MNK Publication

International Journal of Latest Research in Science and Technology **ISSN (Online):2278-5299**
Volume 9, Issue 3: Page No. 26 -32 ,May-June,2020
https://www.mnkjournals.com/journal/ijlrst/index.php

REVIEW OF BOOK: NANOTECHNOLOGY FOR CHEMICAL ENGINEERS

Said S. Elnashaie[1,*], Firoozeh Danafar[2] and Hassan H. Rafsanjani[2]
[1]Chemical and Biological Engineering Department, University of British Columbia (UBC), Vancouver, Canada
[2]Chemical and Environmental Engineering, Shahid Bahonar University of Kerman, Kerman, Iran
*Corresponding Author Email : saidelnashaie@gmail.com

Received : 25, June 2020; **Accepted** :29, June 2020 ; **Published** :30, June 2020

*Abstract :**This review starts by introducing the Nano-scale, to readers uncommon to this scale, in comparison to more common scales. This is followed by introducing the meaning of nanotechnology and its evolution to Nano-engineering using System Theory (ST) and in comparison with the evolution of Chemical Technology to Chemical Engineering. After that a description of the application of nanotechnology is briefly presented. The paper finishes up with the production of Carbon Nano Tubes (CNTs), which is one of the important products for alloys and plastic composites. A short conclusions and prospective research is given at the end.***

Introduction: Nanotechnology is one of the hottest two subjects for chemical engineers; the second is Sustainable Development (SD). This paper is a review of one of the very few books about nanotechnology for chemical engineering. The size of the presentation dictates that the presentation be brief and summarizes everything and eliminate few parts and concentrates on the production of one of the important products which is the CNTs, this will cover production in fluidized bed using Chemical Vapor Deposition (CVD) catalyst. The presentation covers both experimental results as well as mathematical modeling of the units, and comparison between them to determine the unknown parameters. The mathematical model can be used for scaling up and also for design of other configurations; it also presents the principles for modeling and design of other nanotechnology processes. Further suggested research is also discussed.

Brief Description of the book: The book describes the basic principles of transforming Nano-technology into Nano-engineering with a particular focus on chemical engineering fundamentals. It provides vital information about differences between descriptive technology and quantitative engineering in various fields of nanotechnology. The fundamentals of nanotechnology are also covered along with detailed explanation of several specific Nano scale processes from chemical engineering point of view. This information is presented in form of practical examples and case studies that help the engineers and researchers to integrate the processes which can meet the commercial production. It is worth mentioning here that, the main challenge in nanostructure and Nano devices production is nowadays related to the economic point of view. The uniqueness of this book is a balance between important insights into the synthetic methods of Nano-structures and nanomaterial and their applications with chemical engineering rules that educates the readers about Nano scale process design, simulation, modeling and optimization.

Keywords- Nanotechnology,Carbon Nano Tubes ,CVD

Dimensions

Small and ultra-small scales: 1 meter= 100 cm, thus 1cm = $10^{(-2)}$ (10 to the power -2= 1/100) meter, 1 millimeter (mm) =0.1 cm= $10^{(-3)}$ meter, 1 micrometer = $10^{(-6)}$ meter = $10^{(-3)}$ mm=µm (micrometer), nanometer (nm) = 10^{-9} meter

Nanometer= one of a billionth of a meter= 10(-9) m= one of a millionth of a mm= 10(-6) mm

1 micrometer = 10(-6) m & nanometer= 10(-9) m, Micrometer= 1000 nanometer, 1 nanometer= 10 angstroms; 1 angstroms= 10(-1) nanometer

Large Scales:
1 Km = 1000 m, 1Gm= 1000 Km = 10(+6) m

Diameters of Some Atoms

- Diameter of Hydrogen Atom: 0.1-0.5 nm
- A water molecule is 0.0001 micron (0.1 nm) in size according to: www.fphcare.com/humidification/humidity.asp.
- **Is the size of water molecule varied?** No, water molecules are always the same size. However, water molecules can pack together in different ways, so water itself come in different forms (liquid, ice, snow, fog, etc.).
- C-C bond ~ 0.1 nm ; Glucose < 1 nm , Hemoglobin 1-10 nm ; Viruses 10-100nm
- Diameter of Hydrogen Atom: 0.1-0.5 nm
- A water molecule is 0.0001 micron (0.1 nm) in size according to www.fphcare.com/humidification/humidity.asp.
- Diameter of Hydrogen Atom: 0.1-0.5 nm
- C-C bond ~ 0.1 nm ; Glucose < 1 nm , Hemoglobin 1-10 nm ; Viruses 10-100nm
- **DNA molecules** have a consistent **width of about 2.5 nanometers** (a nanometer is one billionth of a meter; human hair has a thickness of roughly 20,000 nm to 180,000 nm), but **the length of DNA molecules varies greatly**. Scientists usually describe the length of DNA using a unit called kb or kbp. One kb is 1000 base pairs, the base pair being the basic repeating nucleotide unit of the DNA chain. Each base pair has a length of 0.33 nm. Plasmid DNA might have a length of 1-200 kb, or 0.33 nm to 66 nm. Bacterial chromosomal

DNA length would be perhaps 3800 kb, or 1300 nm (1.3 microns). The length of human chromosome number 1 DNA is 200,000 kb, or 67,000 nm (67 microns). Of course, within the cell, DNA is coiled into a ball much smaller than its length.

1. Chemical Engineering from Technology to Engineering

1.1 Differences between technology and engineering in general and focusing on this difference as related to chemical engineering

Although, the two terms "technology" and "engineering" are interlaced, the principles of each subject and their capabilities are quite different. Generally, definition of technology is broader than that of engineering, and from a normative standpoint, it is a part of co-evolution process with society and wills for creating and utilizing the artifacts that fulfill human needs or desires. Producing and employing objects and it does not depend upon, thinking, using design equations, theories, etc. Accordingly, skills and arts without specific knowledge are sufficient in creating and managing the technology. Understanding and improving the existing technology, or resolve the problems pertinent to it requires utilizing principles of science and engineering knowledge.

- **Diameters of some atoms:** Diameter of Hydrogen Atom: 0.1-0.5 nm. A water molecule is 0.0001 micron (0.1 nm) in size according to:
- www.fphcare.com/humidification/humidity.asp .

Is the size of water molecule varied? No, water molecules are always the same size. However, water molecules can pack together in different ways, so water itself come in different forms (liquid, ice, snow, fog, etc.). C-C bond ~ 0.1 nm ; Glucose < 1 nm , Hemoglobin= 1-10 nm ; Viruses =10-100nm. DNA molecules have a consistent **width of about**

2.5 nanometers (a nanometer is one billionth of a meter; human hair has a thickness of roughly 20,000 nm to 180,000 nm), but **the length of DNA molecules varies greatly**. Scientists usually describe the length of DNA using a unit called kb or kbp. One kb is 1000 base pairs, the base pair being the basic repeating nucleotide unit of the DNA chain. Each base pair has a length of 0.33 nm. Plasmid DNA might have a length of 1-200 kb, or 0.33 nm to 66 nm. Bacterial chromosomal DNA length would be perhaps 3800 kb, or 1300 nm (1.3 microns). The length of human chromosome number 1 DNA is 200,000 kb, or 67,000 nm (67 microns). Of course, within the cell, DNA is coiled into a ball much smaller than its length.

II. Chemical Engineering from Technology to Engineering

II.1. Differences between technology and engineering in general and focusing on this difference as related to chemical engineering :

Although, the two terms "technology" and "engineering" are interlaced, the principles of each subject and their capabilities are quite different. Generally, definition of technology is broader than that of engineering, and from a normative standpoint, it is a part of co-evolution process with society. Technology emerges from ideas and wills for creating and utilizing the artifacts that fulfill human needs or desires. The outcome of technology is just producing and employing objects, and it does not depend upon, thinking, using design equations, theories, etc. Accordingly, skills and arts without specific knowledge are sufficient in creating and managing the technology. Understanding and improving the existing technology, or resolve the problems pertinent to it requires utilizing principles of science and engineering knowledge. Technology is more descriptive and empirical than engineering.

Technology emerges from ideas and wills for creating and utilizing the artifacts that fulfill human needs or desires. The outcome of technology is just producing and employing objects, and it does not depend upon, thinking, using design equations, theories, etc. Technology is more descriptive and empirical than engineering. It is not enough to create a technically successful product but it must also meet essential requirements to introduce a new product that performs as well as expected and do not cause unintended harm to the public, specially the environment and also achieves sustainability. Engineers take this responsibility to identify, understand, and interpret constraints on design in order to produce successful results. They attempt to predict how well their designs will perform to their specifications prior to full-scale production. In developing technology, engineers carefully consider the constraints including available resources, physical or technical limitations, flexibility for future modifications, and other factors, such as cost, safety, marketability and serviceability. Engineering is then defined as creative application of scientific, economic, social, and practical principles to design, construct, operate, develop and maintain structures, machines, devices, apparatus, systems, materials and/or manufacturing processes as required for an intended function, economics of operation or safety to life and property. With full cognizance of the object or process, engineers forecast behavior of their designed equipment and/or plants under specific operating conditions. Engineering is the ability to create technology and to solve problems, improve the process and construction of product by applying the engineering principles. Engineering principles involve a systematic /iterative approach to accomplish goals to meet human needs and/or society concerns. Engineers should know how to define a solvable problem, test the potential solutions, and to reach an optimal solution by making tradeoffs among multiple concerns, such as functional, ethical, economic, social, etc. factors. Engineers apply mathematics, other sciences and economics accompanied with their logic and tacit knowledge to design novel processes or to find appropriate solutions to existing problems or to improve the status quo. This job is performed by proper mathematical models (design equations) that allow analyzing the system and/or its operation. Engineers respond to the interests and needs of society and affect society and environment by bringing about technological changes. Consequently, it is to note that engineers have an important role in the co-evolution process of society and technology. Engineering is more quantitative and less empirical than technology. Distinction between engineering and technology comes from differences in educational programs. Engineering curriculums is oriented towards development of conceptual skills, and include a sequence of fundamentals and courses built on a foundation of complex mathematics as well as science courses. Technology programs are geared toward applications, and provide the students with only introductory mathematics and science courses accompanied with a qualitative introduction to engineering fundamentals. Relying on these differences engineering and technology programs are evaluated/accredited using two separate sets of accreditation criteria. Technology has been created to satisfy human wishes and requirements. Much of modern technology is a product of science and engineering, and existing technological tools are used in both fields. Technology education relies on study of the human-made world, including artifacts, processes, and their underlying principles and concepts, and the overall aim of technology education is to provide students to participate effectively in technologically-dependent world. There are no constraints in developing and using technology. However, in engineering design a great attention is made on constraints including the laws of nature, or science, time, money, available materials, environmental regulations, manufacturability, and reparability. In this regard, engineering utilizes concepts in science and management as well as technological tools to accomplish their responsibilities. Graduates from engineering programs are called engineers, while graduates of technology programs are called technologists. Clearly, engineering graduates' career differs from those with technology background, technologist. Engineers graduate are with a breadth and depth of knowledge that allows them to function as conceptual designers and operators in product and process development. Once engineers enter the workforce, they typically spend their time planning, while technologists spend their time making plans work.

II.2. Nano-engineering :

Basis for synthesizing new materials is shifting to small systems, namely, micro emulsions, **Nano-particles,** etc. Properties and behaviors of such systems, where the particles are very small, differ dramatically from bulk. Accordingly, transport phenomena, chemical reactions and thermodynamics pose new conceptual and practical challenges. The main platforms include synthesis of nanostructures and incorporate them as building blocks into final products. Unit operations significantly contribute to successful commercialization of many discoveries in the chemical industry. Understanding and controlling nanotechnology unit operations will be equally important for the commercialization of nanotechnology. In manufacturing systems, besides development of unit operations, scale-up and scale-down, process integration and intensification also presents new challenges. On the other hand, as nanotechnology progresses toward manufacturing and commercial stages, the effects of Nano-materials on environmental/ public health will be an important issue that needs consideration. Before we present a brief description of the applications of nanotechnology we present two important issues related to it as shown below

II.3. Water-Engineering :

Increase in population, gives severe shortage of water in most parts of the world. To resolve this problem, water harvesting, water recycling or reusing and momentum gaining are considered initiatives. These techniques are not new to chemical engineers and they certainly can help in designing and managing water treatment and distribution in both industrial and urban areas. There are many conventional methods to remove the impurities/pollutants in water treatment including adsorption, aeration, biological oxidation, chemical oxidation and RO. Among them, the promising process is adsorption, because the used adsorbent can be regenerated by suitable desorption process and it is highly effective and economical. The most widely used adsorbents are activated carbon and zeolite. However, these adsorbents suffer from slow kinetics and low adsorption capacities that encourage researchers to investigate new adsorbents. Carbon nanotubes (CNTs), a new and exciting part of nanotechnology, have been proven to possess great potential as superior adsorbents for removing many kinds of organic and inorganic pollutants Compared with other adsorbents.

II.4. Systems and System Theory (ST) :

- **First Most fundamental classification:**
  1- Isolated System (batch/adiabatic no matter or energy in or out)
  2-Closed System (batch/non-adiabatic no matter in or out)
  3- Open System (continuous, matter in and out)
- **Another Classification:**
  1- Lumped System: No variables change with space
  2-Distributed System: Variables change with space
- **A Third Classification that Usually Combines with the Above Two:**

1- Homogeneous System: Formed of one phase
2- Heterogeneous System: Formed of more than one phase with mass and heat transfer between the phases

II.5. Mathematical Modeling Tools :

Chemical engineers are involved in quantitative analysis and understanding of various phenomena utilizing mathematical modeling. By advent of novel technologies like bio and nanotechnology, this task becomes more important and complicated. They mainly focus on understanding of gas and liquid systems compared to the area of solids handling. Accordingly, the fundamentals for solids flow remain empirical in nature. Solids handling is of considerable importance in processes involved in synthesis of nanostructures and hence research in this areas, such as flow of cohesive powders, flow of gas particle in risers and fluidized beds, etc. are vital. Improved physico-chemical modeling accompanied with microscopic modeling can help to predict the macroscopic behavior of solids; nevertheless, their behavior at microscopic level, especially for reacting systems is still in its infancy. Besides improved modeling techniques, new mathematical tools, which suit the complexities and un-certainties' in the chemical engineering systems such as black box modeling, artificial neural networks, fuzzy logic, phase-space reconstruction, cellular automata etc. have been brought into the profession. These new mathematical tools have offered great possibilities of system prediction under specific circumstances, when not enough information is available. Novel analysis and simulation techniques, like motion simulation and animation/virtual prototype and computational fluid dynamics, finite element analysis, life cycle analysis, and even project management, are also likely to play a strong role in the future of chemical engineering.

III. Nano-new Materials

In a multidisciplinary world of science/engineering, chemical engineers are not just involved in designing and controlling chemical plants; they are now dealing with the formation of new materials. Main tracks for future researches in chemical engineering involves tailoring of materials with controlled structures, targeted properties and new applications. New materials offer novel optical, magnetic, electronic& mechanical characteristics and/or significantly enhanced properties, such as high surface area. Novel materials are for new applications and solve increasing problems of energy and environment. New products with noticeable properties and new functions will revolutionize much of how we will live in the years ahead. Nano-products

III.1. Carbon Nano Tubes (CNTs)

Chemical engineers are involved in developing new processes to produce nanotechnology-based products, including Nano-structures materials like **CNT**s, metal nanoparticles, thin films etc. or materials including nanostructures, like Nano composites, Nano fluids, Nano crystalline metal, Nano sensors, etc. The unique properties of nanostructures have sparked the attention of scientists, engineers and manufacturer to generate materials and devices with new physical characteristics and chemical/biochemical functionalities for a wide variety of applications. For nanostructures, which have the size of below 100 nm, the theories of classical and quantum mechanics are no longer valid and a rich variety of unexpected properties are possible. For instance Nano fluids, well dispersion of nanostructure in a fluid, enhance the thermal conductivity of the fluid. Another example is, incorporating CNTs into plastics can lead to a dramatically increased modulus of elasticity and strength in structural materials . A great novelty with CNTs is that they can achieve high stiffness along with high strength. Bringing these new types of products to the commercial arena is now the main objective of major chemical firms and industries. This will definitely achieve through technical programs and through investments to find appropriate materials, processes, and applications. All products that a chemical company sells to its customer need to have a clearly defined physical shape in order to meet the designed and the desired quality standards. Clients buy the product which is the most efficient. The main key characteristics demanded for Nano-structures to capture high value markets include: producing uniform size of nanoparticle with low levels of agglomeration and high dispensability. According to these researches ,a key obstacle in the development of new materials lies in avoiding any inability to directly control the structure formation at multiple hierarchical levels. So, new developments increasingly concern highly targeted and specialized materials, active compounds and special effect chemicals, which are complex in terms of molecular structure. Dominant elements in producing the most efficient products are control of the end-use properties and expertise in design of the relevant process, permanent adjustments to diversity and varying demands along with rapid reacting to market conditions..

III.2. Preparation of Nano Materials

- **Synthesis technologies and challenges**

Referring to their wide range of applications, synthesis and manufacturing of nanotechnology-based products is one of the most active fields in Nano-science and Nano-engineering. Nevertheless, advances in this field mainly depend upon the ability to synthesize nanostructures of controlled properties. It is well recognized that properties of nanostructure materials greatly depend on size, shape, composition, morphology, and its crystalline structure. Accordingly, various approaches have been developed to control these parameters and, therefore, meet the requirements for diverse applications. Despite of numerous technologies for fabrication of Nano-structures, typically, there are two drastically different approaches, **top-down** and the **bottom-up**.

III.3. Top Down

The top-down approach is analogous to making a stone statue which is starting from bulk size and getting Nano size. A bulk piece of solid materials is taken and modified by milling, carving or cutting to create the desirable shape and size. The top-down process involves material wastage and is limited by the resolution of the tools employed. The smallest sizes of the structures made by these techniques are also restricted. Anyway, the top-down approaches have been practiced with great success by the electronics industry in fabrication of integrated circuits.

III.4. Bottom Up

The bottom-up approach for creating nanostructure involves starting from unit base of material (atom or molecule) and getting the bulk size with controlling the unit base arrangement. This approach can be analogous to building a house. Lots of building blocks is taken and put in a specific place to make final bigger structure. There is less wastage in this technique, however, is limited in how big the structures can be made. Producing nanostructures are generally carried out through chemical reaction and strong covalent bonds will hold the constituent parts together. This approach is the more preferred and efficient method for fabricating a wide variety of Nano-structures with controllable size and properties. Chemical synthesis, self-assembly, and molecular fabrication are all examples of bottom-up techniques.

III.5. Other Methods

Such as **C**hemical **V**apor **D**eposition (**CVD**); which is a process borrowed from electronic industry and is a catalytic cracking of hydrocarbon to deposit carbon in the form of Carbon Nano Tubes (CNTs)?

IV. Applications of Nanotechnology

IV.1. Nanotechnology in Biotechnology : The size of nanometer is of central importance in the nature and biological systems. Cells are the main element of the living organisms that can be much smaller than the sub-micron size domain. A wide range of biomolecules, like proteins and viruses, are in the Nano-scale range . Accordingly, nanotechnology has become a part of the world of biotechnology for understanding the biological systems and their phenomena.

IV.2. Nanotechnology in Petroleum industries : Nanotechnology is offering new and improved methods in different areas of the oil and gas industries from exploration and well drilling to refining and distribution. Properties of nanostructures such as lightness, corrosion resistance and mechanical strength make them significant elements to be used in the oil industry machines, specially drilling machines. Nanotechnology represents breakthrough elements, thanks to the development of innovative monitoring techniques and smarter Nano-sensors. Also novel advanced catalysts.

IV.3. Nanotechnology in Material Science :

Nano-**C**omposites (**NC**s) are broadly defined as **N**ano-**F**illers (**NF**s) bonded to a matrix. **NC**s of ceramic, metallic and polymer matrixes have shown outstanding properties in comparison with composites of the same material but using microstructures. The benefits include improved mechanical properties, scratch resistance, barrier properties, fire resistance, and dimensional stability. Also, a small amount of **NF**s can cut weight and cost compared with the usual loading of conventional fillers. **NC**s can be classified as structural or functional depending on its role filler in each situation.

IV.4.Nanotechnology in Environmental Science :

Nanotechnology innovations have also raised great applications in the environmental sector. Nanostructure-based materials are aimed to improve the environment through direct applications in detecting and removing pollutants from soil and ground water. Nano-sensors capable of detecting a low concentration of toxic gases are imperative for environmental monitoring and chemical safety as well as control of chemical processes and agriculture.

IV.5. Nanotechnology in Energy Sector :

World demand for energy is expected to become about 30 terawatts by the year 2050.

Compounding this challenge is to protect our environment by increasing energy efficiency and developing clean energy sources. Solutions require scientific breakthroughs and truly revolutionary developments. Within this context, nanotechnology presents exciting and requisite approaches for addressing these challenges. Those areas that nanotechnology helps to improve efficiency of energy sources are wide. Application of nanostructure in the energy sector is for energy production, distribution and storage. For example, electrodes comprising carbon nanotubes have been used to produce high-power lithium batteries, solar cells, fuel cells and several other electrochemical applications . Lithium-ion batteries (LIB) consisting of nanostructures also improve storage capacity as well as an increased life-span. Lithium ion batteries have several applications, ranging from portable electronics to electric vehicles, due to their superior energy density over other rechargeable battery technologies. Using nanostructure also offers LIB of smaller size and lower weight that may attract more attentions. Another example is of positive effect of nanostructure is their application in solar Cells. For example, solar cells with Nano-scale semiconductor materials have been developed by mimicking natural photosynthesis in green plants. Solar energy is considered a promising renewable source of energy.

IV.6. Nanotechnology in other specific fields :

Different nanostructures (nanoparticles, nanotubes, Nano-crystals) contribute to the fabrication of gas sensors . The main advantage of these sensors is the nanoscopic size of the sensing element and the corresponding nanoscopic size of the material required for a response. In addition, the mechanical robustness of the sensing elements and its low buckling force increase the sensor life time. As an example, the electrical resistivity of single wall nanotubes has been found to change sensitively on exposure to gaseous ambient containing NO_2, NH_3, and O_2. Nano sensors response is at least an order of magnitude faster than those currently available and they could be operated at room temperature or at higher temperatures for sensing applications.

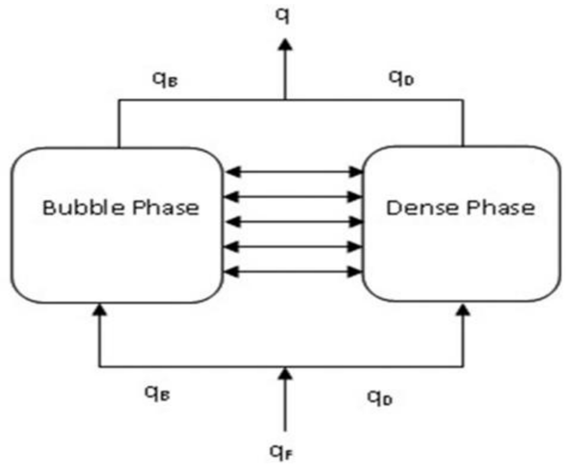

Fig.1.Schematic Presentation of Bubbling Fluidized Bed Catalytic Reactor to be Used for Modeling

The experiments are carried out in bubbling fluidized bed catalytic reactor with a **CVD** catalyst for cracking of methanol to produce **CNT**s. This type of fluidized bed is formed of a dense phase and a bubble phase, the bubble phase is surrounded by a cloud where the concentration of solid in it is lower than in the dense phase. A well verified assumption is to consider the cloud to be a part of the dense phase and therefore the bubble phase has no reactions and their **O**rdinary **D**ifferential **E**quations (**ODE**s) are linear and not **P**artial **D**ifferential **E**quations (**PDE**s) because their dynamics are very fast and can be considered always in pseudo-steady state compared with the slow dynamics of the dense phase. Therefore the ODEs of the bubble phase can be solved analytically and the mass and heat transfer integral for exchange between the dense phase and bubble phase can be evaluated analytically and the fluidized bed dynamic model is reduced to a model similar to a dynamic CSTR (Continuous Stirred Tank Reactor). As described in [2], **CNT**s grow in a fluidized bed reactor through CVD catalyst of pure Ethanol, as a carbon precursor, in presence of particulate catalyst consisting Nano-particles of iron and cobalt supported on alumina. These particulates make the bed of fluidized bed. Temperature inside the reactor could be controlled by the furnace surrounding the reactor. Accordingly, the process can be considered isothermal and the fixed point selected for the furnace can be taken as process temperature (T). The importance of isothermal condition in the reactor is avoiding formation of amorphous carbon as well as getting high productivity[3-5] Besides that, isothermal conditions are particularly useful for the elucidation of kinetics. It is reasonable to assume the CVD process isothermal with a temperature equal to the furnace due to high rate of heat transfer between the furnace and the bed.

In formulating the model a kinetic network is used as shown in [1]. And relating the catalyst activity to the **CNT**s formation by assuming each active site is covered by one **CNT**; the term for catalyst activity (ψ) is defined as:

$$\Psi=(\alpha_0 - \Upsilon)/ \alpha_0 \qquad (1)$$

For fresh catalyst, no active site is covered by **CNT**, that means $\gamma = 0$ so $\psi = 1$. The number of formed **CNT**s varies with time. As **CNT**s are formed on the active sites, the catalyst activity lessens, hence it becomes zero at the end of reaction, where all active sites were occupied by **CNT**s ($\gamma = \alpha_0$ so $\psi = 0$). Based on eq. (1) above , the catalyst activity, which is also time dependent, can be written as:

$$(d\,\psi/dt) = - (1/ \alpha_0).\ (d\,\gamma/dt) \qquad (2)$$

With some other details given in [1] a model of **ODE**s is formulated having hydrodynamic parameters of fluidization given in [6] and kinetic parameters of the suggested reaction network [1]. The model ODEs are highly non-linear(exponentially dependent upon temperature (T)). This highly non-linear model is accurately solved using MATLAB software [6]. The hydrodynamic parameters are kept constant according to hydrodynamic correlations in the literature [7] and the kinetic parameters are adjusted to fit the experimental results as shown in Fig.2. The matching between the experimental results and model with the adjusted kinetic parameters is shown to be excellent (Fig.2).

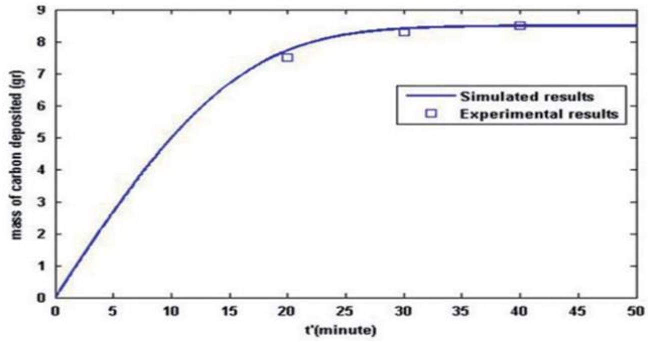

Figure 2: Mass of carbon formed versus time. Results for Experiments and Model with adjusted Kinetic Parameters

Such model can be used to investigate the characteristics of this Bubbling Fluidized Bed Catalytic Reactor as shown in Fhg.3 for carbon formation and catalyst deactivation vs. time and Fig.4 for the effect of temperature on the profile of weight of CNTs vs. time.

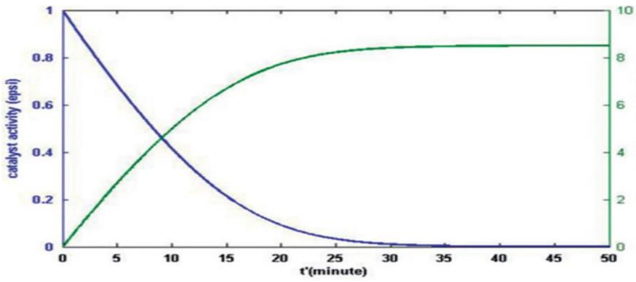

Fig. 3. Mass of CNTs deposition and catalyst activity vs. time using the verified mathematical model

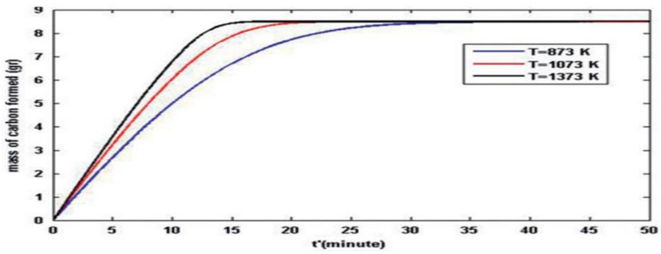

Figure 4: Effects of process temperatures on the carbon formation.

Such a verified model can also be used to scale the unit up to industrial scale (design) and to investigate other configurations such as Reactor-Regenerator units where the **CNT**s is produced in the reactor which is a fast fluidization riser and the regenerator is where the **CNT**s are extracted and the catalyst is refreshed and recycled to the reactor

REFERENCES:

[1] Elnashaie,Said Salah Eldin, Firoozeh Danafar and Hassan Hashemipour Rafsanjani, “Nanotechnology for Chemical Enginers”, 278 Pages, Publisher: Springer, 2015

[2] Fakhru’l-Razi, A., Danafar, F., Dayang Radiah, A.B., Mohd Salleh, M.A., An innovative procedure for large-scale synthesis of carbon nanotubes by fluidized bed catalytic vapor deposition technique. Fullerenes, Nanotubes and Carbon Nanostructures 17, 652–663,

2009

[3] Dasgupta, K., Joshi, J.B., Banerjee, S., Fluidized bed synthesis of carbon nanotubes – a review. Chemical Engineering Journal 171, 841–86, 2011

[4] Dasgupta, K., Joshi, J.B., Singh, H., Banerjee, S., Fluidized bed synthesis of carbon nanotubes: Reaction mechanism, rate controlling step and overall rate of reaction. AIChE Journal 60, 2882–2892, 2014

[5] Pirard, S.L., Pirard, J.-P., Bossuot, C., Modeling of a continuous rotary reactor for carbon nanotube synthesis by catalytic chemical vapor deposition. AIChE Journal 55, 675–686, 2009

[6] Elnashaie,S.S.E.H. and Frank Uhlig "Advanced Numerical Techniques with MATLAB for Chemical and Biochemical Engineers. A Simplified Bifurcation Colourfull Approach", 590 pages, Publisher: Springer,USA, January 2007

[7] Elnashaie, S.S.E.H. and Elshishini, S.S. "Dynamic Modeling, Bifurcation and Chaotic Behavior of Gas-Solid Catalytic Reactors", 660 pages, Publisher: Gordon and Breach Science Publishers, London, UK (July, 1996).