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Dispersion of carbon nanotubes clusters in pulsating and vortex in-line apparatuses

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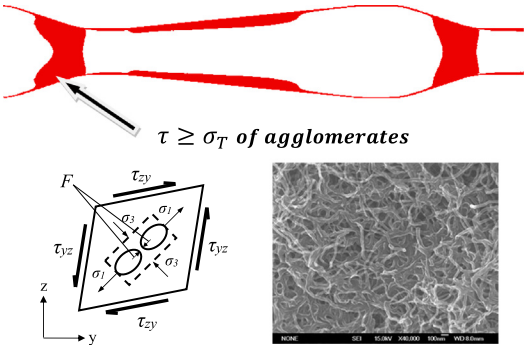
HIGHLIGHTS

- Agglomerates dispersion in pulsating in-line apparatus is more effective than in vortex one and in ultrasonic bath.
- Shear flows of pulsating in-line apparatus disintegrate carbon nanotubes agglomerates to the size 500 nm and less.
- Assessed effective volume of pulsating and vortex in-line apparatuses in deagglomeration process is close to 99%.

GRAPHICAL ABSTRACT



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ABSTRACT

The unique properties of nanoparticles have a high potential in the formation of numerous products, however, nanoparticles tend to enlarge in production, i.e. to form agglomerates (clusters), which leads to significant deterioration or even disappearance of the unique properties of nanostructured materials. In this paper, the process of nanoparticles agglomerates dispersion was investigated by means of powerful shear flows.

The efficiency of agglomerates dispersion process of carbon nanotubes 'Taunit' was studied on two experimental setups: based of the pulsating flow type apparatus (PFA) and vortex jet apparatus (VJA), with subsequent comparison of the deagglomeration quality with ultrasonic bath.

The theoretical model taking into account the fractal structure of nanomaterials and their morphological characteristics was used to determine the interaction forces between the nanoparticles, as well as the strength of the agglomerates.

To interpret and predict experimental results the k-ε turbulence model for both apparatuses was built by CFD simulation. The apparatuses effective volume, which is capable to deagglomerate carbon nanotubes with diameter of 100 nm was determined and was close to 100% for PFA and in the range of 7–36% (depending on the distance between the primary particles) for VJA.

1. Introduction

The term 'nanotechnology' was first introduced by Taniguchi (1974). The most important part of nanotechnology is nanomaterials, i.e. materials with ordered nanoscale structure fragments

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Nomenclature

A	Hamaker constant, J
C	molar concentration of ions, mol/m^3
d_a	projected area diameter, m
D	fractal dimension of agglomerates
e	electron charge, $e = 1.6022 \cdot 10^{-19}$ C
E	specific energy input, J/kg
F	particle interaction force, N
F_a	van der Waals attractive force, N
F_r	electrostatic repulsion force, N
H	separated distance between primary particles, m
I	ionic strength, mol/m^3
k_b	Boltzmann constant, $k_b = 1.38 \cdot 10^{-23}$ J/K
L	agglomerate size, m
L_0	primary particle size, m
m	mass of fluid in the apparatus, kg
n	number of dispersing elements of PFA
N	power costs, W
N_{AV}	Avogadro number, $N_{AV} = 6.0221 \cdot 10^{23}$ mol^{-1}
N_{cav}	cavitation number
p	local pressure, Pa
p_{sat}	saturated vapour pressure, Pa
P	deagglomeration probability
ΔP	pressure drop in the apparatus, Pa
Q	suspension flow rate, m^3/s
Q_{app}	agglomerate 'slip' probability through the apparatus
t	processing time, s
T	temperature, K
u	characteristic flow velocity, m/s
V	suspension velocity, m/s
V_p	volume of a particle, m^3
z	valence of ions

Greek letters

δ	Heywood shape factor
$\dot{\gamma}$	shear rate, s^{-1}
δ_a	shape factor of agglomerates
δ_0	shape factor of primary particles
ε	specific energy dissipation rate, W/kg
ε_r	relative permittivity of the medium, 80.103 water at 20 °C
ε_0	electric constant, $8.8542 \cdot 10^{-12}$ F/m
ε_a	porosity of agglomerates
θ	packing factor for primary particles in agglomerate
κ	Debye–Hückel constant, m^{-1}
λ_K	Kolmogorov microscale length, m
μ	dynamic viscosity of suspension, Pa s
ν	kinematic viscosity of suspension, m^2/s
ρ	density, kg/m^3
σ	surface charge density, C/m^2
σ_T	tensile strength of agglomerates, Pa
τ	shear stresses, Pa
φ_{eff}	proportion effective volume of the apparatus
Φ	cumulative distribution function of particles, %
ψ_d	surface potential of particles, V

ranging in size from 1 to 100 nm which have unusual functional properties.

The concept of solid-state nanostructures has been proposed by (Gleiter (1992, 1981); he also practically implemented the method of producing a compact material with grains (crystallites) of nanometer size. Since that time, compact and disperse materials consisting of nanometer particles, were called nanocrystalline. Nanomaterials compared to conventional bulk particles exhibit some unique physical properties including electrical, catalytic, magnetic, mechanical, thermal features (Mauter and Elimelech, 2008) that make the nanomaterials a relevant topic in medicine, pharmaceutics, electronic, agriculture and other industries. In addition nanoscale structures such as nanoparticles and nanolayers have extremely large surface area to volume ratio and potentially different crystallographic structures which may lead to a radical alteration in chemical reactivity.

For the most complete manifestation of the unique properties of nanostructures in materials it is necessary to prevent the agglomeration process, and this in turn requires a decrease in the concentration of the initial materials and nanoparticles in their environment.

Combining (agglomeration) of nanoparticles occurs due to aspiration of the system to reduce excess surface energy, which is inherent in a fragmented matter, especially for the nano scale state (nano particles have enormous amount of free surface energy). Once nanomaterial agglomerated, solid agglomerate with sizes ranging from hundreds of nanometers to tens of microns does not allow to use the main advantage of nanoscale primary crystallites. This leads to significant decrease in process performance. Therefore, additional operations have to be used for nanoparticles preparation as modification methods aimed at eliminating of agglomeration phenomena like ultrasound disaggregation, modifying by surfactants, and addition of encapsulating substances.

The process of agglomerates dispersion is most often carried out in an aqueous or monomer solution by devices with exertion of high stresses on the constituent particles. There are three fundamental types of agglomerate dispersing by external stress (Bałdyga et al., 2009): *erosion* of the agglomerate surface, where small fragments from the outer surface of the agglomerate are detached; *fragmentation* of the agglomerate, which yields several fragments, the size of which being in the same order of magnitude; *shattering* of the agglomerate, which means rupture into a large number of fragments considerably smaller than the original agglomerate. Herewith, the erosion is dominant for small stresses, fragmentation occurs at high stresses and shattering is expected at extremely high stresses. Additionally, the type of deagglomeration may depend on the type of stress that is exerted to the agglomerate. Deagglomeration in colloidal suspensions mainly results from the interaction with the continuous phase, i.e. from viscous forces, eddies formation and pressures fluctuations. The stress on the agglomerates is, thus, closely related to the flow field (Babick, 2016; Dietzel, 2016): (1) laminar *shear flow*: particles experience shear and normal stresses which induce particle rotation and deformation (e. g agitated vessels with rotating discs (Urban et al., 2006)); (2) laminar *elongation flow*: excessive stretching of the agglomerates caused by parallel velocity gradient to the direction of flow (e.g. in nozzles and diffusers (Wengeler and Nirschl, 2007; Teleki et al., 2008)); (3) *turbulent flow*: pressure fluctuation or shear forces (rotor-stator mixers (Bałdyga et al., 2008)), stirred tanks (Ding et al., 2009), colloid mills (Urban et al., 2006); (4) *cavitation field*: intense, local agitation of the flow field by collapsing bubbles (cavitation caused by ultrasonication (Ding and Pacek, 2008), high velocity (Bałdyga et al., 2009)).

In this paper deagglomeration process of carbon nanotubes in the new type of apparatuses like the vortex jet apparatus and pulsating flow type apparatus was investigate.