocity is higher at T= 1073.15K compared to at T= 973.15 and T= 1173.15K.



(a)



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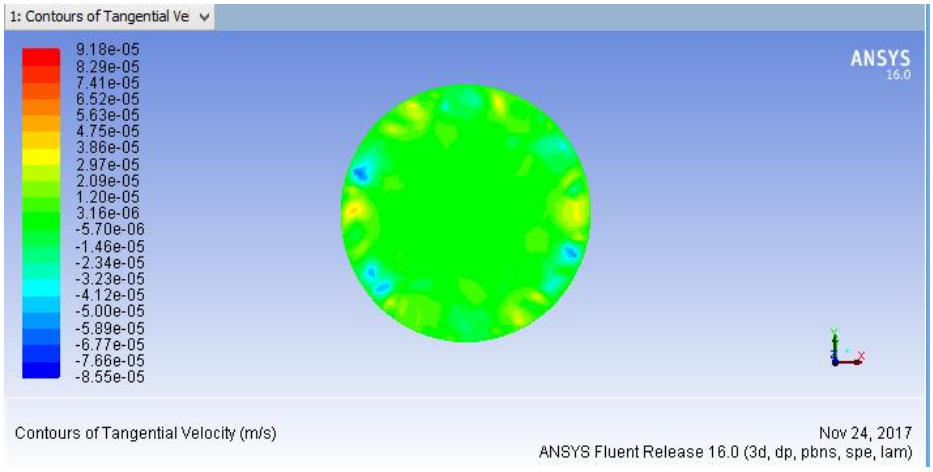

(c)

Figure 15: Contours of Tangential Velocity for Case G at Z= 0. (a) 1073.15K (b) 973.15K and (c) 1173.15K

Figures 16 - 18 show the axial velocity graph at different positions on the boat. The Axial velocity for cases T= 973.15K and 1173.15K can be observed to be constant at different position; this is because of the reduction in temperature which in turn reduced the yield of CNT. Axial velocity for the case with T= 1073.15K can be seen to have higher magnitude than that of the case with T = 973.15K and T= 1173.15K which is as a result of increase in temperature at wall. Increase in temperature increases the axial velocity up to a certain point where the temperature of the fluid is high within the modelled reactor.

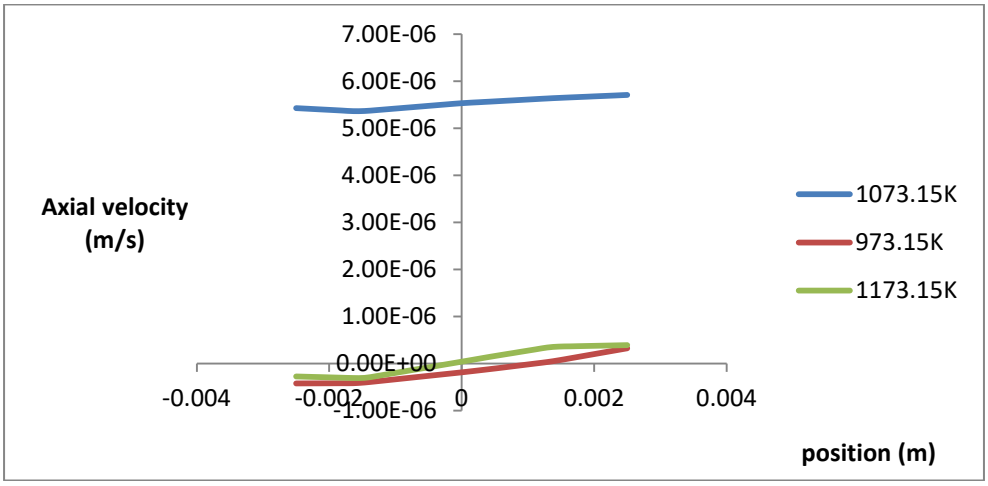

Figure 16: Graph of Axial Velocity for Case G at Z= -240

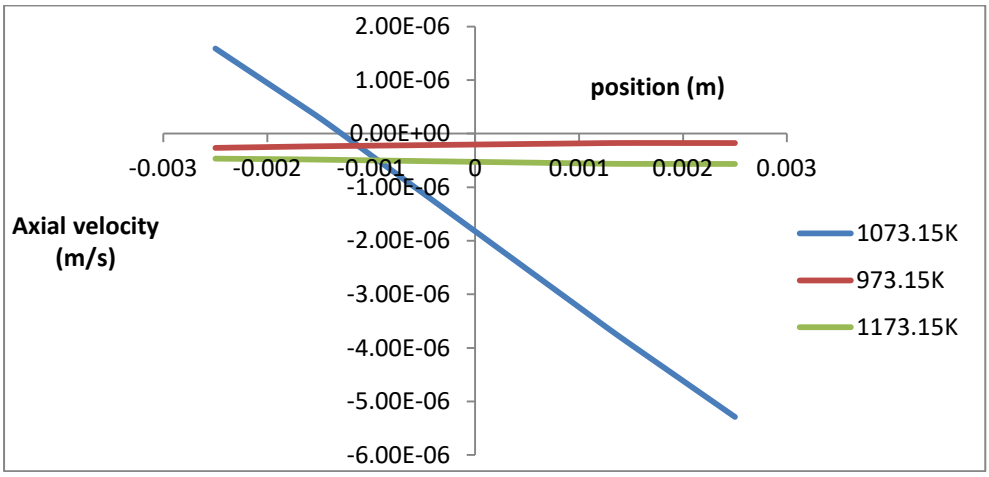

Figure 17: Graph of Axial Velocity for Case G at Z= -280

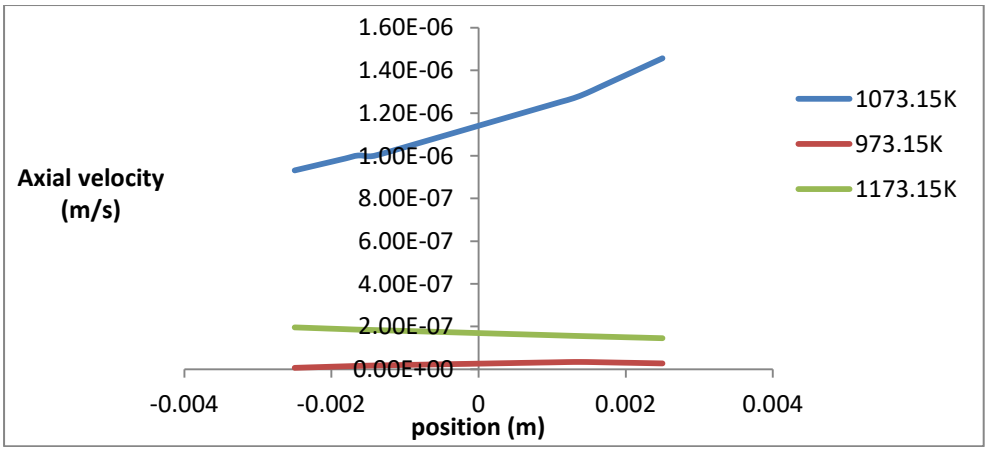

Figure 18: Graph of Axial velocity for Case G at Z= -310

Conclusion

Chemical vapour deposition reactor for the production of CNT was modelled and the effect of process parameters on the CNT deposition successfully investigated. Tangential velocity along the Z – direction and axial velocity along the x – direction were used to show the effect of velocity within the furnace. Based on the results obtained, it can be concluded that the absence of carrier gas and catalyst reduces the Tangential and Axial velocity magnitude within the reactor and there by reduces the deposition rate of CNT. Further increase in temperature above the optimum (1073.15K) lowers the velocity profile within the reactor and thereby decreases the yield of carbon nanotubes. Linear approximation provides less than 5% as reported by Zahed *et al.,* (2014) and hence, conforms better to experimental results.

Nomenclature

M_i : Dynamic viscosity of the gas mixture
I : Unity tensor ($kgm^{-1}K^{-1}$)
P : Pressure (pa)
R : Universal gas constant (8.314 $J.mole.K^{-1}$)
τ : Viscous stress tensor ($N.m^{-2}$)
ω_i: Species mass fraction
T : Temperature (K)
j_i: Diffusive mass flux vector (kg.m-2)
R_k^g: Forward reaction rate of the kth gas phase reaction ($mole.m^{-3}.s^{-1}$)
R_{-k}^g: Reverse reaction rate of the kth gas phase reaction ($mole.m^{-3}.s^{-1}$)
i,j : With respect to the ith/jth species
R_I^S: Reaction rate for the lth surface reaction($mole.m^{-2}.s^{-1}$)
t : Time (s)
Cp: Specific heat of the gas mixture ($Jkg^{-1}K^{-1}$)
$\underset{V}{\rightarrow}$: Velocity vector ($ms^{-1}$)
Mi: Mole mass of the ith species ($kg.mole^{-1}$)
fi : Mass fraction of the ith species
H : Molar enthalpy ($Jmole^{-1}$)
CNT yield = $\frac{outlet}{inlet}$ x 100%

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