408a Simulations of Flow around Multiwall Carbon Nanotubes

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The hydrodynamic behavior of flow around carbon nanotubes and around nanowires is of interest for possible applications, such as developing microfluidic devices, reducing drag on surfaces, and even for improving carbon nanotube synthesis processes. Nanoscale roughness on a surface results in ultra-hydrophobic behavior – the well known "lotus leaf effect" – that has been shown to reduce drag for laminar flows [1]. These drag reduction effects appear to be due to the formation of a thin air layer between the nano-indentations, limiting, thus, the effective contact area between the flowing water and the surface. The present work explores the case when more water is present, to the point that it can completely wet the nano-indentations (this is called a transition to a Wenzel state [2]). The hydrophobic character of the carbon nanotubes is maintained even in the Wenzel state because the graphite-water interfaces that comprise the surface of carbon nanotubes (CN) in water are hydrophobic. The flow of water past these hydrophobic surfaces can be characterized by slip, that is the velocity at the CN-water interface is not zero (as would be the case when the standard no-slip velocity boundary condition is applied in hydrodynamics).

The method of choice for the simulation of the behavior of fluids in the vicinity of CNs is molecular dynamics (MD). Such studies have been conducted recently using nonequilibrium MD for the case of flow around infinite CNs [3,4]. A significant finding from these simulations is that the MD results for the drag on the nanotubes were in very good agreement with predicted behavior from macroscopic Stokes-Oseen equations [3]. This conclusion suggests that simulations based on macroscopic equations that include the continuum approximation can provide reliable results for drag and for flow around CNs. Based on this premise, the present study is conducted using conventional computational fluid dynamics (CFD) and continuum Navier-Stokes equations to simulate the microscopic flow fields around nanotubes. The use of conventional CFD allows the simulation of flow around not only one but multiple nanotubes. The nanotubes can be attached on a surface, and they can exhibit different patterns instead of being infinitely long.

The purpose of this study is to present empirical correlations for determining the drag coefficient on nanotubes as a function of the flow and of the CN dimensions. The specific simulated physical problem is the flow of water with low velocity around a number of identical vertically-oriented nanotubes attached to a flat surface. The nanotubes were arranged in two basic patterns: (a) a linear array of nanotubes placed one next to the other on a line perpendicular to the direction of flow and (b) a forest of nanotubes that were placed according to a diamond pitch. The tubes were modeled as smooth, rigid circular cylinders. The simulations were three-dimensional, and were conducted for various tube dimensions, water velocities, and tube spacing. In addition to simulations with no-slip boundary conditions on the nanotube-water interface, simulations with slip were also performed in order to compare the two limiting cases of no-slip and complete slip. The characteristic length and the characteristic fluid velocity that are appropriate for the definition of the Reynolds number in the case of a flow field around surface-attached nanotubes have been determined to be the geometric mean of the tube diameter and height and the average fluid velocity along the tubes, respectively. With the appropriate definition of the Reynolds number, the results obtained by CFD and the computational methods described here can be used to model applications that involve water flowing around nanotubes, as well as other fluids. They can also improve our understanding of microfluidics with surface nano-indentations.

References

1. Ou, J.; Perot, B.;, Rothstein, J.P. Phys. Fluids, 2004, 16(12), 4635.

2. Cabrone, G.; Mangialardi, L. Eur. Phys. J. E, 2005, 16, 67.

3. Walther, J. H.; Werder, T.; Jaffe, R. L.; Koumoutsakos, P. Phys. Rev. E, 2004, 69, 062201.

4. Kotsalis, E. M.; Walther, J. H.; Koumoutsakos, P. Int. J. Multiphase Flow, 2004, 30, 995.