Nanotubes in the human respiratory tract – Deposition modeling

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Abstract

Deposition of inhaled single-wall carbon nanotubes (SWCNT) and multi-wall carbon nanotubes (MWCNT) in the respiratory tract was theoretically investigated for various age groups (infants, children, adolescents, and adults). Additionally, possible effects of the inhalative flow rate on nanotube deposition were simulated for adult lungs. Theoretical computations were based on the aerodynamic diameter concept and the assumption of particles being randomly transported through a stochastic (close-to-realistic) lung structure. Deposition of nanotubes was calculated by application of well validated empirical deposition formulae, thereby considering Browian motion, inertial impaction, interception, and sedimentation as main deposition mechanisms acting on the particles. Results of the simulations clearly show that for a given inhalation scenario (sitting breathing) total, bronchial, and acinar nanotube deposition increase with subject's age, whereas extrathoracic deposition is characterized by a decrease from younger to older subjects. According to the data provided by the model, MWCNT, whose aerodynamic diameters exceed those of SWCNT by one order of magnitude, are deposited in specific respiratory compartments to a lower extent than SWCNT. A change of the physical state from sitting to heavy work results in a common decline of bronchial and extrathoracic deposition of nanotubes. Total deposition is slightly increased for SWCNT and moderately decreased for MWCNT, whereas acinar deposition is significantly increased for SWCNT and decreased for MWCNT. Based on the results of this contribution it may be concluded that SWCNT bear a higher potential as health

Nanoröhrchen im menschlichen Atemtrakt – Depositionsberechnungen

Zusammenfassung

Die Deposition inhalierter ein- und vielwandiger Nanoröhrchen (SWCNT, MWCNT) im Respirationstrakt wurde für unterschiedliche Altersgruppen (Säugling, Kind, Jugendlicher, Erwachsener) theoretisch untersucht. Zusätzlich wurden mögliche Auswirkungen der inhalativen Flussrate auf die Ablagerung von Nanoröhrchen in der Adultlunge simuliert. Die theoretischen Kalkulationen basierten zum einen auf dem Konzept des aerodynamischen Durchmessers und zum anderen auf der Annahme eines auf Zufall beruhenden Transports der Teilchen durch eine stochastische (nahezu realistische) Lungenstruktur. Die Deposition der Nanoröhrchen wurde unter Anwendung von hinreichend validierten, empirischen Formeln zur Teilchenablagerung ermittelt, wobei Brown'sche Bewegung, Impaktion, Interzeption und Sedimentation als hauptsächliche Depositionsmechanismen zur Darstellung gelangten. Die Ergebnisse der Simulationen zeigen recht klar, dass für ein gegebenes Inhalationsszenario (Atmung bei sitzender Tätigkeit) sowohl die totale als auch die bronchiale und azinäre Deposition von Nanoröhrchen mit zunehmendem Alter der Probanden ansteigen, während die extrathorakale Teilchenablagerung durch einen entgegengesetzten Trend gekennzeichnet ist. Gemäß den Modelldaten erfolgt die Deposition von MWCNT, deren aerodynamische Durchmesser die der SWCNT um eine Größenordnung übertreffen, in einem geringeren Maß als jene der SWCNT. Eine Veränderung des

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hazards than MWCNT, because they are accumulated in sensitive lung regions with higher doses than MWCNT.

Keywords: Carbon nanotube, deposition model, aerodynamic diameter, lung

physischen Zustands von sitzender zu schwerer körperlicher Aktivität resultiert gemeinhin in einer Verringerung der bronchialen und extrathoraklen Nanoröhrchendeposition. Die Totaldeposition ist im Falle von SWCNT leicht erhöht, im Falle von MWCNT moderat verringert, wogegen die azinäre Deposition bei SWCNT eine deutliche Erhöhung und bei MWCNT wiederum eine Reduktion erfährt. Basierend auf den hier vorgestellten Ergebnissen kann die Schlussfolgerung gezogen werden, dass SWCNT ein höheres Gefährdungspotenzial in sich bergen als MWCNT, da sie in größeren Mengen in für Krankheiten empfänglichen Lungenregionen zur Ablagerung gelangen.

Schlüsselwörter: Kohlenstoff-Nanoröhrchen, Depositionsmodell, aerodynamischer Durchmesser, Lunge

1 Introduction

Since the 1990s, nanotechnology could successively establish in the industrial sector, which, among other, has resulted in the production of numerous innovative materials and devices [1]. Essential developments of nanotechnology include the so-called nanoparticles, which represent particulate structures with at least one dimension less than 100 nm [2]. The latest innovation are carbon nanotubes (CNT) being composed of sheets of graphite that have been rolled up to form seamless cylinders. The lengths and diameters of CNT are dependent on the type and duration of the synthesis procedure, which enables the generation of extremely variable particle sizes [3]. Single-wall carbon nanotubes (SWCNT) are characterized by diameters of several nanometers, whereas multi-wall carbon nanotubes (MWCNT) include numerous concentric SWCNT and, thus, measure 10 nm to 100 nm in diameter (Fig. 1). Both types of nanotubes reach lengths of more than 10 μm, resulting in aspect ratios (i.e., ratios of the tube lengths to the tube diameters) between 100 and >1000 [2]. Due to the layered structure of CNT several exceptional properties may be observed for these nanomaterials. These include an extraordinary tensile strength, a hardness exceeding that of diamond, and an electric conductivity similar to that of copper. Based upon numerous material tests, CNT may be attributed to the strongest and stiffest materials discovered hitherto [2,4].

Despite of their continuous triumphal procession in industry, CNT have excited enhanced interest of physicians during the past decade, because their geometric properties are comparable with those of fibrous materials and especially with those of asbestos [5]. Based upon these comparative studies, health risk assessments for nanotubes have been subjected to an intense debate. Due to their extremely small sizes, nanoparticles are taken up into the human body through the respiratory system, the skin, or the gastrointestinal tract. Based on the investigations of Donaldson *et al.* [3], CNT may be evaluated as increasingly pathogenic, because (1) their size ranks on the submicron level, which enhances their toxicity compared to larger particles, (2) their tubular shape is very similar to the

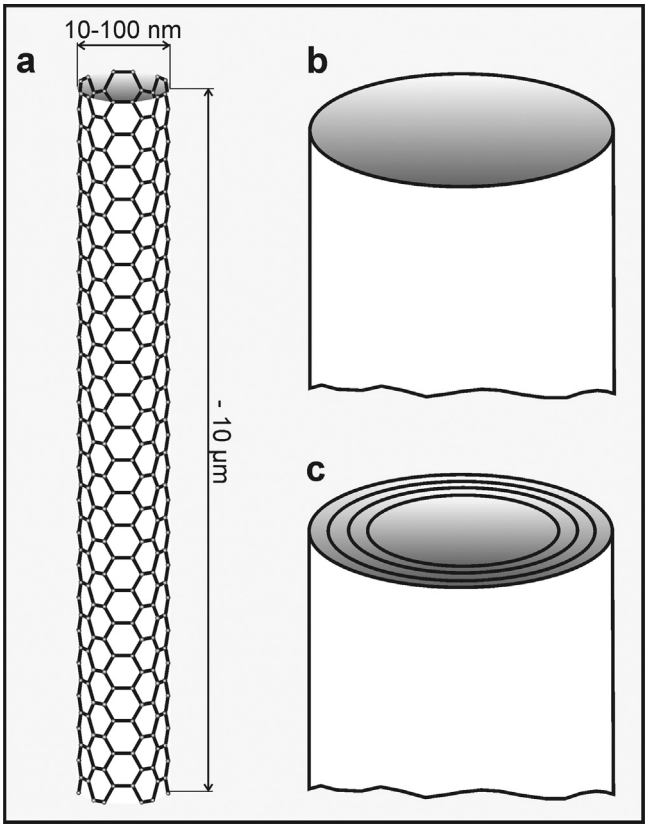

Figure 1. a) Structure and dimensions of a single-wall carbon nanotube; b) Sketch illustrating the main structural difference between single-wall carbon nanotubes and multi-wall carbon nanotubes.