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COMPUTATIONAL STUDY OF THE INTERACTION BETWEEN A NEWTONIAN FLUID AND A CELLULAR BIOLOGICAL MEDIUM IN A STRAIGHT VESSEL

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Abstract. In this work, we solve numerically the governing equations for quasi-steady Newtonian flow past and through a cellular biological medium, which is attached to the surface of a straight vessel. The flow past the cellular biological medium is described by the Navier-Stokes equations. For the modeling of momentum transfer within the cellular biological medium, we consider that the cellular biological medium constitutes a biphasic fluid-solid mixture with poroelastic behaviour. The system of governing equations is solved numerically with the mixed finite element method. The computational domain is discretized using an unstructured, variable density triangular element mesh. From the numerical solution we obtain the spatial distributions of: (i) the fluid velocity and pressure, and (ii) the displacement and stresses of the solid matrix within the cellular biological medium. Also, the components of the overall hydrodynamic force exerted by the flowing fluid on the cellular biological medium are calculated. A parametric analysis is performed with regard to the Reynolds and Darcy numbers that characterize the flow past and through the cellular biological medium.

1 INTRODUCTION

The interaction between a flowing fluid and a cellular biological medium (e.g. biofilm, or tissue) attached to the surface of a vessel is of key importance in several natural phenomena, and processes of physiological and technological significance. The biodegradation of organic contaminants by microbial biofilms in soil and aquifers, the in vitro construction of artificial tissues from human stem cells in synthetic porous scaffolds, the flow of blood in vessels containing thrombus and atheromatous plaque formations, are some of the processes in which fluid-cellular biological medium interactions are important.

In all the aforementioned processes, the interaction between the flowing extracellular fluid and the deformable solid matrix (cells plus extracellular matrix) plays multiple important roles: (a) affects the internal architecture (spatial arrangement of cells and extracellular matrix) and the external morphology (overall size and shape) of the cellular biological medium [1], (b) enhances the mass transfer rate of chemical species (nutrients, wastes, chemical signaling molecules, etc) within the cellular biological medium [2], and (c)regulates the function of cells through the action of mechanical stresses, which are either applied directly on the outer surface of the biological cell, or transmitted indirectly through the extracellular polymeric matrix [3].

Significant research effort has been directed toward the elucidation of the exact mechanisms through which the complex interaction between a flowing fluid and a cellular biological medium occurs. Along this direction, it is standard practice to employ experimental techniques that allow the study of the effect of a well-controlled flow field on the function and morphology of individual biological cells, layers of cells, or cellular biological media samples. In particular, flow chambers with parallel plate configuration have been used in several studies to observe the response of cellular biological media to fluid shear.

Mathematical modelling is an indispensable tool, which is complementary to experimental investigation and provides qualitative interpretation and quantitative correlation of the fluid-structure interactions in these systems in terms of velocity, stress fields, etc. A comprehensive survey on the available approaches for theoretical modelling of momentum transport in cellular biological media, with focus on the formulation of governing equations and the calculation of material properties, is given in [4].

In this work, we present preliminary results from computer simulations of flow past and through a poroelastic biomaterial, which is attached to the surface of a straight vessel. Fluid flow in the clear fluid regions is described by the Navier-Stokes equations, and momentum transfer in the cellular biological medium is described in the context of biphasic mixture theory. The effect of the Reynolds and Darcy numbers that characterize the flow past and through the biological medium is investigated.

2 MATHEMATICAL MODEL

We consider the quasi-steady flow of an incompressible Newtonian fluid in a straight vessel with rigid solid walls, and a cellular biological medium attached to the wall of the vessel as shown in Figure 1. In the clear fluid region, which is denoted by Ω_f, fluid flow is described by the Navier-Stokes and continuity equations

$$\nabla \cdot \mathbf{v}_f = 0 \qquad \text{in } \Omega_f \quad (1)$$

$$\rho_f \mathbf{v}_f \cdot \nabla \mathbf{v}_f = -\nabla P_f + \mu_f \nabla^2 \mathbf{v}_f \qquad \text{in } \Omega_f \quad (2)$$

where $\mathbf{v}_f$ is the velocity, P_f is the pressure, ρ_f is the density, and μ_f is the viscosity of the fluid. The flow in the vessel is driven by a prescribed, constant pressure drop ΔP_{ref} between the inflow and outflow boundaries of the vessel. Further, the gradient of the velocity components along the flow direction (x-axis) is nil at the inflow and outflow boundaries because the flow is considered to be fully developed there. At the fluid-solid interface the fluid velocity is nil based on the no-slip and no-penetration assumptions.

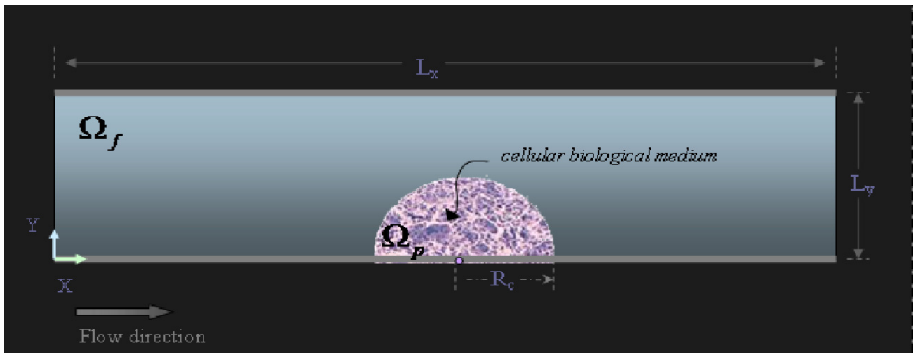

Figure 1: Schematic representation of the flow geometry

The cellular biological medium is treated as a biphasic mixture consisting of: (a) a viscous fluid phase denoted by *f* (extracellular aqueous solution), and (b) an elastic solid phase denoted by *s* (cells and extracellular matrix). The mathematical formulation of the mass and momentum balances for the cellular biological medium is based on the theory of mixtures, which was developed for the mathematical description of momentum, mass, and energy transport in multicomponent, multiphase systems at a scale of observation with resolution much larger than the characteristic length of the individual constituents and phases (the structure of the system at finer spatial scales is disregarded completely). The mathematical foundation of the theory relies upon the concept that the constituents of the mixture can be modeled as superimposed, interacting continua. In this way, a material point is assigned for each constituent at every point in space, which is occupied by the mixture. Exhaustive reviews on the theory of mixtures are given in [5,6]. The governing conservation laws for each constituent of the mixture contain the usual terms (that appear in formulations for a single phase), and an additional term which accounts for the interaction between the reference constituent and the other constituents of the mixture.

We consider that the fluid (*f*-constituent) behaves as a Newtonian fluid, and the solid (*s*-constituent) behaves as a linearly elastic isotropic solid. For the systems under consideration, it is reasonable to neglect the convective momentum transfer and mass production–consumption (for time scales of observation much smaller than the characteristic time of cell division). Furthermore, we assume that the flow is in quasi-steady state. Under these assumptions, in the context of biphasic mixture theory, the equations that govern momentum transfer in the cellular biological medium are

$$\nabla \cdot \mathbf{v}_f = 0 \qquad \text{in } \Omega_p \quad (3)$$

$$\mathbf{0} = \nabla \cdot \boldsymbol{\sigma}_f + \mathbf{F}_{s \to f} \qquad \text{in } \Omega_p \quad (4)$$

$$\mathbf{0} = \nabla \cdot \boldsymbol{\sigma}_s + \mathbf{F}_{f \to s} \qquad \text{in } \Omega_p \quad (5)$$

The stress tensors and the interaction force are given by the following constitutive expressions

$$\boldsymbol{\sigma}_f = -\phi_f P_f \mathbf{I} + \mu_f \left[\nabla \mathbf{v}_f + \left(\nabla \mathbf{v}_f \right)^{\mathrm{T}} \right] \qquad (6)$$

$$\boldsymbol{\sigma}_s = -\phi_s P_f \mathbf{I} + \lambda_s \left(\nabla \cdot \mathbf{u}_s\right) \mathbf{I} + \mu_s \left[\nabla \mathbf{u}_s + \left(\nabla \mathbf{u}_s\right)^{\mathrm{T}}\right] \tag{7}$$

$$\mathbf{F}_{f \to s} = -\mathbf{F}_{s \to f} = \frac{\mu_f \phi_f}{k_{eff}} \mathbf{v}_f + P_f \nabla \phi_s \tag{8}$$

Here, ϕ_a is the volume fraction of the αth constituent in the cellular biological medium (with $\phi_f + \phi_s = 1$), $\mathbf{u}_s$ is the solid displacement, μ_s and λ_s are the Lamé parameters for the solid, and k_{eff} is the hydraulic permeability of the material.

The mathematical formulation is completed with the boundary conditions at the interface between the cellular biological medium and the free fluid. We consider continuity of the fluid velocity and, further, that the normal stress exerted on the interface by each constituent of the cellular biological medium equals the total normal stress weighted by the corresponding volume fraction [7].

3 NUMERICAL SOLUTION

For the numerical solution of the governing equations of the problem we used the Galerkin finite element method. The spatial discretization of the computational domain is performed with triangular elements. An unstructured, variable density triangular element mesh is generated by combining a Delaunay triangulation algorithm with a force-based mesh smoothing methodology, so as to optimize the mesh quality. A typical mesh used for the numerical calculations is shown in Figure 2.

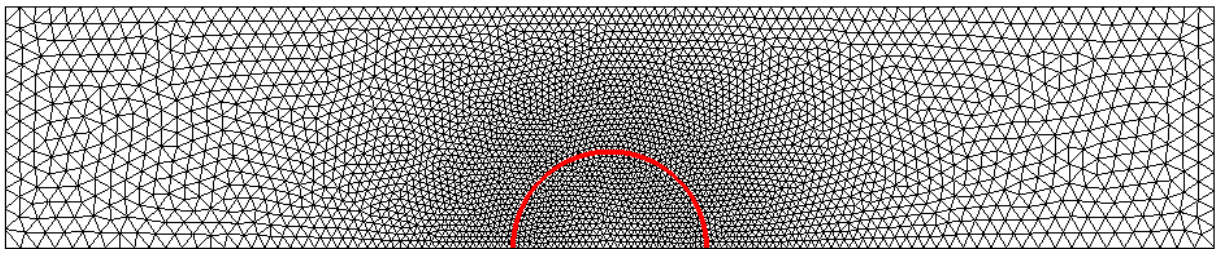

Figure 2: Typical unstructured mesh of triangular elements.

For the approximation of the fluid pressure we use 3-node linear basis functions, while the fluid velocities and solid displacements are approximated by 6-node quadratic basis functions. For the solution of the non-linear systems of equations that result from the discretization of the fluid momentum balances we employ a combination of Picard iterations and the Newton-Raphson method. Due to the assumptions postulated in section 2, the governing equations and boundary conditions of the problem constitute a one-way coupled system, so that the fluid and solid constituents momentum balances can be sequentially solved.

4 RESULTS AND DISCUSSION

In this section, we present preliminary results regarding the effects of the *Reynolds* and *Darcy* numbers that characterize the flow *past* and *through* the cellular biological medium, respectively. These dimensionless numbers are defined as follows

$$Re = \frac{\rho_f \langle U \rangle R_c}{\mu_f} \tag{9}$$

$$Da = \frac{k_{eff}}{R_c^2} \tag{10}$$

where $\langle U \rangle$ is the magnitude of the average velocity for flow in a clear vessel, under the same pressure drop. All other parameters of the system are held constant for the simulations. The size ratio of the radius of the semicircular obstacle to the width of the vessel is equal to 0.4, the length to width ratio of the vessel is equal to 5.0, and the Young's modulus and Poisson's ratio for the solid are set equal to 1MPa, and 0.45. Figure 3 shows the fluid streamlines in the vessel for three different values of the Reynolds number (0, 1, and 10) and two different values of the Darcy number (10^{-2} and 10^{-4}). We observe that as the *Re* number increases, the flow pattern past and through the obstacle changes qualitatively and, gradually, obtains an asymmetrical structure. This effect becomes more pronounced for the lower *Da* number, where an extended recirculation region is formed behind the obstacle. Interestingly, the recirculation zone extends into the permeable biological medium (Figure 3F). Furthermore, we observe that as the *Da* number decreases, the fluid streamlines begin to divert significantly from the permeable obstacle, meaning that the amount of fluid passing through the cellular biological medium undergoes noticeable decrease.

Figure 4 shows the corresponding maps of longitudinal and lateral displacement of the solid in the cellular biological medium. An increase in the *Re* number affects the solid displacement field both quantitatively and qualitatively. The values of the horizontal and vertical displacement increase in response to the elevated values of the forces experienced by the solid due to fluid flow (namely, term $\mathbf{F}_{f \to s}$ in the momentum balance for the solid). In addition, the gradual loss of symmetry of the flow affects strongly the solid displacements (see for example Figure 4F). The *Da* number also has an important effect on the displacements. A decrease in the value of *Da* leads to an increase of the solid displacements. This is attributed to the increase of the fluid-solid interaction force, $\mathbf{F}_{f \to s}$, caused by the decrease of the permeability of the medium.

In Figure 5, the effect of Re on the dimensionless drag and lift forces exerted by the fluid on the cellular biological medium is depicted for two different Darcy numbers, namely Da=10^{-2} and Da=10^{-4}. The dimensionless drag and lift forces (per unit length) are defined by the following expressions:

$$F_{drag} = \frac{1}{L_y \Delta P_{ref}} \oint_S \mathbf{e}_x \cdot \boldsymbol{\sigma}_f \cdot \mathbf{n} dS \tag{11}$$

$$F_{lift} = \frac{1}{L_y \Delta P_{ref}} \oint_S \mathbf{e}_y \cdot \boldsymbol{\sigma}_f \cdot \mathbf{n} dS \tag{12}$$

Here, L_y is the width of the vessel, and ΔP_{ref} is a reference pressure drop.

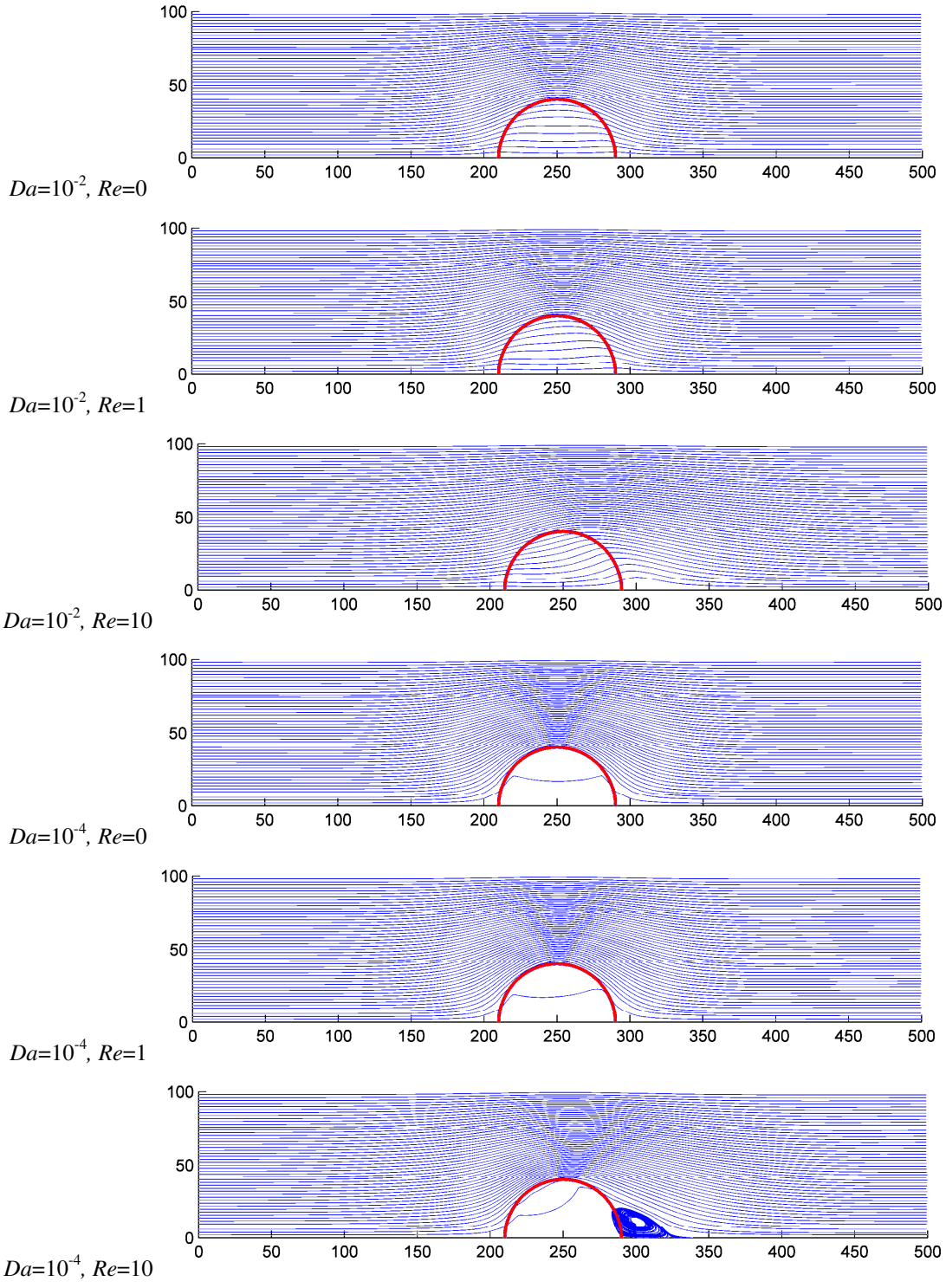

Figure 3: Fluid streamlines for representative values of the Reynolds (*Re*) and Darcy (*Da*) numbers.

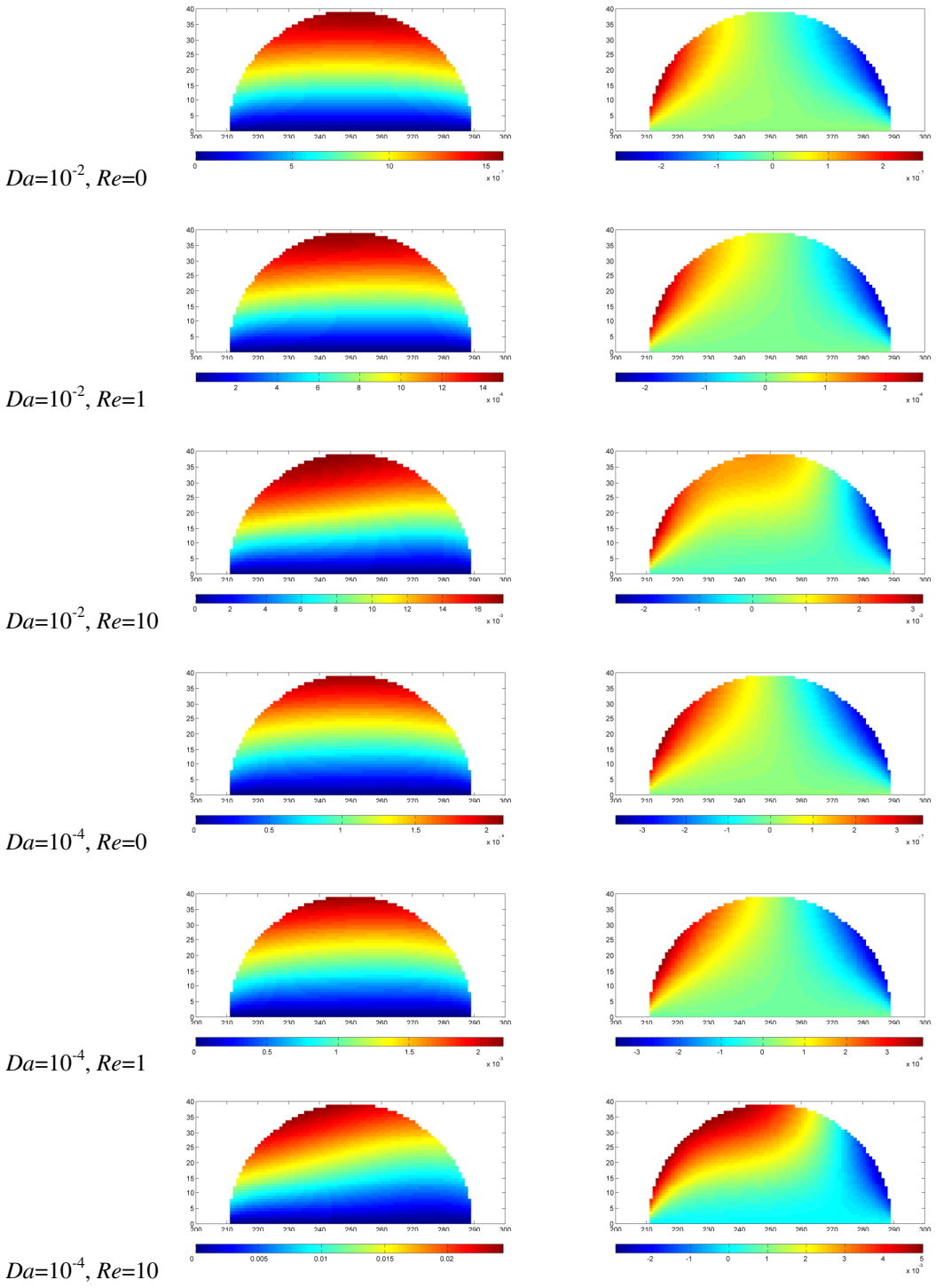

Figure 4: Maps of the longitudinal (left column) and lateral (right column) displacements of the solid in the cellular biological medium for representative values of the Reynolds and Darcy numbers.

In Figure 5, we observe that an increase in the *Re* number is followed by an increase in the values of both the drag and lift forces, as expected. Interestingly, an increase in the *Da* number leads to a decrease in the value of drag and an increase in the value of lift.

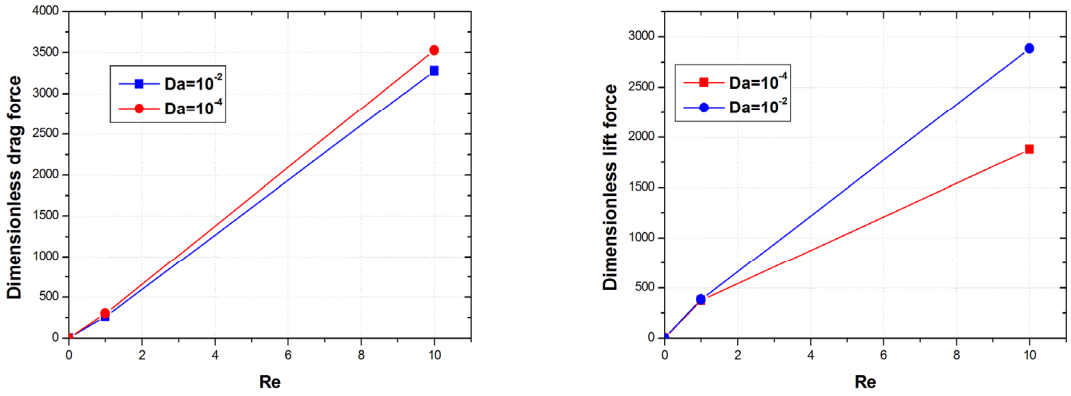

Figure 5: Effect of *Re* on the dimensionless drag and lift forces for two different *Da* numbers.

5 CONCLUSIONS

- As the Reynolds number increases and the Darcy number decreases, an extended downstream recirculation region forms which reaches into the cellular biological medium.
- The drag force exerted by the flow on the cellular biological medium increases for increasing Reynolds number and decreasing Darcy number, while the lift force increases for increasing Reynolds number and increasing Darcy number.

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