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Network and Nakamura tridiagonal computational simulation of electrically-conducting biopolymer micro-morphic transport phenomena

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ABSTRACT

Magnetic fields have been shown to achieve excellent fabrication control and manipulation of conductive bio-polymer characteristics. To simulate magnetohydrodynamic effects on non-Newtonian electro-conductive bio-polymers (ECBPs) we present herein a theoretical and numerical simulation of free convection magneto-micropolar biopolymer flow over a horizontal circular cylinder (an "enrobing" problem). Eringen's robust micropolar model (a special case of the more general micro-morphic or "microfluid" model) is implemented. The transformed partial differential conservation equations are solved numerically with a powerful and new code based on NSM (Network Simulation Method) i.e. PSPICE. An extensive range of Hartmann numbers, Grashof numbers, micropolar parameters and Prandtl numbers are considered. Excellent validation is also achieved with earlier non-magnetic studies. Furthermore the present PSPICE code is also benchmarked with an implicit tridiagonal solver based on Nakamura's method (BIONAK) again achieving close correlation. The study highlights the excellent potential of both numerical methods described in simulating nonlinear biopolymer micro-structural flows.

1. Introduction

Magnetic fields are deployed in many biomedical engineering systems owing to their excellent facility in manipulating properties and characteristics of materials and fluids. These include separation processes [1], smart biopolymer synthesis [2] and micro-channel magnetofluid devices [3]. In next generation "smart bio-engineered" polymers, *magnetic manipulation in biomolecular separation from a sample*, is achievable via initially utilizing adhesion to minute magnetized particles, followed thereafter, via detachment by virtue of carefully orientated external magnetic fields. In contrast to *electric manipulation*, magnetic interactions are generally not affected by surface charges, pH, ionic concentrations or temperature. This makes magneto-hydrodynamic processing of biolpolymers particularly attractive to bioengineers. To exploit this technology, magneto-hydrodynamics (MHD) must be used judiciously and engineers frequently conduct computational simulations leading to optimized designs. Magnetic forces have also been exploited in a vast range of modern biophysical applications including hemodynamic control [4,5], magnetic drug targeting [6–8], smart bio-lubrication [9–11], magnetic resonance imaging of the brain [12], hydromagnetic peristaltic pumps [13,14] and magnetic tweezers [15]. In the present study we simulate the enrobing process of a magnetic rheological biopolymer flow. These complex materials exhibit a number of advantages over synthetic polymers. They are commercially cheaper and non-toxic compared to the vast majority of synthetic polymers [16]. Such materials include methanesulfonic acid doped polyaniline (PANI) conductive blends which possess high electrical conductivity which has been experimentally verified with X-ray Photoelectron Spectroscopy. Mallick and Sakar [17] have also reported in detail on magnetohydrodynamic properties of conductive biopolymers, highlighting enhanced electrical conductivity even at room temperature. They have further emphasized the importance of optimizing fluid mechanical models of micro-structural rheological aspects of such polymers. As early as 1964, Eringen [18] pioneered a new branch

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of fluid mechanics- microcontinuum theory- which to date has provided the most elegant and "computable" model for complex liquids exhibiting microstructure. The micro-morophic framework simulates very accurately microscopic rheological (and vortex) effects which arise from rotary motions of the fluid microelements. The micropolar model, also introduced by Eringen [19] provides a simpler (but equally useful) theory for simulating couple stress and gryration effects and infact generalizes the Stokesian polar (couple stress) and other micro-structural model, by incorporating local rotary inertia. As such the micropolar model is a comprehensive and accurate framework which can describe a wide variety of complex non-Newtonian flows including bubbly liquids, liquid crystals, suspension polymers, paints, gels, physiological fluids (blood), synovial lubricants and even contaminated air in the human lungs. Thus far however this model has not been implemented for conducting biopolymers. Bég et al. [20] have reviewed progress in micropolar flow modeling in biomechanics in addition to aeronautics, chemical engineering and materials processing. Transport phenomena in micropolar flows have also been considered with multi-physical effects in [20].

In the context of biopolymeric enrobing flows, thermal convection boundary layer flows from cylindrical bodies are particularly relevant. Hassanien [21] investigated transverse curvature and viscosity effects numerically for the steady state mixed convective boundary layer flow of a micropolar fluid along vertical slender cylinders, showing that micropolar fluids *display drag reduction* as well as *heat transfer rate reduction* when compared to Newtonian fluids. Mahfouz [22] studied computationally the Rayleigh number and spin viscosity effects on *unsteady* natural convection from an isothermal cylinder placed horizontally in a micropolar fluid is investigated, confirming that in comparison with Newtonian fluids, micropolar fluids display a reduction in heat transfer rate at the cylinder surface. Bhargava et al. [23] obtained numerical solutions for the mixed convection flow of an incompressible micropolar fluid near a stagnation point on a horizontal cylinder, with wall transpiration effects showing that micropolar viscosity reduces drag forces and also acts as a cooling agent i.e. reduces surface heat transfer rates. Kumar et al. [24] used the finite element method to investigate the mixed convection on a moving vertical cylinder with suction in a moving micropolar fluid medium showing that temperature distribution is affected moderately by the motion of the cylinder as well with the buoyancy parameter. Gorla et al. [25] have also studied free and foced micropolar thermal boundary layers from a vertical cylinder. The above studies have all been restricted to *electrically non-conducting* fluid regimes i.e. magnetohydrodynamic effects have been ignored. Dunn [26] presented a simplified analytical model of the magnetohydrodynamic natural-convection heat transfer from a finite cylinder at various orientations with respect to an applied magnetic field, showing that the flow regime can be expressed solely as a function of Lykoudis number (magnetic parameter) and a constant. Aleksandrova [27] analyzed the hydromagnetic flow around an infinitely long elliptical cylinder. Aldos and Ali [28] studied the effect of suction on convection from a horizontal cylinder in a cross field hydromagnetic flow using both local numerical nonsimilarity and coordinate perturbation methods. They showed that blowing decreases Nusselt number and suction increases it both for free and forced convection flows. Rao et al. [29] studied numerically the two-dimensional hydromagnetic flow past a circular cylinder, describing the effects of a strong magnetic field on wake formation and stagnation point characteristics. El-Amin [30] studied porous drag force, Joule heating and viscous dissipation effects on hydromagnetic forced convection flow from a horizontal circular cylinder under transverse magnetic field, with variable wall temperature conditions using a second-level local non-similarity numerical method. Ganesan and Loganathan [31] presented finite difference numerical solutions for the unsteady magnetohydrodynamic convection from a moving vertical cylinder with constant heat flux showing that an increase in the magnetic field decelerates the flow and elevates thermal boundary thickness. El-Kabeir et al. [32] employed the group theoretic method to simulate coupled magnetohydrodynamic heat and mass transfer from an impermeable horizontal cylinder to porous medium saturated with a non-Newtonian power law fluid. Several researchers have also discussed *magneto-micropolar flows with heat transfer*, where the *nonlinearity* of the differential flow conservation equations has generally necessitated numerical analysis. For example Mansour et al. [33] investigated hydromagnetic mixed thermal convection from a horizontal cylindrical body using numerical methods. In the present study we extend the non-magnetic study by Nazar et al. [34] to consider hydromagnetic effects on micropolar free convection boundary layer from a constant heat flux horizontal circular cylinder. Such a study has important applications in the simulation of magnetic field control of ECBP flows with heat transfer and has to the authors' knowledge, not appeared thus far in the technical literature. We study the effects of Hartmann number (*Ha*), Grashof number (*Gr*), micropolar vortex viscosity parameter (*K*) and Prandtl number (*Pr*) on the linear velocity, micro-rotation and temperature profiles using Network Simulation Methodology (NSM) [35]. Validation of numerical solutions is achieved with the Nakamura tridiagonal implicit finite difference scheme (NTS) [36]. The present study, as elaborated earlier, is motivated by further investigating *enrobing hydrodynamics of magnetic non-Newtonian biopolymers*. We employ micromorphic magnetofluid mechanics to investigate the industrial manufacturing processes for biologically-orientated applications of complex fluids including magnetic hydrogels (for bioassays), [37] rheological magnetic directed particle assembly [38], magnetorheological thin film biopolymers [39,40], magnetic "barcoded hydrogel microparticle" suspensions (of interest in multiplexed detection) [41] and microfluidic-based fabrication of magnetohydrodynamic hydrogel compositions [42]. These applications, many of which have been pioneered at the Massachusetts Institute of Technology (MIT), in recent years, have stimulated interest in how such materials can be magnetically manipulated during large-scale manufacture (industrial) for mass production and deployment in the biotechnology and magnetic medicine markets. It is envisaged that the present study will therefore stimulate some interest among researchers in further addressing this intriguing branch of computational biofluid mechanics.

2. Dynamics of magneto-thermo-micropolar biopolymeric fluids

In this study the electrically conducting thermal micropolar constitutive model i.e. *magneto-thermo-micropolar non-Newtonian fluid model* is implemented to simulate microstructural chacateristics of conducting biopolymers. Such a fluid is a special subclass of the much more complex electrically-conducting *thermo-micromorphic* fluid. In thermo-micropolar fluid mechanics, the classical continuum and thermodynamics laws are extended with additional equations which account for the conservation of micro-inertia moments and the balance of first stress moments which arise due to the consideration of micro-structure in a fluid. Hence new kinematic variables (gyration tensor, microinertia moment tensor), and concepts of body moments, stress moments and microstress are combined with classical continuum fluid dynamics theory. Thermo-micropolar fluids can accurately simulate liquids consisting of randomly orientated particles suspended in a viscous medium and offer an excellent framework to study advanced