NTA2022

2nd International Conference on
Nanotechnology: Theory and Applications,
Cairo, 19 – 21 Dec., 2022

Ref. 046

Modeling, Simulation and Optimization of a Bubbling Fluidized Bed Reactor (BFBCR) Using Chemical Vapor Deposition (CVD) Catalyst for the Production of Carbon Nano Tubes (CNTs)

Said Salaheldeen Elnashaie[1*], Firoozeh Danafar[2] and Hassan Hashemipour Rafsanjani[2]

[1]University of Waterloo, Ontario, Canada, sselnashaie@gmail.com
[2]University of Kerman, Kerman, Iran

KEYWORDS

Bubbling **F**luidized **B**ed **C**atalytic **R**eactor (**BFBCR**) , **C**hemical **V**apor **D**eposition (**CVD**) Catalyst , **C**arbon **N**ano **T**ubes(**CNT**s), Reactions Kinetics , Physico-Chemical Parameters

SHORT SUMMARY

***CNT**s can be used as additions to metals and polymers for harder and lighter alloys and composites. **CNT**s can be produced by hydrocarbons cracking in a bubbling fluidized bed reactor using **CVD** catalyst. This process is investigated here both experimentally and by mathematical modeling, together with comparison of both approaches. The mathematical model is used vs. the experimental results in order to adjust the model parameters to fit the experimental ones. The verified model is used to simulate the reactor and find the optimal design and operating conditions.*

EXTENDED ABSTRACT

CNTs are important nanoparticles with many applications, specially the use of them as additions to metals and polymers to make alloys and composites of high strength and low density. One of the most efficient techniques for **CNT**s production is a special kind of hydrocarbons cracking in a bubbling fluidized bed reactor using **CVD** catalyst.

This fluidized bed is formed of dense phase, bubble and cloud / wake phases. This paper is investigating this process both experimentally and mathematical modeling; the work includes comparing the experimental results with a model formed of two phase bubbling fluidized bed, with optimal assumptions.

Carefully chosen assumptions are introduced into the model in order to reduce it into nonlinear **O**rdinary **D**ifferential **E**quations (**ODE**s). The catalyst activity is related to the rate of **CNT**s formation and the catalyst activity is defined in relation to the rate of **CNT**s formation. The model equations are completed with the rate of reaction(s) and other physico-chemical parameters.

The nonlinear **ODE**s with initial kinetic and other parameters are solved numerically using **MATLAB** subroutine with automatically adjusted integration step size to ensure high accuracy. The mathematical model is checked vs. the experimental results in order to adjust the model kinetic and physico- chemical parameters to fit the experimental ones.