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Carbon Nanotubes in Pharmaceutics: Structure, Functionalization, and the Path to Clinical Translation

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Abstract: *CNTs, including single-walled (SWCNTs) and multiwalled (MWCNTs), are a highly versatile class of nanomaterial because of their unique structural, mechanical, and physicochemical properties as well as for their wide range of feasible applications in pharmaceutical sciences. Their high aspect ratio, hollow tubular structure and π-conjugated surface can facilitate drugs loading and release processes as well as interactions with therapeutic molecules, in which the functionalization via covalent, non-covalent or hybrid modes could improve solubility, biocompatibility and targeting ability. CNTs have been widely studied as drug and gene/RNA delivery, imaging, theranostics (therapeutics-diagnostic) formulation and tissue- engineering material –illustrating enhancement in cellular uptake, decrease systemic toxicity, multi- functional therapeutic potentialities. several tremendous advancements, issues with kinetics, biodistribution, chronic toxicity, immunity and approval standardization continue to restrict translation into clinical trials. Precision pharmaceuticals may be made possible by new developments like bioelectronic scaffolds, stimulation-responsive systems, artificial intelligence-driven design, and hybrid CNT-based nanotechnology. The article outlines an approach for the safe and efficient integration of CNTs into next-generation medicinal product and healthcare devices by providing a thorough analysis of their structural features, functionalization techniques, medical uses, medicinal considerations, and translational challenges.*

Keywords: *SWCNTs*

I. INTRODUCTION

Some of the most revolutionary areas in the pharmacy field in the last decade is nanotechnology, which makes it possible to create sophisticated methods of delivery that increase the effectiveness of therapies and reduce side effects. Because of their distinctive combination of their structural, mechanical, and kinetic characteristics, carbon nanotubes (CNTs) have garnered a lot of interest from different nanostructured materials [1]. Several layers of graphene sheets are rolled into transparent tubes to create carbon nanotubes, which are cylindrical allotropes of carbon. CNTs are divided into nanotubes with single walls (SWCNTs) or multi-walled carbon nanotubes (MWCNTs) by determining the total number of layers [2]. They are great options for loading and transporting a variety of therapeutic compounds because of their exceptional surface area, large aspect ratio, and empty core [3]. In the pharmaceutical industry, CNTs' peculiar structure offers a number of benefits. Their tubular spaces are capable of holding drugs or substances for a regulated release, and their π-conjugated carbon structure enables beneficial relationships with volatile compounds through π–π stacking [4]. Additionally, CNTs' outstanding durability, electrical insulation, and chemical resistivity allow for a variety of uses that go beyond traditional drug delivery, such as biosensing, bioimaging, and photothermal treatment [5]. These characteristics make CNTs one of the most adaptable molecules for the medications products of the future [6]. Pristine CNTs have significant limitations in biological processes, despite these encouraging qualities. They have poor dispersibility and erratic relationships with biological elements due to their intrinsic hydrophobicity and propensity to gather in solutions of water [7].

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Furthermore, because of their significant aspect ratio and organ reactivity, unaltered CNTs might trigger cytotoxicity, oxidative stress, and inflammatory reactions [8]. In order to overcome such challenges, scientists have created a variety of functionality techniques that alter the outermost layer of carbon nanotubes (CNTs), increasing their solubility, biocompatibility, and specificity [9]. Two main groups may be employed to classify surface functionalization: Covalent and non-covalent alterations. Non-covalent enhancement, which permits the bonding of surfactants, polymers, or biomolecules despite modifying the fundamental electronic configuration of CNTs, depends on weak connections like van der Waals forces, negatively charged consequences, and π–π stacking [10]. Covalent functionalization, on the other hand, entails the creation of chemical bonds across CNT substrates while different functional groups, among them amine, hydroxyl, or carboxyl moieties, which are frequently added by amidation as well oxidative processes [11]. In addition to offering anchorages for additional conjugation of targeting ligands, polyethylene glycol (PEG), or medical payloads, covalent modifications can greatly improve aqueous dispersibility [12]. In addition to having better therapeutic performance, functionalized carbon nanotubes (f- CNTs) allow for controlled and site-specific drug release, which lowers systemic effects [13]..Over the past two decades, CNTs have been explored for a wide range of biomedical and pharmaceutical applications. In oncology, CNTs have been used to deliver anticancer agents such as doxorubicin and paclitaxel with enhanced intracellular uptake and reduced resistance [14]. Gene therapy approaches have utilized CNTs as carriers for DNA, siRNA, and CRISPR- Cas9 components, enabling efficient transfection and gene silencing [15]. Additionally, CNT- based scaffolds have demonstrated remarkable potential in regenerative medicine, facilitating tissue repair and neural regeneration through improved cell adhesion and electrical conductivity [16]. In theranostics, CNTs combine therapeutic and diagnostic capabilities, allowing simultaneous drug delivery, real-time imaging, and localized hyperthermia [17].Despite substantial progress, the clinical translation of CNT-based pharmaceutics remains limited. Key challenges include incomplete understanding of their long-term biocompatibility, biodistribution, clearance, and potential immunogenicity [18]. Regulatory hurdles related to large-scale synthesis, batch-to-batch consistency, and standardization of toxicity assessment further impede clinical approval [19]. Therefore, ongoing research must focus not only on optimizing the physicochemical design of CNTs but also on establishing standardized evaluation frameworks to ensure their safety and reproducibility in human applications [20].This review aims to provide an in-depth analysis of the current state of carbon nanotube research in pharmaceutics, emphasizing their structural characteristics, surface functionalization strategies, and translational potential. By highlighting both the advancements and the persisting challenges, this article seeks to outline a realistic pathway for CNTs to transition from experimental nanocarriers to clinically approved pharmaceutical tools.

II. STRUCTURAL CHARACTERISTICS OF CARBON NANOTUBES

2.1 Types of Carbon Nanotubes

Carbon nanotubes (CNTs) are cylindrical nanostructures composed of rolled-up graphene sheets, characterized by exceptional mechanical, electrical, and chemical properties that make them highly attractive in pharmaceutics and nanomedicine. Based on the number of concentric graphene layers, CNTs are generally classified into two main categories: single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) [21]. These two forms differ significantly in structure, dimensions, synthesis methods, and physicochemical characteristics, all of which influence their potential biomedical applications.

Single-Walled Carbon Nanotubes (SWCNTs)

SWCNTs consist of a single cylindrical graphene layer with a typical diameter ranging between 0.4 and 2 nanometers and lengths that can extend up to several micrometers [22]. Structurally, each SWCNT can be described by its chiral vector, defined by a pair of integers (n, m), which determines the rolling direction of the graphene sheet and thereby influences its electronic properties [23]. Depending on the (n, m) configuration, SWCNTs can exhibit metallic or semiconducting behavior, properties that are particularly valuable for biosensing and electrochemical drug delivery systems [24].The one-dimensional, hollow, and smooth surface of SWCNTs allows for a large specific surface area—

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up to 1300 m^2/g—making them excellent candidates for high-capacity drug loading [25]. Their tubular cavity can encapsulate therapeutic molecules, while their outer surface can be functionalized to enhance solubility and target specificity [26]. The relatively small diameter of SWCNTs facilitates their cellular uptake via endocytosis or passive diffusion, providing efficient intracellular drug delivery [27]. However, pristine SWCNTs are known for poor aqueous solubility and a tendency to aggregate due to van der Waals interactions, which can limit their dispersibility and biocompatibility [28]. Functionalization through covalent or non-covalent modification significantly mitigates these challenges by introducing hydrophilic groups or biomolecules, improving biological compatibility and reducing potential cytotoxicity [29].

Multi-Walled Carbon Nanotubes (MWCNTs)

MWCNTs are composed of multiple concentric graphene cylinders, typically 2 to 50 layers thick, separated by an interlayer spacing of approximately 0.34 nanometers [30]. Their outer diameter ranges from 2 to 100 nanometers, while their length can reach several micrometers, often exceeding that of SWCNTs [31]. Due to their multi-layered structure, MWCNTs exhibit enhanced mechanical strength and superior thermal and chemical stability compared to their single-walled counterparts [32]. These features make MWCNTs highly durable and suitable for long-term pharmaceutical and tissue engineering applications.However, the structural complexity of MWCNTs reduces their available surface area relative to SWCNTs, which may limit their maximum drug-loading capacity per unit mass [33]. On the other hand, their larger diameter and greater internal volume can accommodate higher quantities of bulky biomolecules such as proteins, nucleic acids, or polymer conjugates [34]. In drug delivery, MWCNTs often serve as robust scaffolds that can be modified with polymers, targeting ligands, or therapeutic agents to achieve controlled release and tissue-specific delivery [35].In terms of biological interactions, the increased rigidity and size of MWCNTs may influence their cellular uptake and biodistribution. Several studies suggest that smaller-diameter SWCNTs are more efficiently internalized by cells, whereas larger MWCNTs may remain at the extracellular matrix or be taken up by phagocytic cells [36]. Despite this, functionalized MWCNTs (f-MWCNTs) have shown improved hemocompatibility, reduced immunogenicity, and enhanced dispersion, making them viable for biomedical use when appropriately engineered [37].

Influence on Surface Area, Loading Capacity, and Biocompatibility

The structural differences between SWCNTs and MWCNTs have direct implications for their pharmaceutical performance. The high specific surface area of SWCNTs provides a larger interface for molecular adsorption, allowing stronger drug-carrier interactions and greater control over release kinetics [38]. Conversely, MWCNTs offer greater mechanical robustness and higher overall loading volume, which can be advantageous for encapsulating macromolecules or multi-drug combinations [39].Biocompatibility remains a critical determinant of CNT utility in pharmaceutics. Pristine CNTs, regardless of type, can elicit inflammatory responses, oxidative stress, or membrane damage due to their needle-like morphology and hydrophobicity [40]. Functionalization plays a decisive role in modulating these effects introducing carboxyl, hydroxyl, or polymeric coatings can substantially improve dispersion, reduce toxicity, and enhance biological compatibility [21]. Notably, studies indicate that SWCNTs, when properly functionalized, exhibit superior compatibility in biological environments due to their smaller diameter and higher flexibility, which facilitate cellular interactions and clearance [42].Overall, both SWCNTs and MWCNTs offer distinct advantages and limitations. The choice between them largely depends on the intended pharmaceutical application SWCNTs are preferred for precision drug delivery and imaging, while MWCNTs are favored for high-capacity, durable, and multifunctional systems. Understanding their structural and dimensional parameters is therefore essential to optimize design, functionality, and safety for clinical translation.

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2.2 Physicochemical Properties

The physicochemical properties of carbon nanotubes (CNTs) largely determine their behavior, performance, and compatibility in pharmaceutical and biomedical systems. These properties arise from their unique atomic arrangement, surface chemistry, and one-dimensional nanostructure.

Surface Chemistry and π-Conjugation

CNTs consist of sp^2-hybridized carbon atoms arranged in a honeycomb lattice, forming a seamless cylindrical structure [43]. This arrangement gives rise to an extended π-conjugated system that contributes to exceptional electrical conductivity, mechanical strength, and chemical stability [44]. The delocalized π-electrons enable strong π–π interactions with aromatic molecules, a feature highly advantageous for adsorbing hydrophobic drugs, biomolecules, or imaging agents [45]. Such interactions form the basis of non-covalent functionalization, which allows the attachment of drugs without disrupting the intrinsic electronic structure of CNTs [46].However, pristine CNTs are chemically inert and hydrophobic, leading to aggregation in aqueous environments and reduced biocompatibility [47]. Surface oxidation and functionalization are thus often employed to introduce polar groups such as –COOH, –OH, or $–NH_2$, which enhance solubility, dispersibility, and conjugation with therapeutic agents [48]. The degree of surface modification can modulate their zeta potential, hydrophilicity, and binding efficiency—critical parameters influencing biodistribution and cellular uptake in pharmaceutical systems [48].

Mechanical Strength, Flexibility, and Thermal Stability

CNTs exhibit extraordinary mechanical strength, with a tensile strength approaching 100 times that of steel and a Young's modulus of approximately 1 TPa [50]. These properties stem from strong covalent carbon–carbon bonds within the graphene layers. Despite this strength, CNTs remain highly flexible, capable of bending without fracture due to their hollow tubular geometry [51]. This combination of rigidity and flexibility has led to their incorporation into composite drug delivery systems, tissue scaffolds, and biosensors, where mechanical stability and resilience are required [52].

Additionally, CNTs display remarkable thermal stability, maintaining structural integrity up to 600–700 °C in air and over 2000 °C in inert atmospheres [53]. This feature is particularly beneficial in sterilization processes or thermal therapies such as photothermal drug release and hyperthermia applications [54]. However, the high aspect ratio and fibrous morphology of CNTs can sometimes induce mechanical irritation or inflammation in biological tissues if not properly functionalized [55].

Electrical Conductivity and Its Role in Biosensing Applications

The π-conjugated structure of CNTs imparts excellent electrical conductivity, which varies according to their chirality and number of walls [56]. Metallic CNTs can conduct electricity more efficiently than copper, while semiconducting CNTs display tunable electronic properties suitable for sensor design [57]. This conductivity has been extensively harnessed in biosensing platforms, where CNTs act as transducers that convert biochemical signals into measurable electrical outputs [58]. Functionalized CNT electrodes can immobilize enzymes, antibodies, or DNA probes, enabling the detection of glucose, cancer biomarkers, or drug metabolites with high sensitivity and specificity [59].In pharmaceutical analysis, CNT-based biosensors facilitate real-time monitoring of therapeutic compounds and metabolic responses, improving precision in drug dosing and diagnostic applications [60]. Moreover, their ability to mediate electron transfer enhances electrochemical reactions, making them integral to nanobioelectronics and electrochemical drug delivery systems [61].

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2.3 Synthesis and Purification Methods

Arc Discharge, Laser Ablation, and Chemical Vapor Deposition (CVD)

CNTs are primarily synthesized through three major techniques: arc discharge, laser ablation, and chemical vapor deposition (CVD). The arc discharge method involves vaporizing graphite electrodes under an inert atmosphere at high temperatures (~4000 °C), producing CNTs with excellent crystallinity but often with metal impurities [62]. The laser ablation technique similarly employs high-power laser pulses to vaporize a carbon target, yielding high-quality CNTs with controlled diameters, though scalability remains a limitation [63].CVD is the most widely used synthesis route for large-scale and cost-effective production. It involves decomposing hydrocarbon gases (e.g., methane, acetylene) over metal catalysts such as Fe, Co, or Ni at moderate temperatures (600–1200 °C) [64]. This method allows precise control over CNT dimensions, alignment, and yield, making it particularly suited for biomedical applications where uniformity and purity are critical [65].

Purification Challenges

Post-synthesis, CNTs often contain metallic catalyst residues, amorphous carbon, and structural defects that must be removed to ensure safety and performance in pharmaceutical use [66]. Common purification strategies include acid washing, oxidation, and ultracentrifugation. However, aggressive treatments can damage CNT walls, create defects, and alter their physicochemical properties [67]. Defect correction through annealing or controlled oxidation is often required to restore stability and enhance biocompatibility [68].

Impact of Synthesis Route on Biocompatibility and Performance

The synthesis technique profoundly influences the purity, morphology, and surface chemistry of CNTs, which in turn determine their biological interactions [69]. CVD-grown CNTs, due to lower defect densities and controllable surface properties, are generally preferred for pharmaceutical applications [70]. Residual metal catalysts, particularly transition metals, can catalyze the formation of reactive oxygen species (ROS), leading to oxidative stress and cytotoxicity [71]. Hence, high-purity CNTs with minimal defects and well-defined surface chemistry are essential for safe and effective clinical translation [72].

III. FUNCTIONALIZATION STRATEGIES

The translation of carbon nanotubes (CNTs) from materials science to pharmaceutics has been driven largely by the development of effective functionalization strategies that modulate their surface chemistry, dispersibility, and biological performance. Pristine CNTs are inherently hydrophobic and prone to aggregation due to strong van der Waals interactions between tubes, which limit their solubility and compatibility in aqueous and biological systems [73]. Functionalization through either non-covalent or covalent modification—addresses these limitations by introducing functional groups, biomolecules, or polymers that improve their physicochemical and pharmacological behavior without compromising their intrinsic properties [74].

3.1 Non-Covalent Functionalization

Non-covalent functionalization involves the adsorption or wrapping of molecules onto CNT surfaces through weak intermolecular forces such as π–π stacking, hydrophobic interactions, or van der Waals forces [75]. This approach is particularly attractive in pharmaceutical applications because it preserves the π-conjugated electronic structure of CNTs, maintaining their intrinsic electrical conductivity and mechanical strength [76].

π–π Stacking and Hydrophobic Interactions

Aromatic molecules, such as pyrene derivatives, porphyrins, and certain drugs, can interact with CNT sidewalls via π–π stacking, leading to stable yet reversible adsorption [77]. For example, doxorubicin a widely used anthracycline anticancer drughas been effectively loaded onto CNTs through π–π interactions, achieving high loading efficiency and

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controlled release profiles [78]. Similarly, hydrophobic interactions between CNTs and lipid molecules have been exploited to form lipid–CNT composites that enhance solubility and facilitate biocompatible interfaces [79]. These systems have shown promise in drug delivery, where the drug–nanotube complex can traverse cell membranes efficiently due to the amphiphilic nature of the conjugate [80].

Surfactant and Polymer Wrapping

Surfactants, including sodium dodecyl sulfate (SDS), sodium cholate, and Pluronic F127, are widely used to disperse CNTs by adsorbing onto their surfaces and reducing inter-tube attractions [81]. Similarly, polymers such as polyethylene glycol (PEG), polyvinylpyrrolidone (PVP), and DNA strands can wrap around CNTs, enhancing dispersion and stability in physiological media [82]. In particular, PEG-wrapped CNTs (PEG–CNTs) demonstrate prolonged circulation times and reduced recognition by the reticuloendothelial system, minimizing immune clearance [83].

Preservation of Electrical and Mechanical Properties

A key advantage of non-covalent approaches is that they do not disrupt the sp^2-hybridized carbon network, thereby maintaining the superior electrical conductivity and tensile strength of CNTs [84]. This preservation is vital in applications such as electrochemical biosensing or electrically triggered drug release, where charge transport is essential for signal transduction or therapeutic activation [85]. However, non-covalent functionalization often results in weaker surface binding and potential desorption under physiological conditions, which can limit long- term stability [86]. To overcome this, researchers are exploring hybrid approaches that combine weak adsorption with secondary stabilization mechanisms such as polymer crosslinking or hydrophobic anchoring [87].

3.2 Covalent Functionalization

Covalent functionalization involves the chemical modification of CNT surfaces through the formation of covalent bonds between the carbon lattice and functional groups or molecules [88]. Although this approach can partially disrupt the π-conjugated system, leading to changes in electrical and mechanical properties, it offers superior stability, solubility, and versatility for drug conjugation and targeting [89].

Oxidation and Carboxylation: One of the most common methods for CNT functionalization is oxidative treatment using strong acids such as nitric or sulfuric acid, which introduce carboxyl (–COOH) and hydroxyl (–OH) groups at defect sites and open tube ends [90]. These hydrophilic groups improve aqueous dispersibility and serve as anchoring points for further conjugation reactions [91]. Carboxylated CNTs (COOH–CNTs) are particularly suitable for pharmaceutical use because they allow straightforward attachment of therapeutic agents via esterification, amidation, or carbodiimide-mediated coupling [92]. However, excessive oxidation may cause tube shortening or structural damage, necessitating controlled reaction conditions [93].

Amidation and PEGylation: Amidation reactions convert carboxyl groups on oxidized CNTs into amide linkages with amine-containing molecules, including drugs, peptides, or polymers [94]. This strategy enables the development of targeted drug carriers with enhanced specificity and reduced off-target effects. PEGylation—the conjugation of polyethylene glycol chains— further enhances solubility, steric stability, and circulation half-life [95]. PEGylated CNTs exhibit reduced opsonization and immunogenicity, enabling stealth behavior that prevents rapid clearance by macrophages [96]. For example, PEG–CNTs loaded with paclitaxel have demonstrated improved tumor accumulation and prolonged systemic retention in preclinical models [97].

Oxidation and Defect Functionalization: Beyond simple carboxylation, controlled oxidation can introduce epoxide, carbonyl, and lactone groups, expanding the reactive sites available for bioconjugation [98]. Functionalization at defect sites or open ends ensures minimal disruption to the sidewall π-system, preserving much of the CNT's electronic character [99]. This is particularly useful for applications in biosensing and theranostics, where maintaining conductivity is critical [100].

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Impact on Dispersibility and Immunogenicity: Covalently functionalized CNTs display significantly improved aqueous solubility and reduced aggregation, enhancing their compatibility with biological systems [101]. Moreover, surface modification can modulate immune recognition, minimizing inflammatory responses [102]. Studies have shown that oxidized and PEGylated CNTs induce minimal cytokine release and macrophage activation compared to pristine forms [103]. Nonetheless, over-functionalization may alter biodistribution or limit drug-loading capacity, necessitating a balance between chemical reactivity and performance [104].

3.3 Targeting and Smart Functionalization

Beyond improving solubility and safety, functionalization strategies increasingly focus on targeted and stimuli-responsive systems, enabling precision drug delivery and on-demand release in response to physiological cues [105].

Ligand Conjugation (Antibodies, Peptides, Aptamers

Targeted functionalization involves attaching biological ligands such as antibodies, peptides, or nucleic acid aptamers that selectively recognize overexpressed receptors on diseased cells [106]. For instance, folic acid (FA) and RGD peptides have been widely conjugated to CNTs for targeting folate receptors and integrins, respectively, enhancing selective uptake by tumor cells [107]. Similarly, antibody-functionalized CNTs (e.g., anti-HER2 or anti-EGFR) enable precise targeting of specific cancer types, improving therapeutic index while reducing systemic toxicity [108]. Aptamer-modified CNTs have also shown promise in gene delivery and biosensing applications, offering high specificity and reversible binding [109].Ligand conjugation not only improves targeting efficiency but also facilitates receptor-mediated endocytosis, promoting intracellular drug delivery [110]. However, maintaining ligand activity during conjugation is critical, as harsh chemical conditions or improper orientation can impair binding affinity [111]. To address this, click chemistry and EDC/NHS coupling methods are commonly used for mild and efficient attachment of biomolecules [112].

Stimuli-Responsive Systems (pH, Redox, Enzyme-Triggered Release

Smart CNT systems exploit endogenous or external stimuli to achieve controlled and localized drug release [113]. pH-responsive CNTs utilize acid-labile linkers that hydrolyze in the acidic tumor microenvironment or intracellular endosomes, releasing the drug selectively at the disease site [114]. Similarly, redox-sensitive CNTs employ disulfide or thioketal linkages that cleave in response to elevated intracellular glutathione levels, typical of cancerous cells [115].Enzyme-triggered release systems use peptide or ester linkers that are specifically cleaved by overexpressed enzymes such as matrix metalloproteinases (MMPs) or esterases in tumor tissues [116]. Such stimuli-responsive designs minimize premature drug leakage, improve pharmacokinetics, and reduce systemic side effects [117]. Moreover, coupling these systems with imaging agents or fluorophores creates multifunctional theranostic platforms for simultaneous diagnosis and therapy [118].

Hybrid Functionalization with Polymers and Biomolecules:

Hybrid functionalization combines both covalent and non-covalent strategies to achieve synergistic improvements in solubility, biocompatibility, and functionality [119]. For example, CNTs functionalized with both PEG chains and targeting ligands offer stealth behavior alongside receptor specificity [120]. Incorporating natural polymers like chitosan, hyaluronic acid, or gelatin further enhances biocompatibility and provides stimuli-responsive degradation [121].Recent advances in polymer-CNT hybrids have enabled the fabrication of responsive nanocomposites for controlled drug release, tissue regeneration, and biosensing [122].

IV. PHARMACEUTICAL AND BIOMEDICAL APPLICATIONS

Carbon nanotubes (CNTs) have emerged as one of the most versatile nanostructures for pharmaceutical and biomedical applications due to their unique combination of high aspect ratio, surface area, tunable functionalization, and electrical

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properties [123]. Their hollow cylindrical morphology allows efficient encapsulation or adsorption of therapeutic molecules, while functionalization enables site-specific delivery and improved biocompatibility [124]. Over the past two decades, CNT-based nanocarriers have been explored for drug delivery, gene and RNA therapeutics, diagnostic imaging, and regenerative medicine, offering multifunctional platforms that integrate diagnosis and therapy in a single construct [125].

4.1 Drug Delivery

The potential of CNTs as drug delivery vehicles stems from their capacity to transport a wide range of therapeutic agents—small molecules, peptides, proteins, and nucleic acids—across biological barriers with high efficiency [126]. Their needle-like structure facilitates penetration through cell membranes, while functionalized surfaces allow conjugation with drugs, targeting ligands, and polymers for controlled and selective delivery [127].

Small Molecules, Peptides, and Nucleic Acid Delivery:

CNTs can load hydrophobic or aromatic drugs through π–π stacking and hydrophobic interactions, while polar drugs can be attached covalently to functional groups on oxidized CNTs [128]. For example, anticancer drugs such as doxorubicin, paclitaxel, and cisplatin have been successfully conjugated to CNTs to enhance tumor targeting and reduce systemic toxicity [129]. Peptide and protein therapeutics benefit from CNT-mediated protection against enzymatic degradation, prolonging their bioavailability [130]. Moreover, CNTs can carry oligonucleotides, siRNA, or antisense molecules for gene silencing applications, offering a potential alternative to viral vectors [131].

Controlled Release Kinetics and Intracellular Targeting:

The surface chemistry and degree of functionalization determine the release kinetics of drugs from CNT carriers [132]. Non-covalent attachment allows for pH- or redox-responsive release, particularly in tumor environments characterized by acidic pH and high glutathione levels [133]. In contrast, covalently attached drugs enable slower, sustained release suitable for chronic therapies [134]. CNTs can also be designed to target specific subcellular compartments. For instance, nuclear localization signals (NLS) or mitochondrial-targeting sequences can be conjugated to CNTs for intracellular precision [135]. Such targeted delivery is crucial in oncology, where the localization of chemotherapeutics to the nucleus can enhance DNA-intercalating drug activity [136].

Examples of Anticancer, Anti-inflammatory, and Antiviral Applications:

Several studies have demonstrated CNT-based delivery of anticancer agents. Doxorubicin- loaded functionalized CNTs (DOX–fCNTs) show higher cytotoxicity against tumor cells than free DOX due to enhanced cellular uptake via endocytosis [137]. Similarly, paclitaxel-loaded PEG–CNTs exhibit improved solubility and reduced systemic toxicity in breast and lung cancer models [138]. CNTs have also been used for co-delivery of multiple drugs or drug–gene combinations, enabling synergistic therapeutic effects [139].In inflammatory diseases, CNTs have been employed to deliver anti-inflammatory agents such as dexamethasone and indomethacin directly to inflamed tissues, achieving controlled local release and reduced systemic exposure [140]. For antiviral applications, CNTs functionalized with antiviral peptides or siRNA have been used to inhibit replication of HIV and influenza viruses, demonstrating potent antiviral effects without significant cytotoxicity [141].Despite their therapeutic advantages, the pharmacokinetics and biodistribution of CNTs remain critical determinants of their safety. Surface modification with PEG or other hydrophilic polymers reduces accumulation in the reticuloendothelial system and prolongs circulation time [142]. However, ensuring complete biodegradation or safe excretion remains a research priority before clinical translation [143].

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4.2 Gene and RNA Therapeutics

CNTs represent an innovative platform for the delivery of nucleic acids and gene-editing systems, addressing major challenges such as poor cellular uptake, enzymatic degradation, and limited endosomal escape [144].

CNT-Based siRNA, mRNA, and CRISPR-Cas9 Delivery Systems

Functionalized CNTs have been developed to deliver small interfering RNA (siRNA), messenger RNA (mRNA), and CRISPR-Cas9 ribonucleoprotein (RNP) complexes [145]. For example, amine-functionalized single-walled CNTs (SWCNT–NH_2) efficiently complex with negatively charged siRNA molecules, facilitating their entry into target cells via endocytosis [146]. Once internalized, CNTs can release siRNA in the cytoplasm, triggering gene silencing of target oncogenes or inflammatory mediators [147]. PEGylated CNTs have also been employed for systemic siRNA delivery in cancer models, demonstrating significant knockdown efficiency with minimal immune activation [148].CNTs have further been used for mRNA delivery, particularly for vaccine and protein expression applications. The π-conjugated structure of CNTs enables electrostatic adsorption of mRNA while protecting it from nuclease degradation [149]. In CRISPR-Cas9 systems, CNTs can act as nanocarriers for delivering Cas9–gRNA complexes, enabling precise genome editing with improved delivery efficiency compared to lipid nanoparticles [150]. These CNT-based systems hold potential for ex vivo gene editing, such as hematopoietic stem cell modification, and for in vivo correction of genetic diseases [151].

Mechanisms of Cellular Uptake and Endosomal Escape

CNT-mediated nucleic acid delivery occurs primarily through endocytosis or direct membrane penetration due to their nanoneedle-like morphology [152]. Once internalized, endosomal escape is a major barrier to effective gene delivery. Functionalization with cationic polymers such as polyethyleneimine (PEI) facilitates proton sponge effects, disrupting endosomal membranes and releasing the nucleic acid payload into the cytoplasm [153]. Alternative strategies employ pH-sensitive linkers or fusogenic peptides that respond to acidic endosomal conditions, enhancing cytosolic delivery [154].Studies have also shown that CNTs can traverse the nuclear membrane under certain conditions, enabling nuclear gene delivery without the need for viral vectors [155]. This unique capability, combined with low immunogenicity and high cellular uptake, positions CNTs as promising non-viral vectors for next-generation gene and RNA therapeutics [156].

4.3. Imaging and Theranostics

One of the most exciting frontiers in CNT research is their integration into imaging and theranostic applications, where diagnostic and therapeutic functions coexist within a single platform [157]. CNTs possess intrinsic optical and electronic properties that make them suitable for multimodal imaging, including near-infrared (NIR), magnetic resonance imaging (MRI), and photoacoustic imaging [158].

CNTs as Contrast Agents (MRI, Photoacoustic, NIR Imaging)

Functionalized CNTs have demonstrated strong optical absorption in the NIR region (700– 1100 nm), allowing for deep tissue imaging and photothermal therapy [159]. When irradiated with NIR light, CNTs convert light energy into heat, inducing localized hyperthermia that can selectively kill cancer cells [160]. This photothermal property forms the basis of CNT-mediated photothermal therapy (PTT), often combined with chemotherapeutics for synergistic effects [161].CNTs can also serve as MRI contrast agents by incorporating or chelating paramagnetic ions such as Gd^{3+} or Fe^{3+} on their surfaces [162]. Gadolinium-functionalized CNTs (Gd–CNTs) have been shown to enhance MRI contrast while reducing toxicity compared to free Gd- chelates [163]. Similarly, CNTs labeled with iron oxide nanoparticles exhibit strong T_2 contrast and can be tracked in vivo for monitoring biodistribution and tumor accumulation [164].Photoacoustic imaging combines optical excitation with ultrasound detection, and CNTs—owing to their high

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photothermal conversion efficiency serve as excellent photoacoustic contrast agents [165]. Their optical tunability allows multiplexed imaging of various tissues or molecular targets [166].

Combined Diagnostic and Therapeutic (Theranostic) Platforms

The convergence of imaging and therapy in CNT-based systems has led to the development of theranostic nanocarriers, which enable real-time monitoring of drug distribution and therapeutic response [167]. For instance, CNTs co-loaded with doxorubicin and NIR dyes enable simultaneous tumor imaging and chemotherapy under a single platform [168]. In another example, CNTs functionalized with gold nanoparticles and PEG chains have been used for combined photothermal ablation and fluorescence imaging [169].Theranostic CNTs also allow clinicians to visualize drug release kinetics and predict therapeutic outcomes, enhancing personalized medicine [170]. The integration of imaging modalities with stimuli-responsive release mechanisms such as NIR-triggered or redox-controlled systems further improves spatial and temporal control over treatment [171]. However, the translation of CNT-based imaging agents to clinical practice requires rigorous safety evaluation, particularly regarding long-term retention and potential metal toxicity [172].

4.4 Tissue Engineering and Regenerative Medicine

CNTs have shown remarkable potential as scaffolding materials in tissue engineering due to their high mechanical strength, electrical conductivity, and ability to promote cell adhesion and proliferation [173]. Their incorporation into polymeric or hydrogel matrices creates hybrid scaffolds that mimic the extracellular matrix (ECM) while providing electrical and mechanical cues essential for tissue regeneration [174].

CNT Scaffolds for Neural, Cardiac, and Bone Regeneration

In neural tissue engineering, CNT–polymer composites have been shown to enhance neuronal growth, axonal alignment, and synaptic activity [175]. Conductive CNT scaffolds facilitate electrical signal transmission, making them suitable for neural repair or neuroprosthetic interfaces [176]. For cardiac regeneration, CNT-containing hydrogels improve the electrical coupling of cardiomyocytes, supporting synchronous beating and tissue maturation [177]. These materials are being explored for cardiac patch fabrication to restore damaged myocardium following infarction [178].In bone regeneration, CNT-reinforced scaffolds exhibit superior mechanical strength and osteoinductive properties compared to conventional polymers [179]. Functionalization with calcium phosphate or bioactive peptides promotes osteoblast adhesion and mineralization [180]. Studies have demonstrated accelerated bone healing and improved mechanical integration in CNT-based bone grafts and orthopedic implants [181].

Electrical Stimulation and Cell Adhesion Enhancement:

The electrical conductivity of CNT scaffolds enables the application of electrical stimulation, which has been shown to modulate cell proliferation, differentiation, and alignment [182]. For example, electrical stimulation through CNT–gelatin scaffolds enhances neurite outgrowth and neural network formation in vitro [183]. Similarly, electrically active CNT–collagen composites support cardiomyocyte contractility and synchronization, critical for cardiac tissue regeneration [184].CNTs also improve cell adhesion by providing nanoscale topography that mimics native ECM features [185]. Functionalization with bioactive molecules such as laminin, fibronectin, or RGD peptides further enhances cell attachment and signaling [186]. In addition to neural and cardiac applications, CNT-based scaffolds are being investigated for skin, vascular, and skeletal muscle regeneration, leveraging their tunable elasticity and conductivity [187].While CNT scaffolds offer distinct advantages, their long-term biocompatibility and degradation behavior remain under scrutiny [188]. Embedding CNTs within biodegradable matrices such as chitosan, polylactic acid (PLA), or gelatin can mitigate potential cytotoxicity while retaining functionality [189]. Future research aims to integrate CNTs with growth factors, stem cells, and smart polymers to develop next-generation bioelectronic scaffolds that support both tissue regeneration and real-time monitoring [190].

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V. PHARMACOKINETICS, BIODISTRIBUTION, AND TOXICOLOGY

5.1 Absorption, Distribution, Metabolism, and Excretion (ADME)

The in vivo behavior of CNTs absorption, distribution, metabolism, and excretion (ADME) has emerged as a critical determinant for their biomedical viability. After systemic administration (e.g., intravenous injection), functionalization and dispersion status strongly influence circulation half-life, organ distribution, and clearance routes [191]. Early reviews noted that surface chemistry, particularly hydrophilic functionalization such as PEGylation, significantly improves biocompatibility and facilitates favorable pharmacokinetics compared to pristine CNTs [191, 192].Routes of administration studied include intravenous (IV), intratracheal (pulmonary), and in some cases oral or peritoneal exposure. In IV administration, properly functionalized CNTs avoid immediate aggregation and can circulate, allowing potential delivery to target tissues [191]. For example, PEG-functionalized CNTs have shown extended blood circulation and reduced rapid sequestration by the reticuloendothelial system (RES) compared to nonfunctionalized CNTs [193]. However, circulation is often transient: many studies report clearance from blood within minutes to hours post-injection, with rapid uptake by liver, spleen, kidneys, and to some extent lungs [194, 195].Organ accumulation studies reveal common deposition sites. A comprehensive review of biodistribution experiments reported that following pulmonary exposure, CNTs often remain in lungs for months or even years if not cleared; a portion may migrate via the mucociliary escalator to the gastrointestinal (GI) tract, though uptake from GI appears minimal for most CNT types [196]. Upon IV injection, major organs of accumulation tend to be the liver and spleen, with lesser amounts in kidneys, lung, and bone marrow; renal excretion has been observed particularly for some small, well-functionalized single-walled CNTs (SWCNTs) [196]. A more recent in vivo study demonstrated that SWCNTs of different diameters injected in mice show diameter- dependent biodistribution: larger-diameter SWCNTs (1–5 nm) preferentially localize in liver and spleen, while smaller-diameter SWCNTs (0.7–0.9 nm) accumulate more in the lungs. Importantly, pulmonary CNTs were nearly cleared within 60 days in that study [197].Clearance pathways depend on CNT physicochemical properties. Functionalized CNTs (e.g., PEGylated or other hydrophilic coatings) often show improved excretion via hepatic (biliary) and renal routes, likely due to enhanced dispersibility and smaller hydrodynamic size preventing rapid RES sequestration [191, 198]. However, pristine or poorly dispersed CNTs tend to agglomerate and deposit in organs without significant clearance, raising concerns about long-term biopersistence [196, 199].Metabolism of the carbon skeleton itself appears minimal; several studies using transmission electron microscopy (TEM) have observed intact CNT structures in tissue for months post-exposure, indicating that the sp^2 carbon backbone resists in vivo degradation under physiological conditions [191, 192]. Nonetheless, biodegradation has been reported under certain circumstances: macrophage-mediated degradation, oxidative mechanisms, or enzymatic cleavage may gradually shorten CNTs or introduce functional groups, particularly when CNTs are localized in phagolysosomes [200]. The efficiency of biodegradation depends on CNT type (SWCNT vs MWCNT), functionalization, and aggregation state [200].Overall, ADME behavior of CNTs is highly variable and context- dependent. Functionalization, dispersion, size (diameter, length), and dose are key modulators of biodistribution and clearance. For clinical translation, standardized protocols for CNT characterization and in vivo tracking are essential to reliably assess ADME and long-term fate.

5.2 Toxicological Considerations

Toxicity of CNTs remains a critical barrier to clinical use. Both in vitro and in vivo studies have revealed a spectrum of adverse effects but results are often inconsistent due to variation in CNT type, purity, functionalization, aggregation, dose, and exposure route [201]. A recent systematic review of in vitro studies (nearly 200 publications) found wide variability: on a substrate (e.g., CNT-coated surface), ~90% of studies reported negligible cytotoxicity, whereas in dispersion form toxicity emerged at average doses around 4–5 $\mu g\ mL^{-1} \cdot h^{-1}$ [202]. This suggests that mode of presentation (substrate vs suspension) drastically alters cell responses.At the cellular level, proposed mechanisms of CNT-induced toxicity include generation of reactive oxygen species (ROS), oxidative stress, membrane disruption, interruption of electron transport, and leaching of residual metal catalyst impurities [201]. Pristine, poorly purified CNTs or aggregated forms tend to exhibit higher cytotoxicity, more pronounced oxidative stress, and proinflammatory

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effects [201, 203]. Metal impurities (e.g., Fe, Ni, Co) from synthesis catalysts may catalyze ROS formation, aggravating toxicity [191].Functionalization generally reduces cytotoxicity. Hydrophilic modifications, especially PEGylation, decrease CNT aggregation, enhance dispersion, minimize protein adsorption, and lower recognition by immune cells collectively mitigating cytotoxic, genotoxic, and inflammatory responses [191, 192, 198]. For instance, PEG–SWCNTs administered intravenously in mice exhibited minimal signs of organ damage, inflammation, or altered biochemical markers up to 60 days post- injection, as opposed to unpurified, non-functionalized CNTs which induced lung damage, hepatotoxicity, renal failure, and even possible cardiovascular effects [204].Nevertheless, in vitro to in vivo translation is challenging. Many in vitro toxicity assays (e.g., MTT) show artefacts due to CNT–dye interactions or adsorption interference, leading to false positives or negatives [191]. In vivo outcomes depend heavily on dose, CNT dispersion status, functionalization, and exposure route. For example, inhalation or intratracheal instillation studies report persistent CNT in lungs for months, with chronic inflammation, granuloma formation, or fibrosis particularly when CNTs are long, rigid, or aggregated, reminiscent of fibre-like materials such as asbestos [196, 205]. By contrast, properly dispersed and functionalized CNTs administered intravenously often show much lower toxicity, though long-term studies are still limited.Importantly, length and aspect ratio influence toxicity: longer, rigid CNTs are more likely to trigger frustrated phagocytosis by macrophages, leading to persistent inflammation, impaired clearance, and possible mesothelioma-like pathology; shorter or degraded CNTs pose less such risk [206]. Aggregation state and degree of functionalization affect clearance and immune recognition, influencing both acute and chronic toxicity [191].Thus, toxicity of CNTs is not an intrinsic inevitability but strongly context- dependent. Rigorous purification (to remove metal catalysts), proper functionalization (to improve dispersion and stealth), size/length control, and dose optimization are critical to minimize adverse biological responses.

5.3 Immunological Interactions

Upon systemic or pulmonary exposure, CNTs interact with the immune system — particularly macrophages and other phagocytic cells, but potentially also complement pathways, cytokine networks, and adaptive immunity. Macrophage-mediated clearance plays a central role in CNT elimination, especially from lungs, spleen, and liver [200, 207]. In pulmonary exposure, alveolar macrophages engulf CNTs; over time, CNTs may be degraded or fragmented, facilitating clearance — though persistence for months has been documented [200]. Length and rigidity of CNTs significantly influence phagocytosis: long, rigid CNTs are often incompletely internalized, triggering “frustrated phagocytosis,” generation of ROS, release of pro-inflammatory cytokines, and chronic inflammation [206, 205, 208].Complement activation and pro-inflammatory cytokine responses have been reported in some studies, especially with poorly dispersed or raw CNTs; these immune reactions may contribute to tissue damage, fibrosis, or immunotoxicity, particularly after repeated or high-dose exposure [209]. However, functionalization (e.g., PEG, hydrophilic polymer or biomolecule coating) markedly reduces immune recognition, complement activation, and cytokine release — improving immunocompatibility [191, 198, 210].In sum, immune interactions remain perhaps the most variable and complex aspect of CNT toxicology. Geographic and temporal heterogeneity (different tissues, exposure routes, species, functionalization status) complicates generalization; yet, data so far suggest that well-functionalized, appropriately sized/distributed CNTs have potential for minimized immunogenicity — a precondition for safe clinical translation.

VI. REGULATORY AND TRANSLATIONAL CHALLENGES

Despite promising preclinical data, significant hurdles remain before CNT-based therapeutics can be approved for human use. The current regulatory landscape is fragmented. Neither the U.S. Food and Drug Administration (FDA) nor the European Medicines Agency (EMA) has issued standard, nanotube-specific guidelines addressing manufacturing, characterization, safety testing, and long-term monitoring of CNT-based nanomedicines. Consequently, researchers must align with existing frameworks for nanomaterials, which may not fully capture the unique risks and behaviors of CNTs (e.g., biopersistence, fibre-like effects, long- term immunogenicity) [211].Manufacturing scalability and reproducibility pose additional challenges. Variability in CNT synthesis (arc discharge, CVD, laser ablation),

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purification, functionalization, and final formulation result in batches with heterogeneous length, diameter, defect density, and surface chemistry all of which profoundly influence biological behavior [191, 212]. Standardization of CNT production, thorough characterization (size distribution, purity, surface groups, metal residue), and reproducible functionalization protocols are essential but not yet universal [213]. This lack of standardization complicates safety assessment, inter-study comparisons, and regulatory evaluation.Safety testing standards for CNTs remain poorly defined. Traditional toxicology assays may be inadequate or misleading due to CNT-specific artifacts (e.g., adsorption of assay dyes, fluorescence/radiolabel interference). Long-term studies especially chronic exposure, biopersistence, mesothelioma risk, immunogenicity after repeated dosing are scarce [191, 214]. Ethical considerations arise: animal studies may not fully predict human responses; human exposure (especially inhalation) may pose occupational risks akin to fibres; public perception especially given historical concerns about asbestos — may hinder acceptance of CNT-based therapies even if safety data is favorable [215].Finally, regulatory approval requires demonstration of consistent manufacturing quality, batch-to-batch reproducibility, validated safety/surveillance protocols, environmental risk assessments, and clear benefit-risk balance. Given the nascent nature of CNT therapeutics, building such infrastructure will require coordinated efforts from scientists, regulatory agencies, industry, and public stakeholders.

VII. EMERGING TRENDS AND FUTURE DIRECTIONS

Given both the promise and obstacles of CNT-based pharmaceutics, several emerging directions seek to address limitations and pave the way for clinical translation.First, hybrid nanostructures combining CNTs with liposomes, polymers, or other nanocarriers are gaining interest. By embedding CNTs within lipid bilayers, polymer matrices, or hydrogel scaffolds, researchers aim to combine the advantages of CNTs (mechanical strength, high loading capacity, conductivity) with improved biocompatibility, controlled release, and safer clearance profiles [213, 216]. Such composites may reduce CNT exposure to immune cells, minimize aggregation, and facilitate targeted delivery.Second, data-driven and AI-driven design of CNT- based drug carriers is an emerging field. Computational modeling, machine learning, and predictive toxicology could help identify optimal CNT structural parameters (length, diameter, surface chemistry) and predict biological behavior, minimizing trial-and-error in preclinical development [217]. This “rational nanomedicine design” may accelerate translation while improving safety and efficacy.Third, there is growing interest in personalized and precision nanomedicine. Given the tunability of CNT functionalization, it may be feasible to tailor CNT- based carriers to individual patient’s molecular markers, disease state, or pharmacogenomics enabling targeted therapy, controlled release, and minimized off-target effects. Integration with biosensors and wearable devices could form closed-loop delivery systems, where CNTs act as both sensors and actuators [218].Fourth, bioelectronic and theranostic platforms combining CNTs with electronics, sensing, and drug delivery hold promise. CNT-based scaffolds or implants may deliver drugs, monitor physiological signals, and provide feedback paving the way toward “smart implants” or “electro-nanomedicine”. For regenerative medicine, integrating CNTs with stem cells, growth factors, and bioactive polymers could yield bio- electronic tissue scaffolds for neural, cardiac, or bone repair [219].However, to realize these visions, several preconditions must be met: rigorous long-term safety studies (chronic exposure, biodistribution, immunogenicity), standardized manufacturing and functionalization protocols, reproducible characterization methods, and regulatory frameworks tailored for CNTs. Moreover, public and environmental safety considerations regarding nanomaterial release, occupational exposure, disposal, and environmental fate must be addressed in parallel.

IX. CONCLUSION

Carbon nanotubes offer a uniquely versatile and powerful platform for pharmaceutics and biomedicine. Their high surface area, hollow core, tunable surface chemistry, and electrical/thermal properties enable drug delivery, gene and RNA therapeutics, imaging, theranostics, and tissue engineering potentially overcoming limitations of traditional carriers. Yet, their clinical translation remains challenged by pharmacokinetic variability, biodistribution uncertainties, potential toxicity, immunological risks, manufacturing heterogeneity, and regulatory gaps.Current evidence suggests

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that many of these limitations are not inherent to CNTs but arise from uncontrolled variables: poor purification, inadequate functionalization, aggregation, and inconsistent characterization. With carefully designed functionalization (e.g., PEGylation or other biocompatible coatings), size/length control, and rigorous safety evaluation, CNTs could achieve acceptable biocompatibility and clearance. Emerging hybrid nanostructures, AI-driven design, precision medicine approaches, and bioelectronic integration open promising avenues for future translation.To realize the full potential of CNTs in medicine, coordinated interdisciplinary efforts are needed uniting materials scientists, pharmacologists, toxicologists, regulatory agencies, and clinicians. Only with a foundation of standardized manufacturing, comprehensive safety data, and transparent regulatory frameworks can CNT-based nanomedicines transition from promising research tools to safe, effective therapies in the clinic.

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