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Investigation of CNT Growth Regimes in a Tubular CVD Reactor Considering Growth Temperature

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Abstract
In Carbon nanotube (CNT) growth process via Chemical vapor deposition (CVD) method, there are two distinct regimes based on growth temperatures, so called mass transfer controlled and surface reaction controlled regimes, which represent different type of behaviour in growth. Operating in each regime has different characteristic that can influence on other operating condition effects on CNTs growth. Thus study of these regimes is important for better understanding of CNTs growth; also it helps to control of other operating conditions effect on growing CNTs. In this paper these two regimes is established and then relevant processes in reactor is studied in details. Results show that CNTs total production in mass transfer controlled regime has higher order and less sensitivity to the growth temperature compared to surface reaction controlled regime. Also produced CNTs in mass transfer controlled regime has less length uniformity compared to surface reaction controlled regime.

Keywords: carbon nanotube; chemical vapor deposition; growth regimes; growth temperature

Introduction

Carbon nanotube (CNT) has become one of the most famous and applicable nanomaterial due to their superior properties and wide range of applications. Chemical Vapor Deposition (CVD) is a common method for preparing CNTs due to its ability to produce highly ordered CNT material with large yields. Despite a huge progress in CNT research over the years, producing CNTs of well-defined properties in large quantities with a cost effective technique is a challenge. The root of this problem is the lack of proper understanding of the CNT growth mechanism. CNTs synthesis via CVD method involves many parameters such as precursors, operating pressure [1], inlet gas mixture flow rate and growth temperature [2,3] that the latter can affect on CNTs growing behavior significantly. Bases on the growth temperature there are two different types of growth regimes [4] that influence on other parameter effects on CNTs growing. Thus understanding of processes occuring in these two regimes can be helpful to control the quality and quantity of produced CNTs. Therefore in this article a CFD model established for analysis of CVD method and then effects of growth temperature on growth behaviour of produced CNTs via CVD method is studied and discussed in details.

Materials and method

Modelled CVD hot wall reactor (fig. 1) used for CNTs fabrication in this study is a horizontal tubular reactor. Inlet gas mixture enters from inlet, heated up in preheater, and then enters into furnace zone. After surface and gas phase reactions, through the catalytic decomposition of xylene, carbon atoms released and CNTs grow on furnace wall and then gas mixture exits from the outlet.

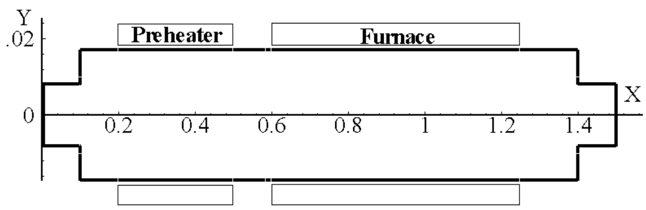

Fig. 1. Geometry of CVD Reactor

Applied CFD model solved conservation of mass, momentum, energy and species (equation (1) - (4)) with the aid of the ideal gas law:
Conservation of Mass:

$$\frac{\partial \rho}{\partial t} = -\nabla.(\rho \vec{V}) \qquad (1)$$

Conservation of Momentum:

$$\frac{\partial \rho \vec{V}}{\partial t} = -\nabla.(\rho \vec{V}\vec{V}) + \nabla.\tau - \nabla p + \rho \vec{g} \qquad (2)$$

That for Newtonian fluids such as existent gases in CVD reactors, viscous stress tensor is as follows: