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CFD modeling and experimental study of multi-walled carbon nanotubes production by fluidized bed catalytic chemical vapor deposition ☆

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ABSTRACT

A parametric study investigating the impact of temperature, gas velocity, and composition of the gaseous phase on the catalytic growth of multi-walled carbon nanotubes (CNT) has been performed. CNTs have been produced by catalytic chemical vapor deposition from methane decomposition over Co–Mo/MgO with average diameter of 188 μm with spherical shape in a fluidized bed reactor. The computational fluid dynamics (CFD) method was used for simulating the hydrodynamics of the reactor and investigating the operational and best velocity for producing high quality CNTs by this system. The operational and best velocities obtained by simulation were 0.015 to 0.05 m/s and near 0.015 m/s. Then the results used in the experiments with different temperature and gas compositions. CNTs products were characterized by Raman spectroscopy, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). The results showed that temperature of 900 °C, methane to hydrogen volume ratio 1:4 and 0.02 m/s are the best quantities of the parameters for CNTs growth.

1. Introduction

A great amount of research on carbon nanotubes (CNTs) has been carried out since its observation in 1991. CNTs have extremely high tensile strength ($\approx$150 GPa), high modulus ($\approx$1 TPa), large aspect ratio, low density, good chemical and environmental stability, and high thermal and electrical conductivity. It has been predicted that CNTs can be novel materials of semiconductor, electric-field-induced electron emitters, quantum wire, catalysts etc. Nowadays, CNTs can be synthesized by arc discharge laser ablation, and chemical vapor deposition (CVD). In order to make CNTs of practical importance, the criteria for assessing any synthesis technique must include the feasibility and potentiality for scale-up production at low cost. So chemical vapor deposition method for single-wall CNT production by using fluidized-bed (FB) reactor has been developed. In the latter fluidized-bed reactor, the residence times of the CNTs can be controlled accurately and the activity of the catalyst is utilized sufficiently to achieve high yields of CNTs. Furthermore, heat and mass transfer is good in a fluidized bed, which is important for the stable growth and high-purity of single-wall CNTs [1–3].

There are three main parameters that have the most important effect on purity and efficiency of CNTs produced by fluidized-bed reactor. These are the concentration, velocity and temperature of feed. They have influence on bed hydrodynamics and kinetic of reaction. In this research, a method has been used for producing CNTs through the catalytic decomposition of methane using a fluidized-bed reactor over the Co–Mo/MgO catalyst which is produced in the Research Institute of Petroleum Industry of Iran, and optimize its production conditions.

Design, scale up and optimization of reactors require the knowledge of hydrodynamics and transport phenomena such as heat transfer. While there are several experimental procedures for optimizing the operating conditions, hydrodynamics and heat transfer of nanotechnology based systems, the use of computational fluid dynamic (CFD) tools for providing valuable information about the mentioned conditions have attracted considerable attention in recent years [4–6].

Two methods have been typically used for CFD modeling of gas–solid flows, namely, Eulerian–Lagrangian method and Eulerian–Eulerian approach. In the Eulerian–Lagrangian approach, the computational demand rises sharply with the number of traced particles, which constrains its applicability to high concentration flows. In the Eulerian–Eulerian method, which is used in the current study, two phases are mathematically treated as interpenetrating continua. The success of a multi-fluid model (MFM) depends on proper description of the interfacial forces and the solid stresses. The interfacial forces are used to describe the momentum transfer between the phases, which significantly affects the hydrodynamic behavior of the mixture. The Eulerian–Eulerian approach based on kinetic theory of granular flow was used by van Wachem et al. [7].

In this investigation in order to optimize the operating conditions of fluidized bed reactor for multi-wall CNT production, the CFD method has been employed for analyzing the bed hydrodynamics, heat transfer and predicting the best feed velocity range for using in this reactor. Then optimized operating condition resulted from CFD modeling employed in the experiments with different temperature and gas compositions. CNTs

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