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Numerical simulation of magnetic nanoparticles targeting in a bifurcation vessel

M.M. Larimi, A. Ramiar*, A.A. Ranjbar

Faculty of Mechanical Engineering, Babol Noshirvani University of Technology, PO Box 484, Babol, Iran

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ABSTRACT

Guiding magnetic iron oxide nanoparticles with the help of an external magnetic field to its target is the principle behind the development of super paramagnetic iron oxide nanoparticles (SPIONs) as novel drug delivery vehicles. The present paper is devoted to study on MDT (Magnetic Drug Targeting) technique by particle tracking in the presence of magnetic field in a bifurcation vessel. The blood flow in bifurcation is considered incompressible, unsteady and Newtonian. The flow analysis applies the time dependent, two dimensional, incompressible Navier–Stokes equations for Newtonian fluids. The Lagrangian particle tracking is performed to estimate particle behavior under influence of imposed magnetic field gradients along the bifurcation. According to the results, the magnetic field increased the volume fraction of particle in target region, but in vessels with high Reynolds number, the efficiency of MDT technique is very low. Also the results showed that in the bifurcation vessels with lower angles, wall shear stress is higher and consequently the risk of the vessel wall rupture increases.

1. Introduction

Fluid flow in bifurcations is a very complex problem of hydromechanics. Unsteady flow and mass transport in bifurcating pipes or vessels are of interest in general and in physiological flows in particular. Flow in bifurcating vessels may be found in blood and lymph-vessels, air-tract and biliary tract. It covers many technical and biomedical applications and many researchers have studied the flow in bifurcation of vessels [1,2] or pipes. Evegren et al. [3], studied Pulsating flow and mass transfer in an asymmetric system of bifurcations. They considered both unsteady- and steady-flow through a three generation system of (non-symmetric) bifurcations. The geometry was consisted of a 90° bifurcation followed by two sets of consecutive symmetric bifurcations. The different inlet conditions affected the flow to the next generation of branches during parts of the cycle. At peak flow and further downstream in the system the effects were negligible. They also found that over a cycle, the mass flow distribution through the outlets can be affected by the inlet velocity conditions and the distribution of a passive scalar is not uniform but depends on the inlet conditions and the Schmidt number.

The flow in a carotid bifurcation model was studied by Bharadvaj et al. [4] and Palmen et al. [5]. In most of investigations on flow in large arteries, blood was modeled as a Newtonian fluid. Gijsen et al. [6] investigated the influence of the non-Newtonian properties of blood on the steady flow in bifurcation vessels. The results showed that in the common carotid artery the non-Newtonian fluid has a flattened axial velocity profile due to its shear thinning behavior.

Lee et al. [7] investigated the direct numerical simulation of transitional flow in a carotid bifurcation. They predicted the complex flow field, the turbulence levels and the distribution of biomechanical stresses present in vivo within a carotid bifurcation. Pin et al. [8] simulated the blood flow at arterial bifurcations by the lattice Boltzmann method. Distribution of physical quantities such as the velocity, shear stress and pressure, as well as the location of fluid separation, was investigated numerically.

On the other hand the accurate prediction of local dynamical behavior of discrete particles released in the fluid flow is an important key for better understanding and optimization of many processes in numerous branches of science and technology. Examples include a wide spectra of phenomena occurring in environmental (pollution dispersion in atmosphere and oceans), engineering (pharmaceutical industry) and biomedical (deposition of hazardous particles in the human respiratory or cardiovascular system) applications. Zhao et al. [9] adopted discrete trajectory model to simulate particle tracks while the Eulerian method for solving the continuous fluid flow. The results showed that particle deposition and concentration are mainly influenced by the ventilation conditions. It was also found that particles with different sizes (1, 2.5, 5 and 10 μm) had different movements in the two ventilated rooms.

* Corresponding author. Tel./fax: +98 111 3212268.
E-mail address: aramiar@nit.ac.ir (A. Ramiar).

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Nomenclature

B	magnetic magnitude
P	pressure
C_D	drag coefficient
Re	Reynolds number
Cc	Cunningham correction factor
Re_p	particle Reynolds number
F	total force acting on the particle
T	temperature
F_D	Drag force
u,v	velocity components in x and y direction
F_M	magnetic force
$\vec{u}_p$	velocity of particles
F_B	Brownian force
V	volume of nanoparticles
F_G	buoyancy force

Greek symbols

F_L	lift force
$_0\mu$	magnetic permeability of vacuum
F_m	magnus force
χ	magnetic susceptibility
F_b	Basset force
ψ	friction coefficient
H	magnetic intensity
ζ	restitution coefficient
J	current density
ζ_i	Gaussian random number
K_B	Boltzmann constant
υ	kinematic viscosity
M	material magnetization
ρ	density
m_p	particles mass
Mn_F	magnetic numbers

Longest and Xi [10] studied the effectiveness of direct Lagrangian tracking models for simulating nanoparticle deposition in the upper airways. The objective of their study was to evaluate the effectiveness of direct Lagrangian tracking methods for calculating ultrafine aerosol transport and deposition in flow fields consistent with the upper respiratory tract. Lagrangian deposition results have been compared with a chemical species Eulerian model, which neglects particle inertia. For the tubular and 90° bend geometries, Lagrangian model results with a user defined BM routine agreed well with the Eulerian model.

Some new applications stemming from this fusion include pumping and mixing of fluids, as well as the incorporation of switches and valves into lab-on-a-chip devices (Pamme [11]). Magnetic forces are used for transport, positioning, separation and sorting of magnetic as well as non-magnetic objects. Bio-assays have been performed on the surface of magnetic particles trapped inside a micro channel. Many areas in microfluidic applications involve manipulation of particles in a controllable manner.

In the design of micro scale devices for cell sorting, cell analysis or cell removal from a sample, it is important to predict the motion of the particles in response to the local flow conditions. For this purpose, various principles and methods have been developed in micro systems, such as the optical tweezers (Furst [12]) and electro kinetic methods (Binyamin et al. [13]). Haverkort et al. [14] performed a Computational simulation of blood flow and magnetic particle motion in a left coronary artery and a carotid artery, using the properties of presently available magnetic carriers. The simulations demonstrated that approximately a quarter of the inserted 4 μm particles can be captured from the bloodstream of the left coronary artery, when the magnet is placed at a distance of 4.25 cm. When the same magnet is placed at a distance of 1 cm from a carotid artery, almost all of the inserted 4 μm particles are captured.

There are many researches related to MDT technique for drug delivery in the literatures. Localized medical drug delivery enables a significant local increase of the medical drug in regions affected by disease and leads to a significant reduction of the always present negative side effects of aggressive medical treatments. Experimental studies on animals and preclinical studies on human patients demonstrated potentials of this approach as shown by Lubbe et al. [15] and [16] and Morsi et al. [17]. Riegleret al. [18] presented the first demonstration of cell targeting using a Magnetic Resonance Imaging (MRI) scanner. They found live human cells, labeled with different iron oxide particles, can be targeted within a vascular vessel model using the magnetic field gradients of an MRI scanner. Liu et al. [19] formulated a hydrodynamic model of Ferro fluids to describe drug carrier flowing in a blood vessel. They found that the enhancement of the magnetic field intensity could slow down the velocity of Ferro fluids and increased the retention of Ferro fluids at the target position. Nacev et al. [20] studied the behavior of ferromagnetic nanoparticles in and around blood vessels under applied magnetic fields. They carried out a detailed analysis to better understand and quantify the behavior of magnetizable particles in-vivo. They found that there are three types of behaviors (velocity dominated, magnetic dominated, and boundary-layer formation) uniquely identified by three essential non-dimensional numbers (the magnetic-Richardson, mass Peclet and Renkin numbers). Kenjeres and Righolt [21] simulated the magnetic capturing of drug carriers in the brain vascular system. They demonstrated that magnetically targeted drug delivery significantly increased the particle capturing efficiency in the target regions.

There are two approaches for the numerical simulation of the multiphase flow: Euler–Lagrange and Euler–Euler approach. The Lagrange discrete phase model is based on the Euler–Lagrange approach where the fluid phase is treated as a continuum by solving the time-averaged Navier–Stokes equations, whereas the dispersed phase is solved by numerically integrating the equations of motion for the dispersed phase, i.e. computing the trajectories of a large number of particles or droplets through the calculated flow field. The dispersed phase consists of spherical particles that can exchange mass, momentum and energy with the fluid phase. In general, interactions between particles can be divided in three classes, based on particle volume fraction. According to Elghobashi [22] and Crowe et al. [23], for particle volume fractions less than 10^{-6}, particle motion is influenced by continuous phase properties while practically there is no feedback from the dispersed phase. This class is called “one-way coupling”. For particle volume fractions in the range of 10^{-6} to approximately 10^{-3}, feedback of the dispersed phase on the properties of the continuous phase fluid dynamics must also be taken into account, this class in known as “two-way coupling”. As the third class, a dense flow is characterized by particle volume fractions