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Numerical investigation of radiative optically-dense transient magnetized reactive transport phenomena with cross diffusion, dissipation and wall mass flux effects

O.A. Bég[a,*], M. Ferdows[b], E.T.A. Bég[c], T. Ahmed[d], M. Wahiduzzaman[d], Md. M. Alam[b]

[a] *Spray Research Group, School of Computing, Science and Engineering, University of Salford, Newton Building, The Crescent, Manchester M54WT, England, UK*
[b] *Department of Applied Mathematics, University of Dhaka, Dhaka 1000, Bangladesh*
[c] *Renewable Energy Research, Israfil House, 243 Dickenson Rd., M13 OYW, Manchester, UK*
[d] *Mathematics Discipline, Khulna University, Khulna 9208, Bangladesh*

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ABSTRACT

High temperature electromagnetic materials fabrication systems in chemical engineering require ever more sophisticated theoretical and computational models for describing multiple, simultaneous thermophysical effects. Motivated by this application, the present paper addresses transient magnetohydrodynamic heat and mass transfer in chemically-reacting fluid flow from an impulsively-started vertical perforated sheet. Thermal radiation flux, internal heat generation (heat source), Joule magnetic heating (Ohmic dissipation), thermo-diffusive and diffuso-thermal (*i.e.* cross-diffusion) effects and also viscous dissipation are incorporated in the mathematical model. To facilitate numerical solutions of the coupled, nonlinear boundary value problem, non-similar transformations are employed and the partial differential conservation equations are normalized into a dimensionless system of momentum, energy and concentration equations with associated boundary thermal conditions. An implicit finite difference method (*FDM*) is utilized to solve the unsteady equations. Verification of the FDM solutions for dimensionless velocity, temperature and concentration functions is achieved with a variational finite element method code (*MAGNETO-FEM*) and also a network simulation method code (*MAG-PSPICE*). The influence of the emerging thermo-physical parameters on transient velocity, temperature, concentration, wall shear stress, Nusselt number and Sherwood number is elaborated. The flow is accelerated with increasing thermal radiative flux, Eckert number, heat generation and Soret number whereas the flow is decelerated with greater wall suction, heat absorption, magnetic field and Prandtl number. Temperatures are also observed to be elevated with magnetic parameter, radiation heat transfer, Dufour number, heat generation (source) and Eckert number with the contrary effects computed for increasing suction parameter or Prandtl number. The species concentration is enhanced with Soret number and generative chemical reaction whereas it is depressed with greater wall suction, Schimidt number and destructive chemical reaction parameter

1. Introduction

Unsteady magnetohydrodynamic (MHD) boundary layer flows continue to stimulate significant interest in engineering sciences and applied physics owing to new emerging applications in magnetic materials processing [1], optimization of Hall and Faraday MHD generators [2], heat transfer control in nuclear reactors [3] and external ionized aerodynamics of flight vehicles [4]. The combined momentum, heat, and mass transfer from a vertical surface is particularly relevant to polymer processing dynamics [5] and also arises in electrochemical treatment of materials [6]. These flows may involve transverse static or alternating magnetic fields, oblique magnetic fields, Hall currents, ionslip effects and Alfven waves. They may also be laminar, transitional or turbulent in nature. The presence of diverse chemical reactions which are executed at different rates, in fluid mechanics processes in hydrometallurgy further necessitates mathematical modeling of thermal-mass diffusion processes including chemical reaction phenomena. Numerous transport processes feature combined buoyancy forces due to both thermal and mass diffusion in the presence of chemical reaction [7]. These processes are observed in chromatography, manipulation of materials, furnace combustion

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[*] Corresponding author. Tel.: +44 (0) 161 295 4570.
E-mail address: O.A.Beg@salford.ac.uk (O.A. Bég).

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systems, solidification of binary alloys and crystal growth dispersion of dissolved materials, drying and dehydration operations in food processing plants, and rocket atomized liquid fuel burning. The presence of foreign mass in water or air may frequently generate some kind of chemical reaction. In many chemical engineering processes such as polymeric sheet extrusion, chemical reactions, which may be homogenous or heterogenous occur between a foreign mass and the fluid material which moves as a sheet. The interaction between homogeneous reactions in the bulk of fluid and heterogeneous reactions occurring on some catalytic surfaces is generally very complex, and this phenomenon may yield and also consume reactant species at different rates both within the fluid and on the catalytic surfaces as elaborated in detail by Aris [7]. Many simplified mathematical models of such processes (often termed *Sakiadis flows*) have been communicated. Das et al. [8] studied the influence of first-order homogeneous chemical reaction of unsteady flow from a vertical plate with the constant heat and mass transfer. Ferdows and Al Mdadall [9] investigated multiple order chemical reaction effects on coupled heat and mass transfer from an extending polymer sheet, observing that velocity, temperature and concentration are all reduced with increasing Schmidt number with fixed order of chemical reaction. They also noted that velocities are enhanced with greater order of reaction with constant Schmidt number and that concentrations are more strongly modified than temperatures with increasing order of chemical reaction. Makinde and Bég [10] employed Arrhenius chemical kinetics to examine inherent irreversibility and thermal stability in reactive magnetohydrodynamic isothermal channel flow, deriving solutions based on a perturbation method coupled with a special Hermite–Pade' approximation technique. They studied the velocity field, temperature field and thermal criticality conditions and computed volumetric entropy generation numbers, irreversibility distribution ratio and the Bejan number for the flow, demonstrating the sensitivity of stability to chemical reaction effects. Uddin et al. [11] studied magnetized reactive nanofluid flow numerically, noting that the flow is accelerated and temperatures increased while nanoparticle volume fraction is suppressed with increasing order of chemical reaction. Rao et al. [12] examined the chemical reaction effects on transient magneto-convection in porous media with heat generation. Zueco et al. [13] used an electrothermal network method and the PSPICE software to analyze double-diffusive reactive convection from a buried cylinder in geological material. Mukhopadhyay et al. [14] examined transport of a species (solute), undergoing a chemical reaction, between a moving surface and a moving stream, showing that concentration boundary layer thickness is reduced with greater Schmidt number and reaction rate parameter, and mass absorption at the plate arises with a constructive chemical reaction. Makinde et al. [15] studied variable viscosity effects on a radially stretching nanofluid surface. Siddheshwar and Manjunath [16] investigated the effects of heterogeneous chemical reaction on the exchange, convective and diffusive coefficients in transient dispersion in a micropolar tube flow, showing that first coefficient arises due to the catalytic wall reaction which also modifies the other two coefficients.

Unsteadiness is also an important in coupled thermal and species diffusion problems. Time can have a significant influence on evolution of concentration and temperature profiles in boundary layer flows. Representative investigations of transient convective heat and mass transfer include Ruckenstein [17], Chang et al. [18] employed a local non-similarity method to study unsteady species diffusion in non-Newtonian boundary layer flows along a porous sheet. Unsteady nanofluid flow from a rotating stretching polymer sheet has been analyzed using a finite element method by Rana et al. [19]. Further studies of time-dependent diffusive boundary layer flows include Hussanan et al. [20] who considered unsteady magnetic convection in permeable materials with special thermal boundary conditions.

The above studies have neglected so-called “cross diffusion” effects. When heat and mass transfer occur simultaneously driving potentials between the fluxes can be of a more intricate nature. An energy flux can be generated not only by temperature gradients but by composition (species diffusion) gradients. The energy flux caused by a composition is called the Dufour or diffusion-thermo effect. Temperature gradients can likewise also create mass fluxes, and this is termed the Soret or thermal-diffusion effect. Generally, the thermal-diffusion and the diffusion thermo effects are of smaller-order magnitude than the effects prescribed by Fourier's or Fick's laws and are often neglected in heat and mass transfer processes. The thermal-diffusion effect, for instance, has been utilized for isotope separation and in mixing between gases with very light molecular weight (Hydrogen, Helium *etc*) and of medium molecular weight (Nitrogen–air) the diffusion-thermo effect was found to be of a significant magnitude. A very good review of the fundamentals of Dufour–Soret convection is provided in Gebhart [21] albeit for non-magnetic scenarios. Boundary-layer flows in the presence of Soret, and Dufour effects and with mixed convection have been addressed by several authors both with and without magnetic fields. Islam and Alam [22] investigated Dufour and Soret effects on transient hydromagnetic convection heat and mass transfer flow in rotating porous media. Mansour et al. [23] obtained shooting solutions for reactive cross-diffusion magnetized boundary layer flow in thermally-stratified porous media. Prasad et al. [24] obtained numerical finite difference solutions for steady-state magnetohydrodynamic double-diffusive natural convection in non-Darcy porous media with Soret (thermo-diffusion) and Dufour (diffusion-thermo) effects included. They showed that increasing Soret number and simultaneously decreasing Dufour number boosts the local heat transfer rate (local Nusselt number) with the converse response computed for the mass transfer rate (local Sherwood number). Bég et al. [25] investigated Soret and Dufour effects on magneto-convection along an extending sheet embedded in a porous medium. Further examples of Soret–Dufour convection include Uwanta et al. [26] who examined magnetized Soret–Dufour flow from a vertical sheet under buoyancy forces. Bég et al. [27] studied Soret/Dufour effects on inclined plate solar panel convection.

Materials processing is frequently conducted at very high temperatures in which thermal radiation becomes significant. The interaction of buoyancy with thermal radiation is also often present in such processes and this permits the modification of flow fields and heat and mass transfer phenomena in order to produce specific characteristics in materials. Both isothermal and non-isothermal scenarios are relevant. Typical examples of materials fabrication applications include super alloy metallurgical liquid metal manufacturing [28], enclosure flows [29] and laser processing of magnetic materials [30]. Thermal radiation by its nature is intrinsically significantly more complex to simulate than conduction or convection. Not only is radiation a quartic temperature function, it also involves spectral effects, wavelength considerations, attenuation, sensitivity to geometrical characteristics and many other aspects. The general equation describing thermal radiation is also *integro-differential* in nature. For this reason it poses a formidable challenge for even numerical methods. Although numerous approaches have been developed for computing solutions to the radiative transfer equation including Chandrasekhar's discrete ordinates method [31] and Hamaker's 6-flux model [32], even these methods have their limitations and are computationally extremely intensive. They are also very difficult to implement for multi-physical flows where other body forces *e.g.* magnetic, gravity, surface tension *etc*, may be present and generally necessitate the use of commercial CFD