# 3

# COMPUTATIONAL MECHANICS

*Work initiated on homotopy analysis method has been continued. A number of industrially significant problems have been considered and it has been demonstrated that the homotopy analysis method gives good results. It is also planned to extend our work on periodically forced suspensions to inertial particles. Work on computational nanomaterials and nanomechanics of complex materials has also been carried out. As part of the progress work on kernel determination for one dimensional carbon nano-structures has been carried out.*

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- ***Mass transfer effects on viscous flow in an expanding or contracting porous pipe with chemical reaction***
- ***The effect of particle inertia on periodically forced triaxial ellipsoids in creeping shear***
- ***Computational nanomaterials and nanomechanics of complex materials***
- ***Kernel determination for one dimensional carbon nanostructures***
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## 3.1 Influence of heat transfer on MHD flow in a pipe with expanding or contracting permeable wall

This investigation deals with the analysis of heat transfer and MHD viscous flow in a porous pipe with expanding or contracting wall as shown in Figure 3.1 below. Using suitable similarity transformations, the governing equations are reduced to a system of coupled nonlinear differential equations. The resulting equations are solved by employing the homotopy analysis method (HAM). The main findings are summarized as follows:

1. For a constant wall expansion ratio α, the dimensionless axial velocity near the center increases with increasing suction while it decreases with increasing injection.
2. For given increase in Hartmann number (M), the dimensionless axial velocity decreases little away from the pipe wall. For every level of injection or suction, for the case of wall contraction, the absolute dimensionless radial velocity decreases with increasing |α| whereas it increases as α increases for the case of wall expansion. The absolute dimensionless radial velocity decreases as M increases.

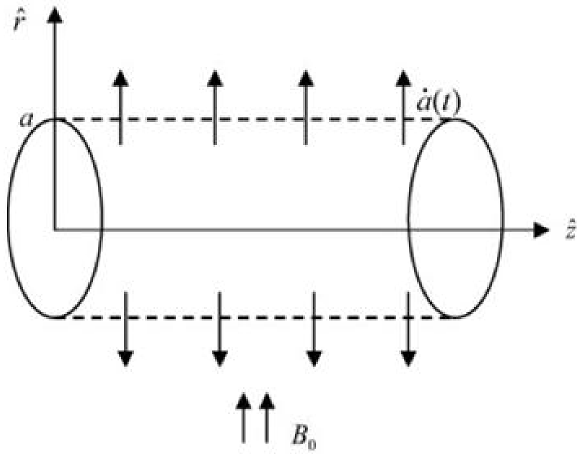

**Figure 3.1 Porous pipe with expanding or contracting wall.**

$\hat{r}$ —Expansion or contraction direction
$\acute{a}$(t)- Rate of expansion or contraction
a- Radius of the pipe
$B_0$- Magnetic Field

3. For every level of suction or injection, θ (dimensionless temperature) increases as α increases for the case of wall expansion while it decreases as |α| increases for the case of wall contraction. Further, θ decreases with increasing Pr (Prandtl number).
4. The absolute wall shear stress increases as M increases.
5. The absolute axial pressure distribution |ΔPr| decreases as M increases.

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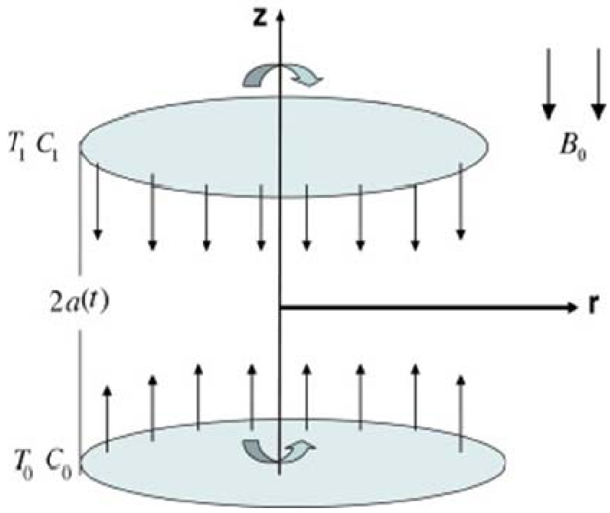
## 3.2 Thermal-diffusion and diffusion-thermo effects on MHD flow of viscous fluid between expanding or contracting rotating porous disks with viscous dissipation

This investigation examines the effects of thermal-diffusion and diffusion-thermo on MHD flow of viscous fluid between expanding or contracting rotating porous disks with viscous dissipation as shown in Figure 3.2. Convergence of the obtained series solutions is analyzed. The results obtained by HAM are in good agreement with numerical solutions obtained by a shooting method coupled with Runge–Kutta scheme. The temperature distribution increases while the concentration decreases with an increase in R (permeation Reynolds number), R* (rotation Reynolds number), Du (Dufour number), and Sr (Soret number).



$C_0$,$T_0$- Concentration and Temperature of Bottom Plate
$C_1$,$T_1$- Concentration and Temperature of Top Plate
2a- Distance between the two plates
$B_0$- Magnetic Field

**Figure 3.2 The model for expanding or contracting porous disks**

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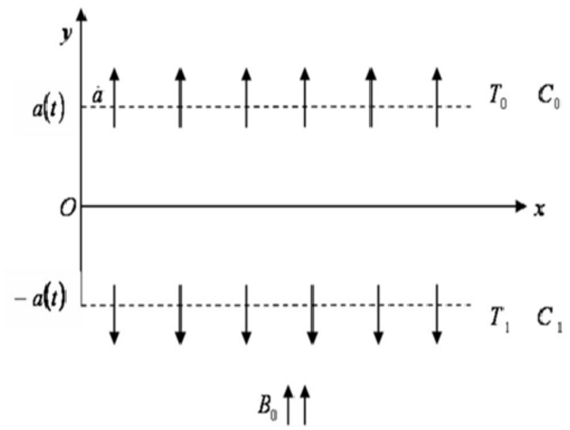
## 3.3 Hydro magnetic flow of a nanofluid in a porous channel with expanding or contracting walls

The present study investigates the hydro magnetic flow of a nanofluid in a two-dimensional porous channel between slowly expanding or contracting walls as shown in the Figure 3.3. Assuming symmetric injection (or suction) along the uniformly expanding porous walls and using a similarity transformation, the governing flow equations are reduced to nonlinear ordinary differential equations. The resulting equations are then solved analytically by by using the homotopy analysis method (HAM).



$C_0$,$T_0$- Concentration and Temperature of Top wall
$C_1$,$T_1$- Concentration and Temperature of Bottom wall
2a- Distance between the two plates
$\acute{a}$- Rate of expansion or contraction
$B_0$- Magnetic Field

**Figure 3.3 Two-dimensional domain with expanding or contracting walls**

The convergence of the obtained series solutions is analyzed through the minimization of the averaged square residual error. A comparison between analytical and numerical solutions is presented for validation in both graphical and tabular forms. The results obtained by HAM are in very good agreement with numerical solutions obtained by the shooting method coupled with a Runge-Kutta scheme. The effects of various physical parameters such as wall expansion ratio, Brownian motion parameter, thermophoresis parameter, and Lewis number on flow variables are discussed. The analysis shows that for the case of contracting walls, the temperature increases for a given increase in Brownian motion parameter, and the thermophoresis parameter. In addition, the nanoparticle concentration increases with an increase in Brownian motion parameter and Lewis number.

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## 3.4 Mass transfer effects on viscous flow in an expanding or contracting porous pipe with chemical reaction

An analysis is performed to study the effects of mass transfer and chemical reaction on laminar flow in a porous pipe with an expanding or contracting wall. The pipe wall expands or contracts uniformly at a time dependent rate. The governing equations are reduced to ordinary differential equations by using a similarity transformation. An analytical approach, namely, the homotopy analysis method is applied in order to obtain the solutions of the ordinary differential equations. The convergence of the obtained series solutions is analyzed. The effects of various parameters on flow variables is discussed. It is noticed that the wall expansion ratio significantly increases the axial velocity and the concentration for the case of wall expansion and it decreases the axial velocity for the case of wall contraction irrespective of injection or suction. Further, it is observed that the concentration $(\phi)$ decreases for a destructive chemical reaction $(\gamma > 0)$ and increases for a generative chemical reaction $(\gamma < 0)$. The concentration reduces as Schmidt number (*Sc*) increases. The corresponding problem related to a porous pipe flow with a stationary wall can be recovered from the present analysis in the limiting case where the wall expansion ratio approaches to zero (i.e., $(\alpha = C)$.

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## 3.5 The effect of particle inertia on periodically forced triaxial ellipsoids in creeping shear

This investigation deals with determining the effects of particle inertia on periodically forced inertial ellipsoids in creeping shear.

Starting from the ellipsoid equation, the position and orientation of an arbitrary rigid body is described in terms of seven generalized co-ordinates, namely Cartesian components of the centre of mass vector (c) and a four component vector of Euler parameters (e) . The Euler parameters are defined in an orthogonal rotation matrix which is in a fixed Cartesian co-ordinate system. These equations are then converted to the body fixed rotating frame. Since Newton’s laws are valid only in a fixed (or a laboratory frame of reference), the moment of inertia of the particle is found in the fixed frame by the Euler transformation. Jeffery’s torque, as derived for constant shear rate, is planned to be used for the periodic torque with the equations derived by Hamilton’s Equations with Euler parameters for rigid body dynamics modelling. The resulting equations were non-dimensionalized. The resulting ODEs will be solved using the ODE solvers (ODE45 and ODE113) with high accuracy as provided by MATLAB. Wolfram Mathematica has been used extensively for the matrix operations and evaluating the definite integrals required.

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## 3.6 Computational nanomaterials and nanomechanics of complex materials

Computational simulations of nanostructures at atomic levels are expensive in terms of cost. CSIR 4PI's High Performance Super computers have been used to simulate and analyse the properties of carbon nantotubes and graphene. Molecular Dynamics Simulations (MDS) are used for modification of existing continuum models to predict behavoiur of nanostructures without conducting experiments. Higher order gradient mathematical models are proposed to replace existing continuum elasticity models by addressing their pitfalls as compared with the lattice dynamics results. Modelling and Simulation of complex materials like graphene; penta-graphene and Meta materials need to be investigated further.

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## 3.7 Kernel determination for one Dimensional carbon nanostructures

Recently, growing interest in terahertz physics of nanoscale materials and devices has drawn more attention to the Carbon Nanotubes (CNTs) phonon dispersion relation, especially in the terahertz frequency range. Since terahertz physics of nanoscale materials and devices are major concerns for CNT wave characteristics, small-scale effects must be considered since the wavelength in the frequency domain is of the order of nanometers. Explicit dispersive solutions are derived in the work, from which small-scale effects can be clearly observed. Such observations are vital for applying continuum models to obtain CNT wave characteristics. To help in development of improved and efficient continuum models for predicting the mechanical response of CNTs it is imperative to determine the best kernel that can capture the physics of small scale effects as discussed above. The most popular approach for determining the kernels is by matching with phonon dispersion curves. Several important kernels have already been discussed. Additionally, one more "BEST FIT" approach used by Sundararaghavan and Waas [2010] is implemented in which the fourier transform of the kernel is directly estimated by matching the atomistic data to the dispersion curves predicted from the nonlocal continuum model theory. The predictions of different kernels are compared. The longitudinal wave dispersion curves in single walled carbon nanotubes (SWCNT) are used to estimate the non-local kernel for use in continuum elasticity models of nanotubes. The dispersion data for an armchair (10,10) SWCNT was obtained using lattice dynamics of SWNTs while accounting for the helical symmetry of the tubes (Sundararaghavan, Waas [2010]).

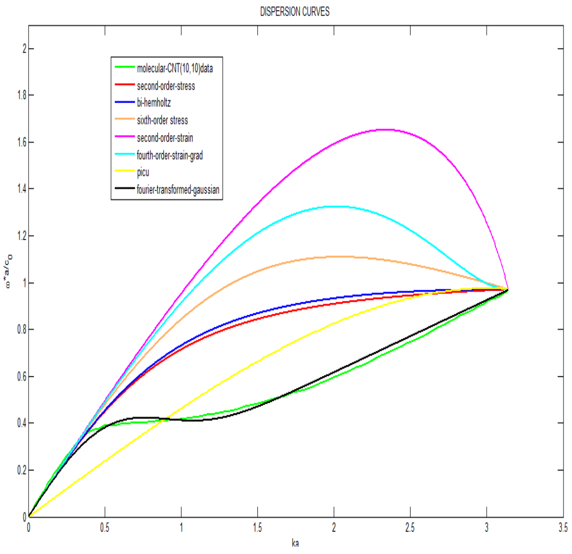

**Figure 3.4 Phonon dispersion curve (comparison with the atomistically computed longitudinal mode of (10,10) nanotube) with various models.**

Dispersion curves (Figure 3.4) for the nanotube computed from this approach are used to obtain the expression for $\alpha(k)$ (the Fourier transform of the non-local kernel) through comparison with the one dimension carbon nanotube model. The Best fit (fourier transformed Gaussian) kernel gives the best fit to the atomistically computed kernel. Gradient theories which reasonably reproduce the phonon dispersion curve for the Born-Kármán model of lattice dynamics (harmonic spring model) are not able to predict complex lattice dynamics found in the case of nanotubes. Picu kernel also fails because it has been constructed for a special case of interatomic potentials depending only on pair interactions (or through embedded functions that are functions of radial distance only). Such an approach cannot be successfully used for CNTs since carbon atom interactions in the CNT are typically multibody potentials that depend on atom coordination (Brenner potential) or three or four body interactions (Force field potentials).

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## 3.8 Nanoscale Effect on Vibration Analysis of Double Walled Carbon Nanotube using Nonlocal Continuum Model

The double walled carbon nanotube is modelled as two single walled carbon nanotubes connected with van der Waals force. Various frequency modes with different initial conditions for the present mathematical model are analysed using a semi-analytical method. The frequency ratio is defined as the ratio between nonlocal frequencies to classical continuum model frequency. The frequency ratio for boundary conditions like Simply Supported (Figure 3.5), Clamped Clamped and Clamped Hinged is decreasing with the increase of the nonlocal effect. However it increases for the Clamped Free boundary conditions of the double walled carbon nanotube. Further it has been observed that increase in the nonlocal parameter decreases the non dimensional frequency for the first four modes.

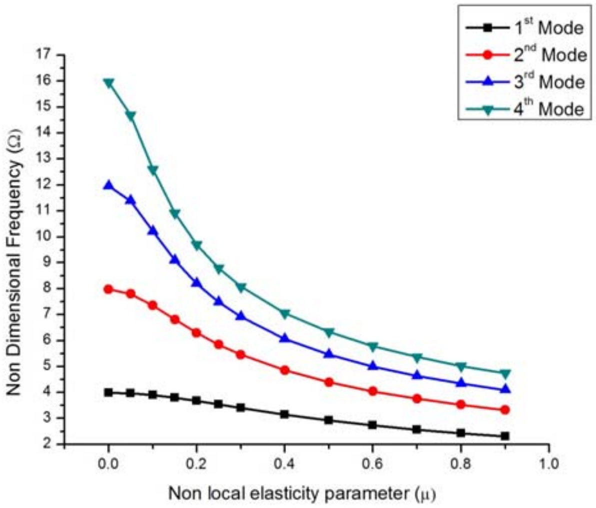

**Figure 3.5 Small scale effects on first four mode frequency parameter for SS condition**

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