

# Chapter 19

## Modelling Liquid Flow Through Carbon Nanotubes

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### ABSTRACT

*In this paper, the structure of a liquid and character of its flow in carbon nanotube is investigated. A review of the literature and the results of experiments show that the simulation of fluid flow for nanoscale systems should be based on the continuum hypothesis taking into account the quantized character of the liquid in the length scale of intermolecular distances. Consideration of the flow characteristics allowed construction of the analogy of behavior of the liquid in a nanotube with a flow of a viscoplastic Bingham fluid. A model of mass transfer of liquid in a nanotube, based on the possibility of forming an empty interlayer between the moving fluid particles and the particles of the wall of the nanotube, is presented.*

### INTRODUCTION

A flow of fluid through microscale and nanotubes represents a fundamental interest for many biological and engineering devices and systems. Therefore, currently, flows in the nanometer size channels are intensively studied.

Popularity of modeling in nanohydrodynamics is supported by the results of numerous experiments conducted over the past two decades, which

revealed significant differences in the behavior of fluids in volumes with dimensions of about 10 and less than the molecular diameters from the predictions of the classical continuum theories. In particular, Holt et al. (2006) showed experimentally that for the tubes with an inner diameter of a nanometer size, there may be an abnormal increase in the rate of mass transfer of water.

Here is an overview of published studies, the basic theoretical principles.

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## **Slippage of the Fluid Particles Near the Wall**

Specifics of the simulation results of Poiseuille flow in the microtubules, when the molecules near a solid wall and the atoms of the wall at a finite temperature of the wall are chaotically moving, are in the fact that in the intermediate range of Knudsen numbers sliding of the fluid particles near the wall is observed.

In the work of American authors Lauga et al. (2006) three possible cases are described: (1) the liquid can be stable (no slippage), (2) slides relative to the wall (with slippage flow), (3) the flow profile is realized; this is when the friction of the wall is completely absent (complete slippage).

In the framework of classical continuum fluid dynamics, in order to describe the experimental data Navier already in 1823 wrote a boundary condition, which considers slippage of fluid along a solid surface.

The results of molecular dynamics simulation for nanosystems with liquid, with characteristic dimensions of the order of the size of the fluid particles, show that a large slippage lengths (of the order of microns) should occur in the carbon nanotubes of nanometer diameter and, consequently, can increase the flow rate by three orders of Kalra et al. (2003) and Holt et al. (2006). Thus, the flow with slippage is becoming more and more important for hydrodynamic systems of small size.

The results of molecular dynamics simulation of unsteady flow of mixtures of water - water vapor, water and nitrogen in a carbon nanotube are presented in the Kotsalis et al. (2004) work. A flow of water through carbon nanotubes with different diameters at temperature of 300 K were considered in the work. The effects of slippage of various liquids on the surface of the nanotube were studied in detail. It was found out that as the diameter decreases, the speed of slippage of particles on the wall of nanotube also decreases. The authors attribute this to the increase of the surface friction.

Experiments with various pressure drops in nanotubes demonstrated slippage of fluid in micro-and nanosystems. The most remarkable were the two recent experiments, which were conducted to improve the flow characteristics of carbon nanotubes with the diameters of 2 and 7 nm, respectively (Holt et al., 2006; Majumder et al., 2006).

In the membranes in which the carbon nanotubes were arranged in parallel, there was a slip of the liquid in the micrometre range. This led to a significant increase in flow rate - up to three - four orders of magnitude.

In the experiments for the water moving in microchannels on smooth hydrophobic surfaces, there are slidings at about 20 nm (Lauga et al., 2006; Cottin-Bizonne et al., 2005). If the wall of the channel is not smooth but twisty or rough, and at the same time, hydrophobic, such a structure would lead to an accumulation of air in the cavities and become superhydrophobic (with contact angle greater than  $160^{\circ}$ ). It is believed that this leads to creation of contiguous areas with high and low slippage, which can be described as "effective slip length" (Stone, 2003; Cottin-Bizonne et al., 2004). This effective length of the slip occurring on the rough surface can be several tens of microns, which was indeed experimentally confirmed (Cottin-Bizonne et al., 2004; Ou et al., 2004; Ou & Perot, 2005).

It should be noted that for practical use of advantages of nanotubes with slippage is necessary to solve many more problems. For example, as Churaev et al. (2002) have already shown, hydrophobic surfaces tend to form bubbles. On the other hand, the surfaces used by Churaev et al. (2002) were rough, and the use of smooth surfaces could have generally reduced the formation of bubbles.

Another possible problem - filling of the hydrophobic systems with liquid. Filling of micron size hydrophobic capillaries is not a big problem, because pressure of less than 1 atm is sufficient. However, capillary pressure is inversely proportional to the diameter of the channel, and filling for nanochannels can be very difficult.

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