
6 Modeling and Optimization of Nanomaterials Production Processes

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6.1 INTRODUCTION

Nanotechnology (NT) applications are predicted to have an impact on almost every part of life and enable significant advancements in materials science, health, manufacturing, and knowledge-based technologies amongst several others [1]. A key fundamental component of NT is nanomaterial (NMT). According to ISO/TS 80004 standard, NMT is a material with both interior and exterior dimensions in the nanoscale (i.e., having an internal structure or surface structure in the nanoscale, with a length range from 1 nm to 100 nm [2, 3]. This incorporates both discrete NMTs (nano-objects) and nanostructured materials. Huge efforts have been targeted at the production of fruitful NMTs, nevertheless, there are still several factors that needed to be investigated [4].

Currently, NMTs are playing a bigger role in the advancement of humanity as a whole. For instance, employing green technology that relies solely on NT is the only way to prevent global warming and climate change in the first place [5] due to the fact that it has been demonstrated that bulk material-based technology cannot compete with nanotechnology in terms of effectiveness [5, 6]. Furthermore, tools to diagnose and manage the epidemic diseases that are raging across the globe are being developed using NMTs. For instance, in 2019, nanoparticles allowed for the diagnosis and management of Covid-19, a disease that was killing a lot of people worldwide [7, 8]. Also, NMTs could be used to identify and cure the monkey pox disease, which is now raging around the world [9]. Nanoscience and NT are predicted to have a major impact on how the world develops in the future [5, 9]. Generally, NMTs are divided into five main categories and several subcategories (see Figure 6.1). The main categories are size (0–3 dimensions), toxicity (fiber-like, bio-persistent granular and CMAR), architectural configuration (composite, organic, inorganic, and carbon-based), origin (artificial and natural), and size of their pores (micropores, mesopores, and macropores) [5].

Several approaches have been used in NMT production however, chemical vapor deposition (CVD) stands tall. This is due to its ability to accurately control NMT properties such as length, diameter, purity, and density, amongst several others. Due to its low cost and ease of use, the CVD process is frequently both theoretically and

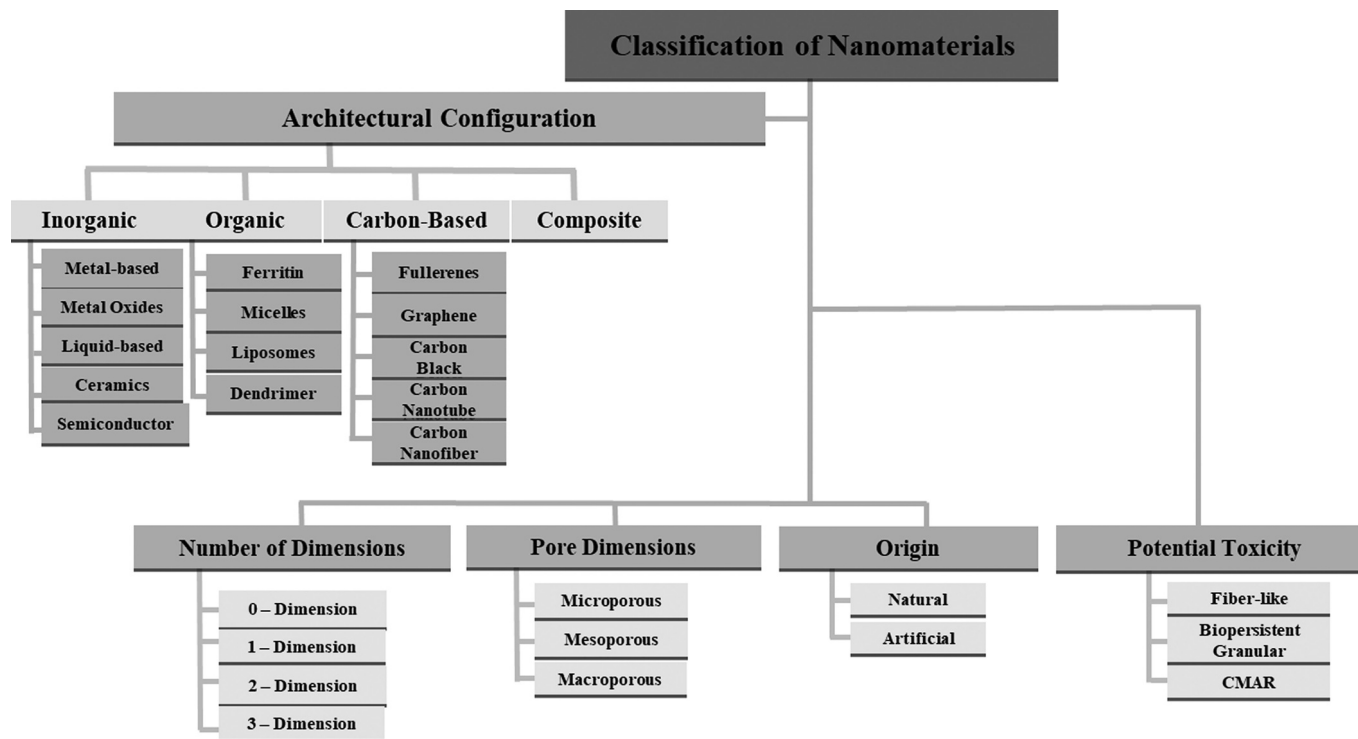


FIGURE 6.1 Classification of nanomaterials.

empirically examined [4, 10]. Production of NMT via CVD is accomplished by using a carbon source in the gas phase (precursor) and an energy source, such as a plasma or a resistively heated coil, to transfer energy into the gaseous carbon molecule [11]. Even though NMT production through CVD is widely preferred, it has some drawbacks which are mainly due to the high toxicity of the gaseous byproducts and the need for specialized equipment [12].

In order to get the most performance out of NMTs, a variety of additional factors, like the NMT tube curvature, have been proven to be important. However, experimental outcomes have consistently fallen short of the rule of mixtures expectations regardless of the type of nanotube influence on various attributes [13, 14]. In addition, to model and optimize NMT production, the simultaneous control of the size and shape of the particles along with their uniformity is crucial [15]. Hence, there is a need to re-investigate NMT production from a modeling point of view. Computational modeling and optimization tools have always played a significant role in the revolution of NMT science [14, 16].

Investigating various models that could be used to maximize NMT, for example, carbon nanotube (CNT) production, is necessary to overcome the challenges associated with studying the behavior of NMTs, such as the expense of laboratory experiments or other conventional methods that require a lot of time and resources. The objective of this chapter is to investigate different models and optimization tools that have been employed in CNT production processes.

6.2 ARCHITECTURAL/STRUCTURAL NANOMATERIALS

As aforementioned, NMTs have subcategories, however, this section will focus on the architectural/structural subcategories. These NMT subcategories include composite, organic, inorganic, and carbon-based. The distinction between these four as well as different applications will be discussed briefly in subsequent sections.

6.2.1 COMPOSITE NMTs

These NMTs consist of nanoparticles coupled with other nanoparticles, nanoparticles mixed with large-scale materials, and NMTs combined with bulk-type materials [17]. Automobile parts and packaging materials, among other things, are already using composite NMTs to enhance their mechanical, thermal, and flame-retardant qualities [5].

6.2.2 ORGANIC NMTs

Organic compounds are transformed into organic nanomaterials at the nanoscale. Ferritin, liposomes, dendrimers, micelles, and organic nanoparticles or polymers are a few examples. Liposomes and nano-capsule micelles are biodegradable, non-toxic nanoparticles with hollow interiors that are sensitive to heat, electromagnetic radiation, and light [18]. A dendrimer's surface is covered in multiple chain endings that can carry out particular chemical processes [5, 18]. In molecular recognition, nano-sensing, light harvesting, and opto-electrochemical systems, dendrimers are employed [5]. In addition, three-dimensional (3D) dendrimers may be helpful for drug delivery since they have interior holes that can contain additional molecules [18, 19].

6.2.3 INORGANIC NMTs

Inorganic NMTs are also divided into six classes: Metals, metal oxides, quantum dots, metal\CNT hybrids, metal oxides\CNT hybrids, and quantum dots\CNT hybrids. Metallic NMTs are defined as nanoscale metals with dimensions between 1 and 100 nm [20]. The most intriguing metals being examined are gold, silver, palladium, platinum, zinc, cadmium, copper, and iron. They display several traits that give them unique NMT qualities [15]. Due to their distinctive chemical, magnetic, electrical, mechanical, and optical properties, metal oxides like aluminum oxide (Al_2O_3), cerium oxide (CeO_2), copper oxide (CuO), iron(iii)oxide (Fe_2O_3), nickel(ii)oxide (NiO), titanium(iv)oxide (TiO_2), zinc oxide (ZnO), zirconium dioxide (ZrO_2), amongst several others, have attracted a lot of study attention [15, 21–25] and have a wide variety of specific applications in numerous technical domains [26, 27].

Another category of inorganic NMTs are quantum dots (QDs). QDs are monodisperse crystalline clusters that have physical dimensions that are lower than the bulk-exciton Bohr radius [28]. A variety of these dots have been constructed, often made of atoms from groups II–VI, III–V, or IV–VI. Furthermore, QDs may include NMTs such as CdS, CdSe, CdTe, ZnSe, CdSe/ZnS, In, amongst several others [15], and have diameters in the range of 2–10 nanometers. To create NMTs, metal oxides, and hydroxides have been successfully placed on CNTs. The resulting NMTs combine the distinctive qualities and capabilities of the two types of components and may also display certain novel features brought on by the cooperative effects between the two types of materials [29]. Notably, CNTs with a lot of chemically active surface area are excellent supports for QDs. An intermediary molecule, such as a polymer that has already been conjugated to either the CNT or the QD, is required for the indirect bonding [30–32].

6.2.4 CARBON-BASED NMTs

Carbon-based NMTs include graphene, carbon nanotube (CNT), carbon nanofiber (CNF), and fullerenes. Figure 6.2 shows the structural model of different carbon-based NMTs. Graphene is an intriguing substance with exceptional qualities like extraordinary transparency, ultra-high electrical and thermal conductivities, and extreme mechanical strength [33–35]. In graphene, carbon atoms are arranged in a honeycomb crystal lattice to form a one-atom-thick planar sheet [1, 36–38]. Unlike graphene, CNT is a cylindrical-shaped molecule with a single or complex roll(s) of graphene sheet(s). Fullerenes on the other hand are hollow cage-like structures. In some cases, graphene and CNTs are classified under the fullerene family [1]. The last example of carbon-based NMTs is CNF. Just like CNT, CNF is also cylindrical, however, the graphene layers in CNF are arranged as stacked plates (or cones). CNT is also referred to as CNF with graphene layers wrapped into perfect cylinders [39]. CNFs are less affected by van der Waals forces and tend to stay scattered for longer periods, in contrast to CNTs, which are affected by the forces and induce the nanotubes to form ropes or reassemble after being dispersed [39]. From the various sub-categories of NMTs, this chapter will focus on CNT production modeling and optimization.

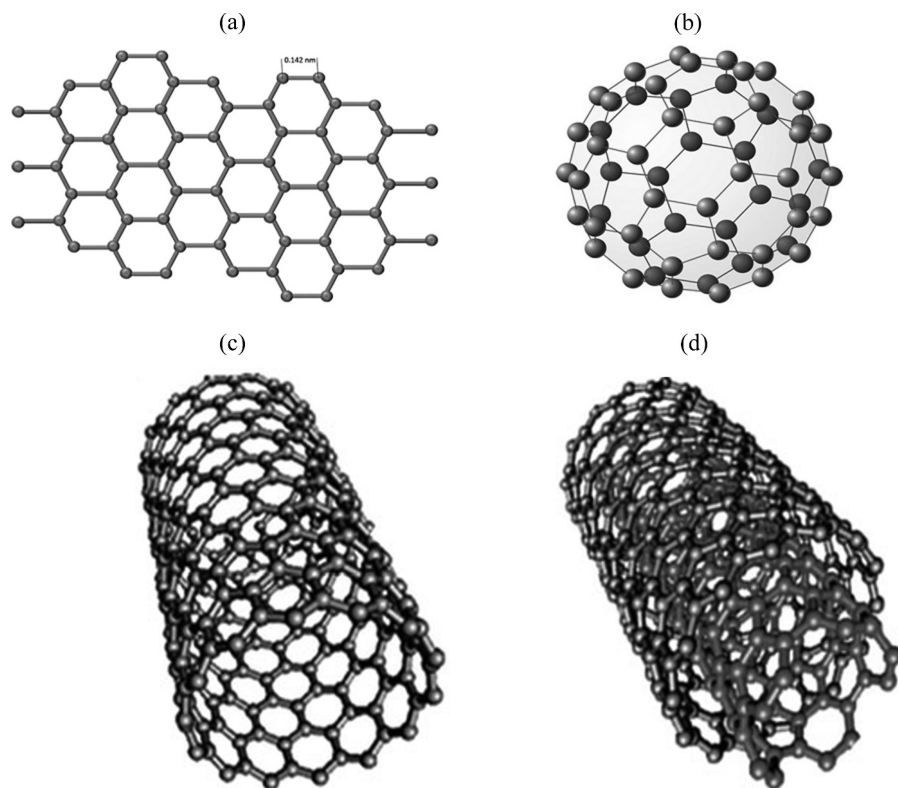


FIGURE 6.2 Schematic representation of carbon-based nanomaterials architecture. (a) Graphene [40] (b) Buckminsterfullerene (C_{60}) [41] (c) SWCNT [42] (d) MWCNT [42].

(a, c & d Reprinted with permission from [40, 42]).

6.3 CARBON NANOTUBES

Carbon nanotubes (CNTs) are hollow cylindrical tubes made up of carbon with nano-sized diameters within the 0.1–100 nm and long lengths above 100 μm [43, 44]. They have a high electrical conductivity and tensile strength that is more than 100 times greater than that of stainless steel, and they are physically and chemically stable [43]. Moreover, CNTs have a wide range of uses, including energy storage, biosensors, medical devices, conductive paints and coatings, semiconductor transistors for environmental applications, microelectronics, and composite plastic materials as electrically conductive fillers or to increase composite strength [43, 45–47]. In the earliest attempts to produce CNTs, high-temperature preparation techniques were used [11, 48, 49], like the arc discharge approach or the laser ablation technique. Currently, CNTs are being created utilizing a variety of processes, including CVD, flame synthesis, sonochemistry, ball milling, and others because of technological advancements in the field [11]. Arc discharge, laser ablation, electrolysis, and CVD are a few of the techniques (see Figure 6.3) that are frequently applied in industry. Further, CNTs can either be single-walled or multi-walled [11, 50]. Although single-walled

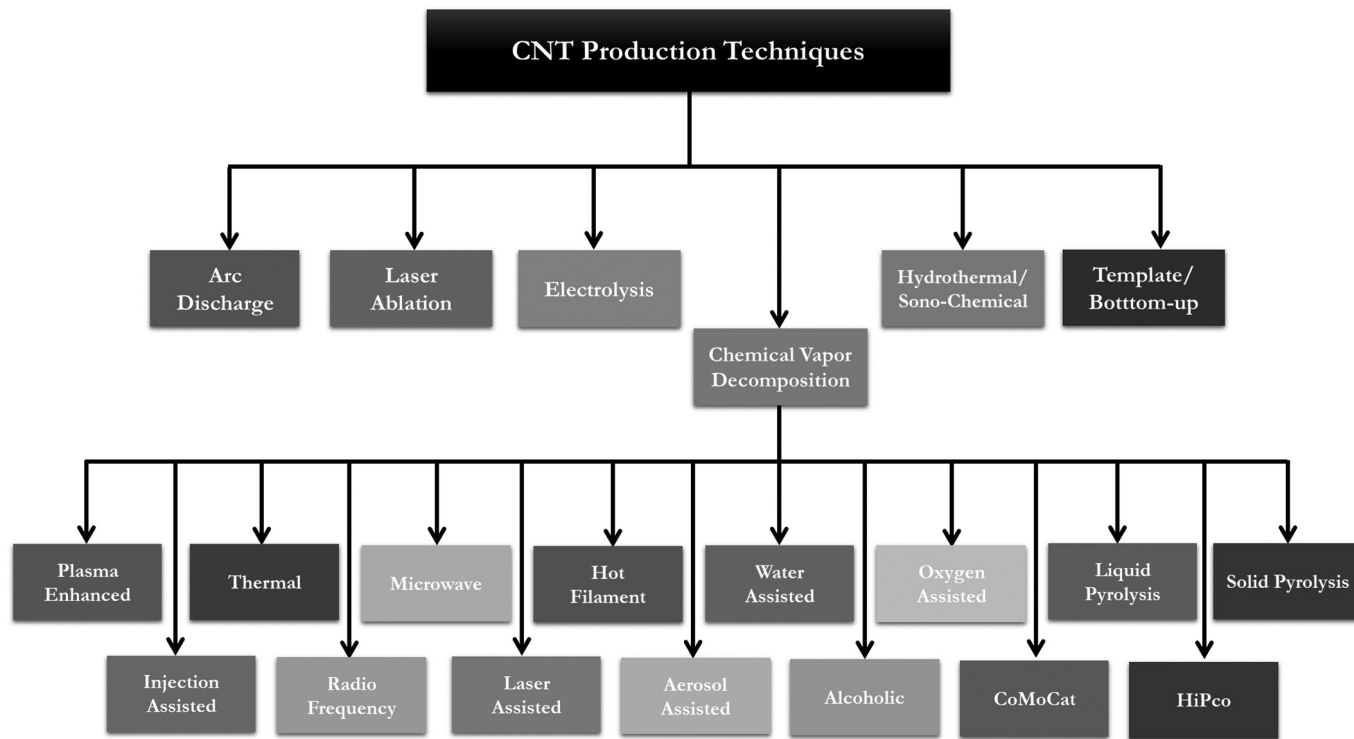


FIGURE 6.3 CNT production techniques
(Image recreated with permission from reference [75]).

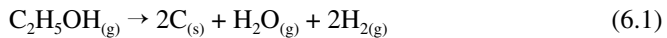
CNTs (SWCNTs) were initially found, multi-walled CNTs (MWCNTs) have not received as much attention [44]. This is due to the higher specific stiffness and strength of SWCNTs when compared to MWCNTs. However, MWCNTs provide better advantages such as having lower resistance, lower power consumption, higher mechanical strength, higher thermal stability, higher conductivity, etc. than SWCNTs [51, 52]. A range of different carbon sources for the production of CNTs has been investigated, including coal [53], plastic tar [54–56], tires [57–59], methane [60–62], carbon dioxide [62, 63], ethanol [49], and aromatic hydrocarbons including benzene, toluene, and xylene [43, 64–66] and several other sources [43, 67–70]. Carbon nanotubes are a significant kind of petrochemical raw material that is extensively employed in the separation, refinement, and processing of chemical industry products like petrochemical, gasoline, and natural gas [71–74].

6.3.1 CARBON NANOTUBE PRODUCTION MODELING

Modeling CNT production is a huge task for most researchers; however, some authors have managed to overcome this using different models which include the kinetic model and its derivatives, process models such as the fused deposition model, as well as machine learning models to predict critical CNT parameters. The sections below describe some of these models and how they have been applied in CNT modeling.

6.3.1.1 Modeling of Ethanol to CNT

Carbon nanotubes have been synthesized in different reactors, using different techniques and carbon precursors. In this case study, the authors employed a fluidized bed reactor using the chemical vapor deposition (CVD) of pure ethanol which serves as a carbon precursor. The experiment was carried out in the presence of a particulate catalyst made of iron and cobalt nanoparticles supported on alumina [49]. The furnace encircling the reactor was able to regulate the temperature within. As a result, the process can be thought of as being isothermal, and the fixed point chosen for the furnace can be considered the process temperature. The isothermal state of the reactor is crucial both for achieving high productivity and for preventing the development of amorphous carbon [49, 76]. The CNT synthesis overall reaction is given by Equation (6.1):



According to [49], the first-order reaction rate which corresponds to EtOH cracking is defined as:

$$r_{\text{EtOH}} = -k_{\text{EtOH}}(C_{\text{EtOH}})D_{\text{p}} \quad (6.2)$$

where r_{EtOH} , C_{EtOH} , and $-k_{\text{EtOH}}$ are ethanol reaction rate ($\text{mol}/\text{m}^3\text{s}$), concentration (mol/m^3), and reaction constant ($1/\text{s}$) respectively and D_{p} implies dense phase. $-k_{\text{EtOH}}$ according to Arrhenius's law is a function of temperature (T) and activation energy (E_{a}) as shown in Equation (6.3).

$$-k_{\text{EtOH}} = k_0 e^{-\frac{E_{\text{a}}}{RT}} \quad (6.3)$$

According to the established mechanism for CNT synthesis, the catalyst dissolves the carbon that has been broken down and deposited on the active sites (nano-particles of transition metals) [49]. Carbon precipitates out as CNTs when the point of carbon saturation is achieved. It is plausible to believe that carbon is deposited in the form of CNTs and that the creation of CNTs on the catalyst is the limiting stage since ethanol degradation occurs in the presence of catalytic nano-particles. Since CNTs are deposited on active sites, the catalyst activity (φ) – a term used to describe how many active sites are present on the catalyst – directly affects how many CNTs are formed. As a result, the intrinsic reaction additionally has to include catalyst activity. Hence, Equations (6.3) and (6.2) with φ become Equations (6.4) and (6.5):

$$-k_{\text{EtOH}} = k_0 \varphi e^{-\frac{E_a}{RT}} \quad (6.4)$$

$$r'_{\text{EtOH}} = -k_{\text{EtOH}} \varphi (C_{\text{EtOH}})_{D_p} \quad (6.5)$$

When the active site on the catalyst is covered by a single nanotube, φ becomes:

$$\varphi = \frac{\alpha_0 - \gamma}{\alpha_0} \quad (6.6)$$

where α_0 is the initial number of active sites and γ is the number of active sites covered with CNT. For fresh catalysts, since none of the active sites are filled with nanotubes, $\gamma = 0$, hence, $\varphi = 1$. In addition, the total CNT formed varies with time. As nanotubes formation progresses on the sites, $\varphi \rightarrow 0$ at the end of the reaction hence, $\gamma = \alpha_0$. Hence, Equation (6.6) can be written as:

$$\frac{d\varphi}{dt} = \left(-\frac{1}{\alpha_0} \right) \left(\frac{d\gamma}{dt} \right) \quad (6.7)$$

Equation (6.7) expresses the catalyst deactivation rate which depends on the carbon deposition rate, which also relates to the ethanol consumption rate. In order to determine the catalyst deactivation rate, α_0 must be known and this can only be done using reasonable approximations which correspond to the composition of the catalyst.

Modeling of CNT production in a fluidized bed reactor is divided into two phases: the bubble phase and the dense phase. While the bubble phase containing the gas phase is seen as plug flow, the dense phase comprising solid catalysts and a cloud of gas phase is regarded as a perfect mixing condition (as a pseudo-homogeneous phase). The gas reactant and gas product are both contained in the bubble phase's inlet and outflow, respectively. Since mass and heat transmission connects these two stages, the process model is dependent on both space and time. According to [49], the dense phase mass balance is given in Equation (6.8) as:

$$q_{D_p}(C_{EtOH})_F - q_{D_p}(C_{EtOH})_{D_p} + \int_0^H (K_{bd}) \delta A \left((C_{EtOH})_{B_p} \right) - \left((C_{EtOH})_{D_p} \right) dy - (1 - \delta) (1 - \varepsilon_d r'_{EtOH} AH) = 0 \quad (6.8)$$

where q_{D_p} is the volumetric flow rate (m^3/s) in the dense phase, K_{bd} is the overall mass transfer coefficient between the two-phase (1/s) δ is the fractional volume of bubbles, A is the reactor cross-sectional area (m^2), ε_d is the dense phase voidage, H is the height of the reactor (m).

The bubble phase mass balance is given in Equation (6.9) as:

$$q_{B_p} \left(\frac{d(C_{EtOH})_B}{dy} \right) = - (K_{bd}) \delta A \left((C_{EtOH})_{B_p} - (C_{EtOH})_{D_p} \right) \quad (6.9)$$

where q_{B_p} is the volumetric flow rate (m^3/s) in the bubble phase.

The molar rate of ethanol converted to carbon can be expressed in Equation (6.10) as:

$$n_{EtOH} = (1 - \delta) (1 - \varepsilon_d) r'_{EtOH} AH \quad (6.10)$$

The mole of carbon formed in the reaction is $n_C = n_{EtOH}$ as the stoichiometric of the reaction (Equation 6.1). Then, the rate for the number of carbon atoms formed can be expressed as in Equation (6.11):

$$Nu_{Catm} = n_C \times N_{Avo} = 2N_{Avo} (1 - \delta) (1 - \varepsilon_d) r'_{EtOH} AH \quad (6.11)$$

By using a software called “wrapping” (available at: www.photon.t.u-tokyo.ac.jp), one can estimate the number of carbon atoms present in each CNT. The mean value of the diameter of the CNT can also be estimated using electron microscopy observations [75]. Equation (6.5) predicts that the rate of CNT creation (Nu_{CNT}) will be as follows:

$$Nu_{CNT} = \frac{Nu_{Catm}}{N_{C-CNT}} = \left(\frac{d\gamma}{dt} \right) \quad (6.12)$$

Combining Equations 6.5, 6.7, 6.11, 6.12, the general equation can be expressed as Equation 6.13):

$$\frac{d\varphi}{dt} = \frac{2N_{Avo}}{N_{C-CNT}} \left(-\frac{1}{\alpha_0} \right) (1 - \delta) (1 - \varepsilon_d) AH k_0 \varphi e^{-\frac{E}{RT}} (C_{EtOH}) \quad (6.13)$$

6.3.1.2 Kinetic-based Derivative Models Employed in CNT Production Modeling

Various models have been employed in modeling CNT production process, some of these processes are presented in Table 6.1. From a survey of some research works

TABLE 6.1
Models Employed in CNT Production and Key Observations

SN	Model Name	Work	Model and Key CNT Reaction	Key Observation(s)	Ref.
1	Simple model based on weight	Effect of temperature on the kinetics of C ₂ H ₄ decomposition over reduced iron oxide catalyst for CNT production	$\text{CNT}_{\text{yield}} (\%) = \left[\frac{W_{\text{cat,CNT}} - (W_{\text{cat}0} - W_{\text{cat,loss}})}{(W_{\text{cat}0} - W_{\text{cat,loss}})} \right] \times 100$ where $W_{\text{cat,CNT}}$, $W_{\text{cat}0}$, $W_{\text{cat,loss}}$ are the weight (g) of the CNT and catalyst deposited, the initial weight of the catalyst, and the weight of the loss of catalyst at the operating condition respectively.	The result from the proposed model shows that the percentage yield of CNT produced is significantly influenced by the iron oxide crystal size and decomposition temperature.	[67]
2	Weight gain Model	Synthesis of carbon nanotubes from conventional biomass-based gasification gas	$\begin{aligned} \text{CH}_{4(\text{g})} &\rightarrow \text{C}_{\text{CNT}(\text{s})} + 2\text{H}_{2(\text{g})} \\ 2\text{CO}_{(\text{g})} &\rightarrow \text{C}_{\text{CNT}(\text{s})} + \text{CO}_{2(\text{g})} \\ \text{CO}_{(\text{g})} + \text{H}_{2(\text{g})} &\rightarrow \text{C}_{\text{CNT}(\text{s})} + \text{H}_2\text{O}_{(\text{g})} \\ \frac{C_{\text{dep}}}{C_{\text{cat}}} &= \frac{W_{\text{t}} - W_{\text{cat}}}{W_{\text{cat}}} \times 100 \end{aligned}$ where $\frac{C_{\text{dep}}}{C_{\text{cat}}}$ is the carbon weight gain per unit catalyst weight, W_{t} and W_{cat} are the total and initial weights (g) of the catalyst after the reactions.	This model followed the assumption that CNT was produced from two carbon sources (CH ₄ and CO). The authors observed that the CNT produced is a function of the initial and total weight of the catalyst.	[62]
3	Kinetic Model	Mechanism and kinetics of growth termination in controlled CVD growth of MWCNT arrays.	$\text{C}_2\text{H}_{4(\text{g})} \rightarrow 2\text{C}_{\text{CNT}(\text{s})} + 2\text{H}_{2(\text{g})}$ $v_{\text{gCNT}} \sim v e^{-\frac{E_a}{k_B T}} K P_{\text{H}_2}^2 \left(\frac{P_{\text{C}_2\text{H}_4}}{P_{\text{H}_2}^2 K} - 1 \right) = v e^{-\frac{E_a}{k_B T}} \left(\xi_{\text{C}_2\text{H}_4} P_0 - K \xi_{\text{H}_2}^2 P_0^2 \right)$ where v_{gCNT} – CNT growth rate, v – pre-exponential frequency factor, E_a – activation barrier, k_B – Boltzmann constant (J/K), T – Temperature (K), K is the equilibrium constant, ξ_i – volume fractions of gaseous specie, P_0, P_i are the total pressure and partial pressures of gaseous specie (bar).	In addition to describing the growth rate as a function of total process pressure, the model also incorporated the effects of partial pressures of C ₂ H ₄ and hydrogen on C ₂ H ₄ decomposition to CNT.	[68]

4	Kato and Wen Model combined with Kinetic Model	Kinetic modeling study of CNT synthesis by fluidized bed CVD	$\text{C}_2\text{H}_{4(\text{g})} \rightarrow 2\text{C}_{\text{CNT}(\text{s})} + 2\text{H}_{2(\text{g})}$ $\left(\frac{dX_{\text{CNT}}}{dt} \right) = 69.97 \times \left(\%_{\text{Fe}} \times m_{\text{cat}} \right)^{0.28} \times e^{-\frac{29000}{RT_K}} \times \left(y_{\text{C}_2\text{H}_4} \right)^{\frac{3}{4}}$ where $\left(\frac{dX_{\text{CNT}}}{dt} \right)$ – CNT formation rate, $\%_{\text{Fe}}$ – composition of Fe in the catalyst (wt.%), m_{cat} – mass of the catalyst (kg), R – gas constant (J/mol K), T_K – bed temperature (K), $y_{\text{C}_2\text{H}_4}$ – molar composition of C_2H_4 (mol%).	The influence of the primary operational parameters on the temporal evolutions of the species molar fractions, the weight of CNTs produced, and the bed properties were numerically investigated in MWCNT production. The proposed model was developed from experimental correlation.	[77]
5	Kinetic Model	A chemical kinetic model for CVD of CNT	$\text{C}_2\text{H}_{2(\text{g})} \rightarrow 2\text{C}_{(\text{g})} + \text{H}_{2(\text{g})}$ $2\text{C}_{(\text{g})} + 6\text{Fe}_{(\text{s})} \rightarrow 2\text{Fe}_3\text{C}_{(\text{l})}$ $2\text{Fe}_3\text{C}_{(\text{l})} \rightarrow 3\text{Fe}_{2(\text{s})} + 2\text{C}_{\text{CNT}(\text{s})}$ $n = \frac{N_A \times \rho}{C_{A0} (1 - X_A) \times M_c}$ where n – number of carbon atoms in the CNT produced, N_A – Avogadro number, ρ – density Fe_3C (g/m³), C_{A0} – initial composition of Fe_3C (mol/m³), X_A – molar conversion of C. M_c – molar mass of C (g).	The result obtained from the model shows deposition temperature and deposition pressure exhibit a decreasing trend with an increase in furnace temperature up to 1000 K. In addition, as the reaction time increases, the deposition temperature decreases.	[78]

(Continued)

TABLE 6.1 (Continued)
Models Employed in CNT Production and Key Observations

SN	Model Name	Work	Model and Key CNT Reaction	Key Observation(s)	Ref.
6	Kinetics model for CNT growth	Temperature and time dependence study of SWCNT growth by CVD	$\text{C}_2\text{H}_5\text{OH}_{(g)} + 2\text{S}_v \xrightarrow{k_1} 2\text{C.S}_{(s)} + \text{H}_2\text{O}_{(g)} + 2\text{H}_{2(g)}$ $\text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{C.S} \xrightarrow{k_2} \text{C}_{\text{SWCNT}}^{g+1} \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{S}_v$ $\text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{C.S} \xrightarrow{k_3} \text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^{d+1} \cdot \text{S} + \text{S}_v$ $\text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{C.S} \xrightarrow{k_4} \text{C}_{\text{SWCNT}}^{g-1} \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{H}_2 + \text{CO}$ $\text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^d \cdot \text{S} + \text{H}_2\text{O} \xrightarrow{k_4} \text{C}_{\text{SWCNT}}^g \cdot \text{C}_{\text{AMOR}}^{d-1} \cdot \text{S} + \text{H}_2 + \text{CO}$ $\frac{d[\text{C.S}]}{dt} = 2.k_1 [\text{C}_2\text{O}_5\text{OH}] [\text{S}_v]^2 - k_2 [\text{C.S}]^2 - k_3 [\text{C.S}] ([\text{C.S}] + [\text{C}_{\text{SWCNT}}] + [\text{C}_{\text{AMOR}}])$ where S_v, is the catalyst site, g and d, are the numbers of SWCNT and amorphous carbons present respectively.	This study discussed the existence of a temperature window and the best period for growth. The authors proposed that the conflict between the growth of SWCNT and that of amorphous carbon can be used to explain temperature and time dependence.	[79]
7	An improved model for CNT growth	Growth of CNTs in a floating catalyst reactor	$\text{C}_8\text{H}_{10(g)} \rightarrow 8\text{C}_{\text{CNT}(s)} + 5\text{H}_{2(g)}$ $G_{\text{CNT}} = \frac{\int_0^t 8CAU_r \left(\frac{D_{\text{in}}}{D_{\text{in}} + D_{\text{out}}} \right) dt}{\frac{\pi}{4} \frac{1}{M_c} n D_{\text{CNT}}^2 \rho_{\text{CNT}} A_s}$ where G_{CNT} is the CNT growth (m), C is the molar composition of CNT (mol/m³), A is the surface area of the reactor inlet, U_r is the velocity of feedstock in the reactor (m/s), D_{in} and D_{out} is the diameter of the substrate and reactor, M_c is the molar mass of C_{CNT} (g/mol), n is the number of nanotubes per unit surface area (1/m²), D_{CNT} is the diameter of the CNT, ρ_{CNT} is the CNT density (g/m³), and A_s is the substrate cross-sectional surface area.	The observation from the developed model shows that catalyst deactivation takes place kinetically when the formation rate of the graphene network is smaller than the carbon deposition rate by the decomposition of CH_4 .	[64]

8.	Modified Kinetic Model	Mathematical Modeling of CNT Formation in Fluidized Bed CVD	$\text{C}_2\text{H}_5\text{OH}_{(\text{g})} \rightarrow 2\text{C}_{(\text{s})} + \text{H}_2\text{O}_{(\text{g})} + 2\text{H}_{2(\text{g})}$ $\frac{d\varphi}{dt} = \frac{2N_{\text{Avo}}}{N_{\text{C-CNT}}} \left(-\frac{1}{\alpha_0} \right) (1 - \delta)(1 - \varepsilon_d) A H k_0 \varphi e^{-\frac{E}{RT}} (C_{\text{Eth}})$ where φ is the catalyst activity parameter, N_{Avo} is the Avogadro Number, $N_{\text{C-CNT}}$ Number of carbon atoms involved in CNT formation, α_0 is the initial number of active sites, δ is the fractional volume of bubbles, ε_d is the dense-phase voidage, A is the reactor cross sectional area (m^2), H is the height of the active part of the reactor (m), k_0 is the preexponential kinetic constant (1/s), E is the activation energy (kJ/mol), R is the gas constant (J/mol K), T is the temperature (K), and C_{Eth} is the ethanol concentration (mol/m^3).	The result from the proposed model shows that catalyst loading, reaction time, and temperature have a significant impact on how quickly the reaction proceeds and, consequently, how much ethanol is present in the exit flow. The mass of CNTs that develop on the catalyst is also influenced by these variables.	[49]
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[49, 62, 64, 67, 68, 77–79], the kinetic model (and its derivatives) is the most widely employed in CNT production modeling. Table 6.1 also presents the key carbon source, the key reaction(s), as well as key observations from the models that have been employed in CNT production process.

6.3.1.3 Machine Learning Models Employed in CNT Production Modeling

With the use of experience and automation, a system can learn and develop through the use of machine learning, an application of artificial intelligence [80–82]. By developing algorithms that can take inputs and use statistical analysis to predict outputs, such systems may reliably anticipate the outputs [83, 84]. Additionally, upon obtaining fresh data, the outputs are updated automatically. Artificial Neural Networks (ANN), Gaussian Process Regression (GPR), Decision Tree Regression (DTR), Prey Predator Algorithm, Linear Regression (LR), Support Vector Machine Regression (SVMR), Density Functional Theory (DFT), and K-nearest neighbors regression (KNNR) are just a few of the machine learning algorithms that have attracted a lot of attention for their ability to predict CNT properties [85–90]. A summary of some of these models is presented in Table 6.2.

TABLE 6.2

Summary of Some Machine Learning Models Employed in Modeling CNT Production

SN	Work	Key Observation(s)	Ref
1	Machine learning methods for MWCNT genotoxicity prediction	In order to accurately forecast the genotoxicity of various types of MWCNTs, the authors constructed a predictive nano-informatics model that is thoroughly validated and based on statistical and machine learning methodologies. A variety of computational workflows which combined unsupervised (Principal Component Analysis, PCA) and supervised classification methods (Support Vector Machine, “SVM,” Random Forest, “RF,” Logistic Regression, “LR,” and Nave Bayes, “NB”) with Bayesian optimization were all employed. The most crucial variables were chosen using the Recursive Feature Elimination (RFE) approach. From their results, RF was the most accurate model for predicting the genotoxicity of MWCNTs with 80% external validation accuracy and also has a high classification probability. The authors concluded that the length, zeta average, and purity were observed to be the most informative MWCNT features in the process.	[86]

(Continued)

TABLE 6.1 (Continued)
Summary of Some Machine Learning Models Employed in Modeling CNT Production

SN	Work	Key Observation(s)	Ref
2	Machine Learning-Assisted High-Throughput Molecular Dynamics Simulation of High-Mechanical Performance CNT	The authors explored chemical detection using cross-sensitive CNT-based field-effect transistors (FET) sensor arrays made of SWCNTs coated with metal nanoparticles. Five purine compounds – adenine, guanine, xanthine, uric acid, and caffeine – were distinguished by integrating the investigation of FET device properties with supervised learning techniques. DFT computations were used to support the interactions between purine compounds and SWCNTs coated with metal nanoparticles. From the results obtained, the method successfully detects the presence of caffeine in 95% of the samples with 48 features using linear discriminant analysis (LDA), and in 93.4% of the samples with only 11 features using SVM approach. The authors concluded that the main advantage of the LDA model is the 95% prediction accuracy.	[91]
3	Development of artificial intelligence-based model for the prediction of Young's modulus of polymer/CNT composites	The authors employed an ANN model to predict the behavior of composites made of polymers and carbon nanotubes (CNTs). A parametric analysis was used to choose and refine the design of the ANN model. The obtained results demonstrated that the suggested model performs admirably during both the training and testing stages, with correlation coefficients of 0.978 and 0.986, respectively.	[87]
4.	Prediction of tensile strength of polymer CNT composites using practical machine learning method	The authors developed a machine learning-based model that can be used to predict the tensile strength of composites made of polymer and CNTs. A database with 11 input variables was constructed using literature data. The primary factors considered for predicting the tensile strength of nanocomposites include polymer matrix type, polymer matrix mechanical properties, CNT physical characteristics, and CNT mechanical properties amongst several others. Gaussian Process Regression (GPR) model was employed in the prediction process. The authors concluded that the GPR model performed well in both the training and testing phases (RMSE = 5.982 and 5.327 MPa, MAE = 3.447 and 3.539 MPa, respectively).	[88]
5.	CNT Growth Rate Regression using SVM and ANN Machines and Artificial Neural Net	The author employed an SVM classifier to train an SWNT dataset which comprise 121 experiments out of a total of 450 experiments. With an accuracy of 95.04%, the SVM classifier predicted parameter values for SWNT growth with 99% probability. In addition, the author also employed ANN to forecast SWNT growth rates and growth lengths. From the result obtained, a peak in growth rate as a function of water concentration and growth temperature was shown in the analysis of the ANN growth rate model. The growth length model demonstrated an 80% reduction in validation errors and was trained using the same growth experiments as the growth rate model. The author concluded that The SWNT length-maximizing water/ethylene ratio was likewise determined by the growth length model.	[89]

6.3.1.4 Other Models Employed in CNT Production Modeling

Besides the kinetic-based model and its derivatives, and the machine learning model, other models that have been employed in modeling CNT production include:

- **Fused Deposition Model (FDM):** The most important additive manufacturing approach is FDM, which describes the process of depositing successive layers of material in a computer-controlled environment to produce a 3D object such as CNT. The limited options of materials that are now accessible and the fact that parts created using FDM method are only employed as conceptual or demonstration parts rather than functional parts are the main drawbacks of employing FDM in industrial applications [14].
- **Coarse Grain Model (CGM):** To transfer atomistic systems onto systems with a coarser resolution, CGM techniques like Monte Carlo simulations are developed. Consequently, CGM modeling approaches can be used to simulate larger systems with longer time scales and less processing [92].
- **Molecular Dynamic Model (MDM):** MDM is one of the most effective modeling CNT techniques because it mimics nanoscale systems using the laws of physics governing particles and motion. The biggest drawback of MDM is that a variety of simulation approaches can be used to make models simpler without compromising the accuracy of the results [93].
- **Density Function Theory (DFT):** Based on quantum physics, DFT investigates the electrical structure of atomic-scale systems. The local density approximation (LDA), which solely takes into account the electronic density at each place in space, is one of the approximations that the DFT models frequently employ. Although DFT models simulate molecular structure and provide the stable state's geometric characteristics through energy minimization, these models have some drawbacks. It is demonstrated, for instance, that LDA is unable to faithfully recreate systems with van der Waals interactions and weak bonds [94].

6.3.1.5 Thermochemical Processes and Reactors Employed in CNT Production Modeling

Various thermochemical processes have been employed in CNT production, however, most of these techniques are employed to break down the main carbon source waste materials (such as plastics, coal, and tires) into the desired carbon source for CNT production. Thermal cracking, pyrolysis, and gasification are the common thermochemical processes that precede chemical vapor deposition (CVD) in CNT production [43, 54, 55, 58, 61, 62]. These processes have been employed both in single-stage [95–97] and double-stage [55, 59, 61, 74, 98, 99] CNT production in reactors which include: fluidized bed reactors [49, 62, 77], fixed bed reactors [54, 57, 59, 98, 100], amongst several others [43, 64, 95, 99]. Figure 6.4 shows a schematic setup of a double-stage (gasification) production process while Figure 6.5 shows a screw kiln pyrolysis-distillation-catalysis process setup.

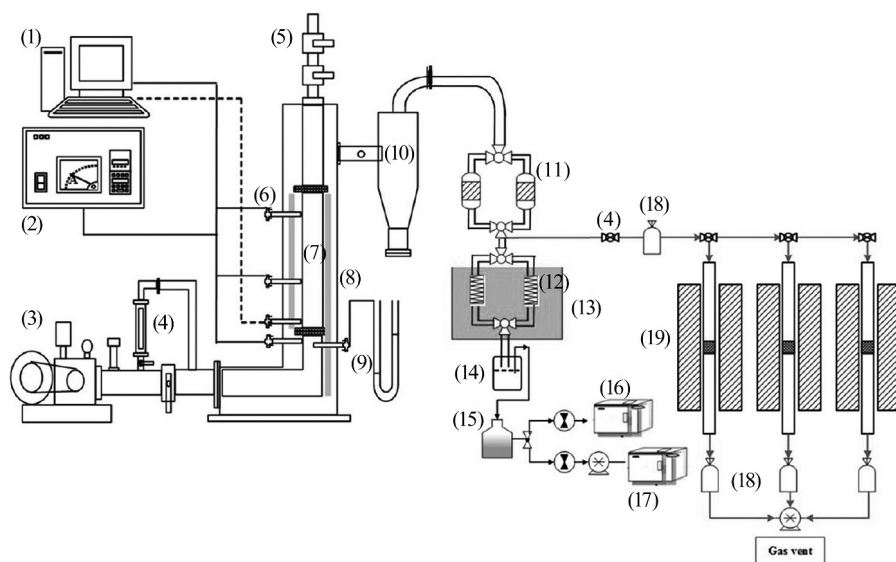


FIGURE 6.4 A schematic setup of CNT production from a fluidized bed gasification process. (1) computer, (2) TIC, (3) blower, (4) flow meter, (5) feeder, (6) thermocouple, (7) sand bed, (8) electric resistance, (9) U-manometer, (10) cyclone, (11) column filter, (12) trapping tube, (13) cooler, (14) gas-washing bottles, (15) backup absorber, (16) GC/TCD, (17) GC/FID, (18) sampling place, and (19) catalysis reactor.

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6.3.2 CARBON NANOTUBE PRODUCTION OPTIMIZATION

The process of choosing the best operating parameters for a process that will optimize the output of the target product and gasification efficiency while lowering overall costs is known as process parameter optimization [83]. The optimization of a full CNT production process in a single stage is quite complex, nonetheless, some authors have carried this out while others have employed a two-stage breakdown for optimum production as well as for coproduction of valuable byproducts. In order to optimize CNT production from solid wastes such as organic and inorganic wastes, several researchers [43, 55–60, 66, 100] have suggested a valuable coproduct such as hydrogen gas. Most of these studies have gone past the laboratory-scale experimentation with different types of catalysts to pilot scale to maximize the production process [70, 102]. Of all these studies, Yang *et al.* [100] optimized CNT production in both production stages (gasification and CVD) stages. In the first stage, waste plastics (a combination of polyethylene and polypropylene) as the carbon source decomposed to CNT and light hydrocarbons in the presence of Ni/Al-SBA-15 catalyst. Meanwhile, in the second stage, the hydrocarbon combines with another catalyst (Ni-Cu/CaO-SiO₂) to produce CNT along with hydrogen gas. The CNT fraction obtained in both cases was around 48 wt.% along with very

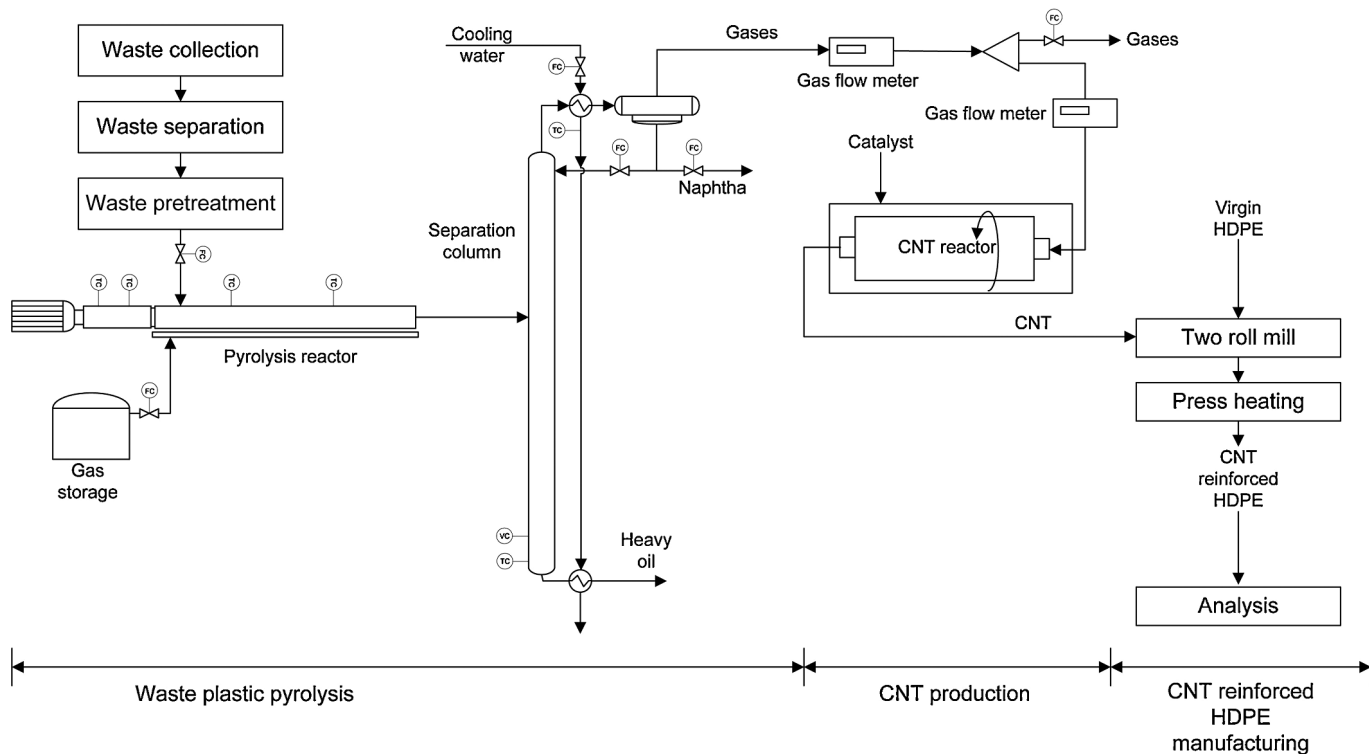


FIGURE 6.5 A setup for CNT production in a screw kiln pyrolysis-distillation-catalysis process.

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high hydrogen with 857.6 mmol/h-g catalyst when the production process was compared and validated with similar studies. The authors concluded that optimum operating conditions such as operating temperature and equivalence ratio all play a crucial role in the process.

Yahyazadeh *et al.* [103] employed Response Surface Methodology (RSM) [104] to optimize CNT growth. In the study, acetylene and Fe/CaCO₃ were used as the catalyst and hydrocarbon source respectively in the catalytic CVD method to create CNTs. The CVD reactor's ideal operating conditions for maximizing CNT production and purity were identified using the RSM approach. The authors employed RSM central composite design (CCD) to investigate the effects of the reaction time (30–60 min), temperature (700–800°C), and catalyst loading (10–30 wt.% Fe). From the result, the most notable influences on CNTs growth were determined to be the reaction temperature and reaction time. The highest CNT yields were obtained by using 10Fe/CaCO₃ at the minimum reaction temperature (700°C) and the shortest reaction time (both of which were 30 minutes). However, according to Raman spectroscopy data, the CNT quality is not at its best under these circumstances ($I_D/I_G = 0.816$). The authors further advised using a reaction temperature of 800°C to produce high-quality CNTs with a low I_D/I_G ratio, as this is related to the creation of graphitic carbon structure rather than amorphous carbon at high temperatures.

In addition, a number of optimization techniques, including Newton-Raphson [105], Gauss-Newton, numerical methods [106], and Lagrange multipliers are accessible for adoption in CNT production optimization. To determine the ideal process parameter combination, statistical optimization techniques such as Taguchi [107, 108], and Factorial [109–113], Design of Experiment (DOE) [114–117] could also be applied.

6.4 CONCLUSION

Nanomaterials (NMTs) have been around for centuries; however, years of intensive research has provided a better understanding of the mechanisms involved in modeling the production processes involved in their production. Extensive investigations are still needed on the production of aligned NMTs (mostly importantly, CNT) and the regulation of their growth. As a result, there is a vast body of theoretical or experimental research devoted to understanding the nucleation and growth of NMTs. The modeling and optimization of the NMT production process is an interdisciplinary field combining physics, chemistry, biology, material science as well as engineering. In order to design products that are directly applicable to the industrial sector and to stay informed about current demands and upcoming difficulties, industry and academia must work closely together to make NMT production successful. Choosing the right model that combines the NMT production with the necessary characteristics and constrained impurities as well as the approach's scalability is of the utmost importance. In the industrial sphere, the utilization of high-quality NMTs is rapidly expanding, making them the next generation's attractive resources with promising applications. Undoubtedly, in the upcoming years, the current gap between basic research on NMTs and their practical use will be closed.

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