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Homotopy-based solution of Navier-Stokes equations for two-phase flow during magnetic drug targeting

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ABSTRACT

As one of the promising innovative methods of drug delivery, magnetic drug targeting (MDT) ideally contains three main steps to treat localized diseases; chemically attaching drugs to magnetic nanoparticles and their injection to a proper local blood stream, control and steering the cluster of particles in the arterial network with a proper external magnetic field and finally, trapping them and releasing the drugs at the diseased part of body. Focusing on the third step, some mathematical models, followed by uncountable numerical simulations, have been developed; keeping in mind this fact that by having answers which are functions of temporal, spatial and other related variables which make it possible to consider this kind of two-phase flows much easier, homotopy analysis method (HAM) was used to solve one of the most comprehensive models developed for such system. An artery-inspired geometry was a straight tube through which the supposed mixture is passing. Due to demanding results, only four steps of Maclaurin series were able to be computed; with this insufficient number of steps, acceptable accordance with numerical results was achieved.

1. Introduction

Treating localized diseases like different kind of cancers, cardivascular episodes like stenosis and thrombosis and of course, cell ejection to some particular tissues are challenged by finding a way to get medication to supposed locations. It is due to linked vessels in body circulatory system. A way by which neither does the majority of ejected drug waste nor toxic drugs affect healthy tissue.

These reasons make targeted drug delivery to be a continuing challenge and active scientific field in medicine throughout last two decades more particularly, magnetic drug targeting (MDT) is considered as a great method to deal with this challenge and lower the proposed deleterious side effects. In an ideal MDT process, chemotherapeutic agents are bound on magnetic nano-particles with some biocompatible composites and then ejected to a proper local blood stream, moving the cluster of particles throughout the bloodstream is observed by real-time imaging, and finally steered them in circulatory system and hold at the diseased location. This project focuses on the last stage of this process.

Different kinds of models are developed for this kind of flows; Nacev et al. [1] stated and solved numerically a system of equations governing the diffusion, convection and magnetic transport of nanoparticles in the blood and into surrounding tissue; Lagrangian [2,3], Eulerian [2,4], two-phase mixture [2,5] and LTNE [6] are ones that researchers use in their projects. In this project we revisit a system of equations using two-phase mixture (as used in [7]) model developed to describe the behavior of magnetic nano drug carriers in a non-Newtonian fluid (blood) under an external magnetic field [8] by using an improved version of Adomian decomposition method in topology named homotopy analysis method (HAM). A great method, developed by Liao [9,10], has shown its credibility in analytical solution of numerous equations with strong nonlinear terms like heat transfer in a porous channel [11] or under magnetic field [12], diffusion and reaction in porous catalysts [13], nonhomogeneous Blasius problem [14] and MHD viscoelastic fluid flow in a channel with a stretching wall [15]. However, till now, no one has used this method in topology to solve such complicated system of equations.

This method introduces an embedding parameter (q) by increasing which from 0 to 1, this transformation is usually from zero-order, the homotopy equation turns from an auxiliary equation (here a linear one) to main nonlinear PDE (or ODE). By having this in mind, briefly, we can find the expanded form of solution of homotopy equation around $q = 0$ as a series; finally, approximate solution of the original equations would be this series in which q is replaced with 1.

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In this paper, we used divergence theorem [16] to turn the numerical form of equations into PDE form that can be considered more mathematically and solved analytically. As it was predictable, demanding results were achieved; consequently, only 4 first steps of Maclaurin series were computed. Further development to compute more terms of Maclaurin series of solutions would be required.

2. Theory

2.1. Numerical form of equations

The model suggested and modified by Cherry et al. [8] is the homogeneous flow (or dusty gas approach) developed by Carrier [17] which considers the cluster of particles as a variable continuum moving throughout local flow. Here are some assumptions taken in this model; firstly, the maximum volume fraction of particles (c) is ¡ 1%; as a consequence, this system can be considered as an incompressible one. Secondly, particle stoke number ($\frac{\tau_p u_{bulk}}{D}$) is so small (in order of 10^{-7}) as a consequence of which, particle response to surrounding flow is instant. Finally, all magnetic particles are assumed to be in saturated state.

The system of equations modified by Cherry et al. is as follows which are continuity (Eq. (1)), scalar transform (Eq. (2)) and momentum transport (Eq. (3)) equations respectively.

$$\int_s u_i ds_j = 0 \tag{1}$$

$$\int_v \frac{\partial c}{\partial t} dv + \int_s c u_j dsj = \int_s (D_{Br} + D_{bl}) \frac{\partial c}{\partial \chi_j} ds_j \tag{2}$$

$$\int_v \frac{\partial(\rho_m u_i)}{\partial t} dv + \int_s \rho_m u_i (u_j.ds_j) = \int_s P ds + \int_v \rho_m g_i dv$$
$$+ \int_v M_j \frac{\partial B_i}{\partial x_j} dv + \int_s \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) ds_j + F_{int,i} \tag{3}$$

Table 1 introduces the variables used in above system of equations.

2.2. Magnetic particles internal force

Here, F_{int}, i is the internal force of magnetic dipoles acting on volume fraction expressed as follows [8]:

The force, every pair of magnetic dipoles acting on each other with volumes V_1 and V_2, is as below where $\hat{r}$ is dimensionless form, with $h = \frac{\sqrt[3]{V_{cell}}}{2}$ which V_{cell} denotes the average volume of numerical mesh grids, of separation between two dipoles and m is magnetic moments of them.

$$\vec{F}_{int} = \int_{v_1} \int_{v_2} \frac{3\mu_0 c_1 c_2}{4\pi |r^4|} (\hat{r} \times \vec{m}) \times \vec{m} + (\hat{r} \times \vec{m}) \times \vec{m}$$
$$- 2\hat{r}(\vec{m}.\vec{m}) + 5\hat{r}(\hat{r} \times \vec{m})(\hat{r} \times \vec{m}) dV_2 dV_1 \tag{4}$$

c, μ_0 and V stand for magnetic particles volume fraction, magnetic permeability and volume of control volume respectively.

Now, assume that subscripts 1 and 2 stand for the control volume equations of which are written by Eqs. (1) to (3) and its surrounding respectively.

However, this integration is divergent when r tends to zero; so, Cherry et al. used the first term of Taylor expansion of this integral around the local domain position and introduced an index, a ratio correction and a weight function to correct the errors; it is unphysical if we compute this force when $r \to 0$, the force tends to infinity, so it is used an index showing this fact that the nearest magnetic dipole to local origin place is more than this supposed index (averagely, $\lambda = 1.88 \times 10^{-6}$). As the consequence, the net internal force applied to control volume can be expressed as two below; the first term ($\hat{F}_s$) is force acted on supposed control volume from distant surrounding (λ to infinity) and the second one is acted by nearer particles.

$$\vec{F}_{int} = \vec{F}_s + \vec{f} \tag{5}$$

where

$$f_x = \frac{3\mu_0 M^2 c}{4\pi} \frac{dc}{dx} \frac{-23.87\lambda - 0.5639}{\lambda^3 + 0.919\lambda^2 + 0.3679\lambda + 0.003827} \tag{6}$$

$$f_y = \frac{-15\mu_0 M^2 c}{4\pi} \frac{dc}{dy} \frac{9.545\lambda + 0.2256}{\lambda^3 + 0.919\lambda^2 + 0.3679\lambda + 0.003828} \tag{7}$$

And

$$\vec{F}_s = (1 - W)\vec{F}_{int}$$

which after expansion is written as below:

$$F_{sx} = c \int_0^{2\pi} \int_\lambda^\infty 3\ c\ \mu_0 \frac{1 - W}{4\pi r^4} R_x(-4m^2)\cos\theta$$
$$+ 2m^2 \sin\theta + 5\ m \cos\theta(\cos\theta - \sin\theta)^2) r dr d\theta \tag{8}$$

$$F_{sy} = c \int_0^{2\pi} \int_\lambda^\infty 3\ c\ \mu_0 \frac{1 - W}{4\pi r^4} R_y(-4m^2)\sin\theta$$
$$+ 2m^2 \cos\theta + 5\ m \sin\theta(\cos\theta - \sin\theta)^2) r dr d\theta \tag{9}$$

More precisely, at every local position of domain, internal force conduced by near magnetic dipole is shown by $\vec{f}$ which is dominated for near distance, and for far distance, it is $\vec{F}_s$ that is dominant. W, conveying this domination, and R_x and R_y are weighting function and correcting ratio in x and y directions respectively showed by followed equations.

If we introduce Θ as below

$$\Theta = \arctan \frac{|\sin\theta|}{\cos\theta} \tag{10}$$

The, correction ratios in x and y directions would be

$$Ratiox = 1 + h^2 \frac{-1.218\Theta + 1.97}{r^2} \tag{11}$$

Table 1
Variables corresponding to Eqs. (1) to (3).

Symbols	Variable name	Units
c	Magnetic particle volume fraction	–
g	Acceleration of gravity	$\frac{m}{s^2}$
t	Time	s
u	Fluid velocity	$\frac{m}{s}$
χ	Spatial coordinate	m
B	Magnetic field	T
D_{Bl}	Diffusivity (particle/blood cell collisions)	$\frac{m^2}{s}$
D_{Br}	Brownian diffusivity	$\frac{m^2}{s}$
M	Magnetization	$\frac{N}{m^2\ T}$
P	Pressure	$\frac{N}{m^2}$
S	Grid cell surface area	m^2
V	Grid cell volume	m^3
μ	Blood dynamic viscosity	$\frac{kg}{ms}$
ρ_m	Density of mixture	m^3