3
COMPUTATIONAL MECHANICS

Sophisticated mathematical modelling aided by powerful computing and visualization has the potential to provide cutting-edge to industry; generation of cost-effective solutions, process optimization and product design are some of the areas where modelling and simulation can play critical to enabling role. The CSIR-4PI Computational Industrial Mechanics Programme (CIMP) seeks to develop and apply tools of mathematical modelling and computer simulation in diverse areas of engineering.

Inside

- *Computational Modelling and Simulations of Nanocomposite Properties*
- *Dispersion of plane waves with higher-order nonlocal continuum model using bi-Helmholtz operator approach*
- *Nanotechnology: Continuum to Atomic Scales*
- *Computational Stability Analysis of Graphene Sheet*
- *MHD flow of a nanofluid in an expanding or contracting porous pipe with chemical reaction and heat source/sink*
- *Thermal-diffusion and diffusion-thermo effects on MHD flow of viscous fluid between expanding or contracting rotating porous disks with viscous dissipation*
- *Influence of thermal radiation on unsteady flow over an expanding or contracting cylinder with thermal-diffusion and diffusion-thermo effects*
- *Mass transfer effects on viscous flow in an expanding or contracting porous pipe with chemical reaction*
- *Impact dispersion using 2D and 3D composite granular*

3.1 Computational modelling and simulations of nanocomposite properties

Nanocomposites have superior material properties comparedto composite materials with micro-mechanical properties. The effective material properties of composites contain randomly oriented nanostructured fibers and are modeled with continuum models. The stress-strain relations based on longitudinal and transverse directional properties are computed. The Mori-Tanaka model or Halpin-Tsai are used to study the mechanical properties of nanocomposite structures. The Molecular Dynamics Simulations are used as an alternative way to determine the mechanical properties of structures made up of nanocompositematerials.

Senthilkumar V

3.2 Dispersion of plane waves with higher-order nonlocal continuum model using bi-Helmholtz operator approach

The continuum models fail at atomic scale. The nonlocal continuum models are good at predicting dispersion characteristics of waves better than the conventional continuum models. The nonlocal continuum approach based on Eringen model predicted the dispersion nature which is in agreement with atomic based Born-Karman model.

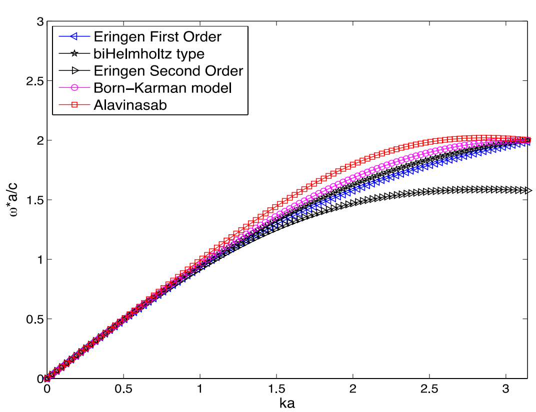

Figure 3.1 The dispersion characteristics gradient models

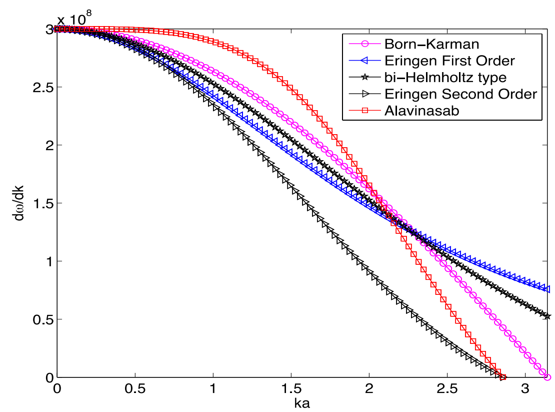

Figure 3.2 The group velocity characteristics gradient models

For the first time, the higher-order stress gradient model with bi-Helmholtz operator has been proposed. The present model has been examined with the other models like Eringen model, Alvinasab model, and Eringen second order model. The Born-Karman model is the realistic model to study the atomic level interaction and small sized structures. From Figure 3.1, it is very clear that the present model has very close agreement with atomic based model compare to all other models. The group velocity also predicted better than other models as shown in Figure 3.2.

Senthilkumar V and Chaudhary T *
*(*IIT BHU, Varanasi)*

3.3 Nanotechnology: Continuum to atomic scales

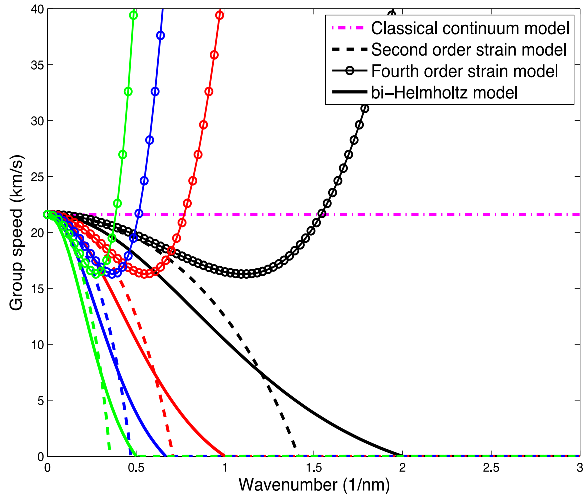

Figure 3.3 Group speed of carbon nanorod with various gradient models

The nonlocal continuum models are modeled with lattice parameters/distance between the atoms etc. The second order strain model, fourth order strain model and bi-Helmholtz models have two small-sized parameters. Depending on the applications, these parameters are considered. The carbon nanorod with ultrasonic frequency analysis are analyzed and the group speeds are studied (Figure 3.3) for the axial waves. It is clear that the bi-Helmholtz model predicts the group speed better than the other gradient models. These small-scale parameters are evaluated using lattice dynamics models. The experimental studies are expensive and difficult to control at atomic level. So molecular dynamics is used to calibrate the small-scale parameters.

Senthilkumar V

3.4 Computational stability analysis of graphene sheet

The equivalent continuum model with nonlocal continuum effect is developed to study the stability analysis of Graphene sheet. Unlike continuum models, the present model involves boundary conditions with small-scale effect. The Differential Quadrature Method (DQM) has been developed to study stability analysis of graphene sheet. Combining matrix methods of analysis for structures and DQM, analyses are carried out. The collocation polynomials are used as basis functions. The computational programming code has been developed and critical stability studies are carried out.

*Senthilkumar V and Shriyans Bagla**
*(*IIT BHU, Varanasi)*

3.5 MHD flow of a nanofluid in an expanding or contracting porous pipe with chemical reaction and heat source/sink

In the present investigation, an analytical approachhas been used to study the influence of chemical reaction on MHD flow of a nanofluid in an expanding or contracting porous pipe in the presence of heat source/sink. The pipe wall expands or contracts uniformly at a time dependent rate. Similarity transformations have been invoked to reduce the governing flow equations into coupled nonlinear ordinary differential equations. Homotopy analysis method (HAM) is employed to obtain the analytical solutions of the ordinary differential equations. The convergence of the obtained series solutions is analyzed. The effects of various physical parameters such as wall expansion ratio, Brownian motion parameter, thermophoresis parameter, Lewis number, chemical reaction parameter and heat source/sink parameter on flow variables have been discussed. Further, for the case of hydrodynamic viscous fluid, we find a good agreement between the HAM solutions and solutions already reported in the literature.

Srinivas S*, Vijayalakshmi A*, Subramanyam Reddy A*
and Ramamohan T R *(*VIT, Vellore)*

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

The present work investigates the effects of thermal-diffusion and diffusion-thermo on MHD flow of viscous fluid between expanding or contracting rotating porous disks with viscous dissipation. The partial differential equations governing the flow problem under consideration have been transformed by a similarity transformation into a system of coupled nonlinear ordinary differential equations. Homotopy analysis method is employed in order to obtain the solutions of the ordinary differential equations. The effects of various emerging parameters on flow variables have been discussed numerically and explained graphically. Comparison of the HAM solutions with the numerical solutions is performed.

Srinivas S*, Reddy A S*,Ramamohan T R and Shukla A K**
*(*VIT, Vellore, **Amrita Vidyapeetham, Coimbatore, Vellore)*

3.7 Influence of thermal radiation on unsteady flow over an expanding or contracting cylinder with thermal-diffusion and diffusion-thermo effects

An analytical study is conducted to present thermal radiation, Dufour, and Soret effects on unsteady viscous flow over a contracting cylinder. The coupled nonlinear partial differential equations are transformed into a system of coupled nonlinear ordinary differential equations by using a suitable similarity transformation. The homotopy analysis method (HAM) and HAM with a nonhomogeneous term are employed to obtain analytical solutions for the system of coupled nonlinear ordinary differential equations. A significant reduction in the averaged square residual error is obtained when the nonhomogeneous term is introduced. A comparison between analytical and numerical solutions is presented for validation. The effects of various emerging parameters on flow variables are discussed. It is found that the temperature distribution increases with an increase in Dufour number, but decreases with an increase in Soret number. The concentration distribution decreases for a given increase in the Dufour number, but increases with an increase in Soret number.

Srinivas S*, Shukla A K **, Ramamohan T R and Reddy A S*
*(*VIT, Vellore, **Amrita Vidyapeetham, Coimbatore, Vellore)*

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

In this work, 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. HAM 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 have been 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 (ϕ) 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 the 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.,$\alpha=0$).

Srinivas S*, Reddy A S* and Ramamohan T R*(*VIT, Vellore)*

3.9 Impact dispersion using 2D and 3D composite granular packing

We present a study of efficient dispersion of an impact onto structured and potentially scalable granular beds. We use discrete element method based dynamical simulations of shock wave propagation and dispersion in 2D and 3D arrangements of granular spheres. The spheres are geometrically packed in a nested columnar structure, which leads to the severe attenuation and spreading of the incident energy within the structure. We further show that by incorporating inhomogeneity in material properties, or by introducing layers of a dissimilar material in the middle of the arrangement, impact mitigation can be enhanced significantly. Such an arrangement can therefore be useful in the design of effective impact decimation systems. Using a 2D arrangement we first show the basic idea behind impact dispersion in such an arrangement. With this understanding the system is scaled to 3D. The influence of the system size and material properties on the wave propagation within the packing is also presented.

Sen S*, Krishna Mohan T R and Tiwari M**
*(*State University of New York, USA ,**DA-IICT, India)*