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# A CFD study on a vertical chemical vapor deposition reactor for growing carbon nanofibers

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## ABSTRACT

A computational fluid dynamic (CFD) study has been carried out to simulate velocity, temperature, and concentration profiles in a vertical chemical vapor deposition (CVD) reactor used for growing carbon nanofibers (CNFs). CNFs were grown over activated carbon fibers (ACFs) wrapped over an especially designed perforated tube which was vertically mounted in the reactor. The numerical model analysis incorporated the conservation equations of momentum, energy, and species. Natural convection effects on the heat-transfer and the exothermic heat generation due to the decomposition of benzene were included. The model simulation results revealed that approximately uniform temperature and concentration profiles existed in the ACF-packed bed. In addition, multiple combinations of the heating length and the wall temperature of the reactor were possible to achieve the prescribed CVD temperature. Under the simulated CVD conditions, the present model predicted an average carbon deposition rate of  $5 \times 10^{-13}$  kg/m<sup>2</sup> s, which corresponded to the yield of ~0.005 g of CNFs per g of ACFs. The simulation results of this study are important for the optimization of the CVD operating conditions to achieve a high and uniform CNF growth in the vertical reactor.

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**Keywords:** Computational fluid dynamics (CFD); Chemical vapor deposition (CVD); Carbon nanofibers (CNFs); Numerical simulation; Packed-bed

## 1. Introduction

Carbon nanotubes (CNTs) are presently used in a number of engineering applications because of their unique physical, electrical and thermal properties (Bansal et al., 1988; Downs and Baker, 1991; Iijima, 1991; Odom et al., 1998; Karanfil, 2006). CNTs are produced by the chemical vapor deposition (CVD) of hydrocarbons at elevated temperatures over the metal oxides supported catalysts (Mukhopadhyay et al., 1999; Colomer et al., 2000). After the production of CNT, the catalyst support is removed in a post-synthesis step.

Carbon nanofibers (CNFs) are relatively newer materials and are grown over activated carbon microfibers (ACFs) used as the substrate (Gupta et al., 2009, 2010; Chakraborty et al., 2011; Mekala et al., 2011, 2012). Use of ACF as a support has the advantage that the post synthesis processing is not required because the prepared hierarchical micro-mesoporous

structure of CNF/ACF can be directly used in end-applications, for example, the fabrication of fuel cell electrodes, and adsorbents for environmental remediation (Kisamori et al., 1994; Maruyama et al., 2002; Li et al., 2004; Tzeng et al., 2006; Dicks, 2006; Gupta et al., 2009, 2010; Mekala et al., 2011, 2012; Chakraborty et al., 2011; Ismail et al., 2011).

In the aforesaid studies (Gupta et al., 2009, 2010; Mekala et al., 2011, 2012; Chakraborty et al., 2011), CNF was grown on ACF in a vertical CVD reactor. There are advantages of using vertical reactors. (1) The foot-print is small. (2) The furnace used for the heating of the reactor may be moved vertically downward immediately after growing CNF. This allows the rapid cooling of the reactor, and therefore, immediate reuse of the reactor in the subsequent CNF-production. (3) The gas flows downward in the tube and then radially outward through the ACF-cloth wrapped over the perforated section of the vertical tube. Such an arrangement causes uniform flow through the ACF.

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