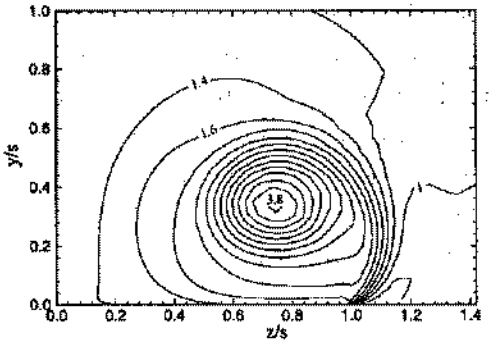
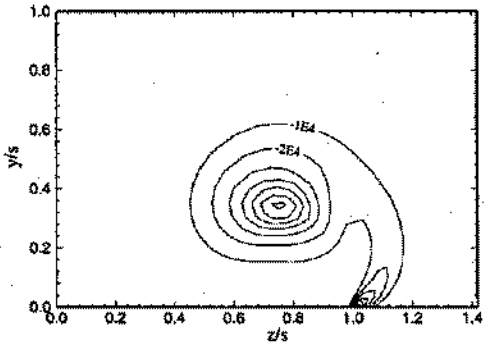
Simulation of Leading-Edge Vortex Flow Using an Embedded Conical Grid

Leading-edge vortex flow is employed in the design of modern high performance aircraft capable of sharp manoeuvres. Its numerical simulation employing conventional grids however gives a poor resolution of the near-apex flow because of the dissimilar length scales of the flow and the grid. The poor resolution of the vortex will give a lower vortex suction and may affect other vortex related phenomena. The problem is overcome by a new type of grid, called the embedded conical (EC) grid.

Work has been carried out to demonstrate that an EC grid provides an accurate capturing of the vortex formation and its development near the apex of a sharp-edged delta wing, by comparing the Euler solutions on the EC grid with that on a conventional H-O grid for a range of incidence. The EC grid solutions show that the vortex, as seen from the contours of velocity, vorticity and pressure fields, is well resolved right from the apex. The peak suction along the vortex axis is attained close to the apex. The near-apex flow remains well resolved even at a very low incidence. The vortex breakdown is well predicted on the embedded conical grid, including the case where the breakdown has just moved upstream of the trailing-edge. The above features of the flow were found to be not satisfactorily resolved on the comparable H-O grid. Vortex resolution



(a)



(b)

Fig. 14: Contours of (a) axial velocity and (b) chordwise vorticity in the first computational plane downstream of the apex ($x = 0.00128$) for a 70° delta wing at 30° incidence, showing the resolution of the near-apex vortex structure on the EC grid

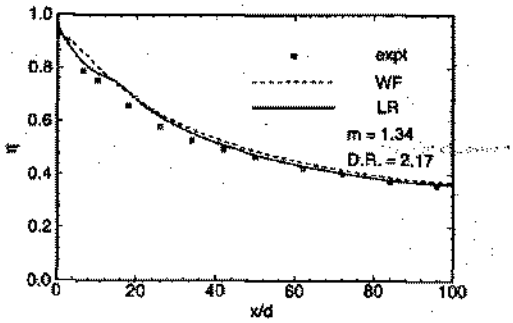


Fig. 15: Comparison of computed film cooling effectiveness using the two turbulence models, with the experiment

near the apex of a 70° delta wing is shown in Fig. 14. The investigation of vortex breakdown employing the EC grid is under progress. The top right panel on the front cover shows breakdown causing a sudden broadening of the vortex core, shown by the near-axis streamlines (note the straight vortex axis ahead of the breakdown), and the loss of suction in the core, shown by the pressure in the transverse planes. *(A. Kumar)*

Film Cooling

Film cooling refers to the employment of a secondary cold fluid injected through discrete slots to thermally insulate a solid surface from a hot gas stream flowing over it. Film cooling is a widely used technique for protecting components, such as high pressure turbine blades, from the hot gases from combustion chamber, rocket nozzles and cones. Numerical study of film cooling on a flat plate where the coolant jet is injected through a two-dimensional slot is being carried out.

The computation employs a pressure based algorithm to solve the Navier-Stokes equations. The turbulence is modelled using a $k-\epsilon$ model with either a wall funcion (WF) approach or a low Reynolds number (LR) model. Comparison of the predicted film cooling effectiveness with the experimental values (Papell, 1960 NASA TN-D-299), for a given test condition is displayed in Fig. 15. *(A. Kumar and G. Madhav*, * Student trainee)*

Laser Welding of an Iron-Nickel Alloy: An Experimental and Numerical Study of Double-Diffusive Marangoni Convection

The laser surface treatment can selectively modify the surface properties of metals such as wear and corrosion. In laser surface melting problems, a laser beam impinges on the surface giving rise to large temperature gradients between the hot region where the beam impinges and the relatively cold edges of the workpiece. This temperature difference along the free surface causes variations in the surface tension which can setup fluid motion, called thermocapillary flow or Marangoni convection. It is important to obtain information on velocity and temperature profiles in the melt to make meaningful predictions of the nature and extent of variation in the resulting microstructure and/or segregation patterns after solidification takes place.

Based on discussions during the workshop on modelling of macrosegregation held at C-MMACS (C-MMACS Annual Report 1994-95) and the importance of the iron - nickel alloy (steel and its variants), a fundamental study of the laser surface melting problem has been carried out with the objective of predicting the segregation patterns by considering an idealized model of mixing of two molten metals. Boundary conditions, initial conditions and dimensions of the weld pool have been obtained from experiments conducted at the Department of Metallurgy, Indian Institute of Science, Bangalore. Effects of thermal Marangoni, solutal Marangoni (variation of surface tension due to changes in concentration), thermal buoyancy, solutal buoyancy,

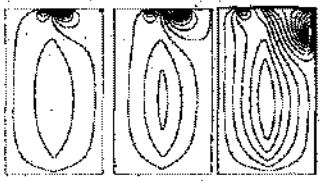


Fig. 16: Development of flowfield during a welding process

property variation with temperature, and compositional dependence of the binary diffusion coefficient have been modelled. Spatial and temporal evolution of the unsteady flow, driven primarily by surface tension gradients and modified by buoyancy effects, has been studied over a range of parameters. Comparison of the predicted iron concentration profiles at various sections with experimentally measured values seems to indicate the validity of using a simple (from a geometry point of view) mixing model for predicting the segregation patterns during laser surface melting. Most analyses neglect the effects of buoyancy in such problems based on a simple scaling argument. While this may provide prediction of gross features such as the cooling rate, the work clearly shows the importance of buoyancy in answering questions related to the existence of oscillatory solutions, temporal evolution of flow and estimation of penetration depths. Fig. 16 shows the flow development during the initial stages of the welding process. *(M.S. Phanikumar, Balaji Sundaram* and K. Chattopadhyay†, * TISCO, Jamshedpur, † Metallurgy Department, IISc, Bangalore)*

Thermal Effluent Disperion Near Madras Coast

As a part of a study aimed at understanding and assessing the environmental impact of a proposed thermal power plant at Pillai Perumalnallur near the Madras coast, a

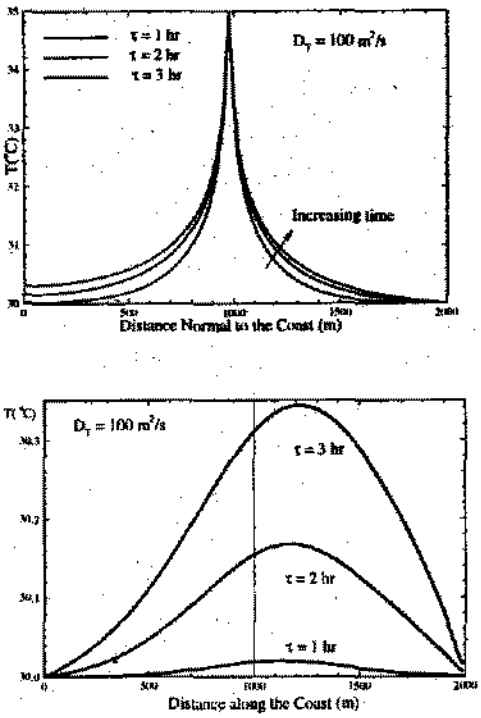


Fig. 17: Temperature variations across the coast, and along the coast

modelling and simulation experiment has been carried out in colloboration with NIO, Goa. Bathymetry of the region of interest as well as observations of hydrodynamics have been obtained from NIO.

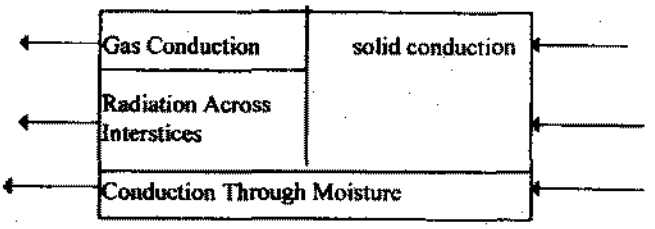
The model, based on the vertically integrated shallow water equations, has been integrated numerically to predict the temperature field in the region for several scenarios. Simulations of temperature field for different dispersivities and discharge locations as well as temperature variations along the coast and across the coast have been made to assess a possible worst scenario situation. Fig. 17 shows the temperature variations across the coast and along the coast for one of the scenarios. *(M.S. Phanikumar and P. Chandra Mohan*, * NIO, Goa)*

Design and Scale up of Coke Ovens

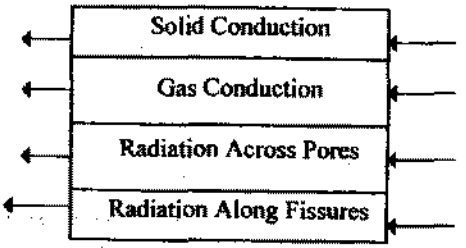
Formation of coke from coal is a very involved and complex process. In this process coal is indirectly heated upto $1300 - 1400°C$ in absence of oxygen to increase the carbon content of coal. An attempt has been made to mathematically model coke oven processes to assist in design and setting up of operations of bottom heated coke ovens. The mathematical model can be used as a cost-effective tool to analyse the various design variables and options, because the assessment of changes in design or operations by tests on experimental ovens are time consuming and expensive. Coal when heated undergoes various reactions as mentioned below:

$$\text{Coal} \rightarrow \text{metaplast}$$
$$\text{Metaplast} \rightarrow \text{semicoke} + \text{PVM}$$
$$\text{Semicoke} \rightarrow \text{coke} + \text{SVM}$$

where PVM and SVM represent primary and secondary volatile matter respectively. These are assumed to be first order parallel system of reactions. Volatile matter consists of several chemical species, such as methane, ethane, carbon mono-oxide, carbon di-oxide, tar, hydrogen, water, ammonia and hydrogen di-sulfide. The yield of each species depends on the type of coal. As the volatile matter is released from the solid matrix of coal, it becomes more porous and as suggested in the reactions above, it forms a metaplast state. With further increase in temperature it resolidifies at about $1023K$ after which there is shrinkage of coal. The entire process is classified into two regimes: a particulate regime and a coke charge regime. The first two reactions represent the particulate charge which takes place below resolidification temperature of coke. The third reaction represents coke charge. The conversion of coal to coke is assumed to be complete when the whole bed attains the temperature of $1023K$.



(a) Particulate charge heat transfer processes



(b) Coke charge heat transfer processes

Fig. 18: Heat transfer processes occuring inside the coke ovens

In the particulate and coke charge heating, coal undergoes structural changes causing significiant porosity changes. Porosity and density of coal can then be estimated from the emperical correlations. A kinetic expression relating the chemical composition of the coal and the amount of volatile gases evolved is used to calculate the chemical composition of the coal at any given time. The activation energy and frequency factor involved in these calculations are temperature dependent. Heat transfer processes which accompany the evolution of gases are presented schematically in Fig. 18 for the particulate and the coke charge heating.

A heat conduction equation with an advection term coupled with kinetics of volatile matter evolution was solved numerically to get the temperature profiles in the bed for different bed heights. The time required to attain the $1623K$ (i.e. the temperature at which the conversion of all the coal and semi-coke to coke is assumed to be complete) for different bed

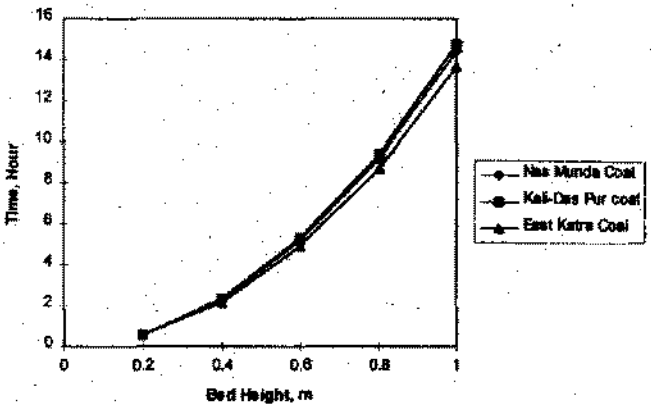


Fig. 19: Time required to attain $1623K$ for various types of coals

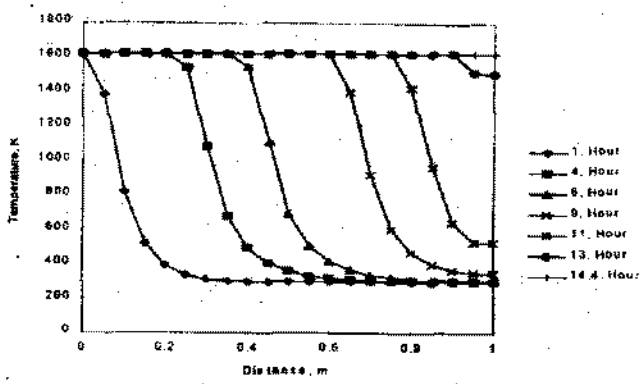


Fig. 20: Temperature profiles in $1m$ length of coal beds in the coke ovens

heights is also calculated. In these calculations it was assumed that the bed acts as a slab and the change in the densities do not change or alter the overall bed height. All the heat transfer processes in the above reactions are incorporated by employing an effective thermal conductivity in the heat conduction equation. All other properties (heat capacity of coal and gas, and porosity of bed) of coal/coke are evaluated by the emperical correlations which incorporate the changes in the densities with temperature and chemical composition.

Time required for attaining $1623K$ is plotted against the different bed heights for different types of coal in Fig. 19. As expected, the figure indicates that the saturation time has increased with increase in height of the bed. Fig. 20 indicates temperature profiles in the bed at different times. There is drastic drop in temperature in each profile and the temperature profile is seen to be moving as a front.

(R.A. Sohony, K.S. Yajnik, P.S. Swathi, M.K. Sharada, K.S. Narasimhan, A.K. Mukherjee*, A. Chowdhary* and J. Roy*, * CFRI, Dhanbad)*

Design of Multi-Layered Road Systems

Design of pavements is an important area in the field of highway engineering as it is an essential element for the structural evaluation of extant pavements for decisions on their maintenance.

Collection of pavement deflection data for the development of a mathematical model for analysis of the multilayer road system as prevalent in India, is in progress. Towards this end an experimental pavement section was constructed in the CRRI test bed for testing under controlled conditions. Deflection data has been generated by FWD over a wide range of wheel loads. Table 6 gives details of the data. The average scaled deflection for various values of radial distance given in table has been plotted in Fig. 21.

Data has also been collected for different environmental conditions on a few typical road sections for this purpose. Some more test sections are being identified for data collection for the further generalisation of the model. Field work on these test sections under different stress levels and for various environmental situations is proposed to be taken up soon.

The project work concerning development of

Load Deflection (microns)							
Load (KPa)	P(1)	P(2)	P(3)	P(4)	P(5)	P(6)	P(7)
490	385	180	76	48	31	20	16
576	455	207	87	52	37	24	20
693	573	244	100	63	43	29	26
796	735	278	112	80	48	33	30

Table 6: Road deflection data for a test point

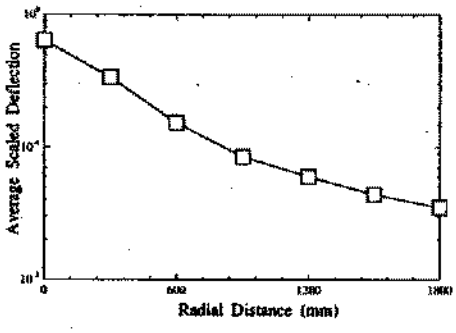


Fig. 21: Averaged scaled deflection (micron/KPa) vs radial distance (mm)

an inverse model and a software to determine the material properties of component layers of multi-layered road systems from surface measurements is under progress. *(Sridevi J., K.S.Yajnik, P.K.Nanda* and V.N.Kumar, * CRRI, New Delhi)*

Strength Contours of Leather Surfaces

Tensile strength (TS) and per cent elongation at break (EB) experiments have been carried out in CLRI, Madras by marking test samples close to each other in the form of a dumb-bell shape on the surface of a chrome tanned cow upper leather. Several test samples were cut according to SLTC/BI standard specification in the direction perpendicular to the back bone from the above cow upper leather and tested. These observations of the strengh at various locations on the leather surface have been used to obtain strength contours using a software package developed at C-MMACS. This is expected to help in design of leather products. *(M.I. James, M.K. Sharada, K.S. Yajnik, B. Lokanandam*, B. Sivaramakrishnan* and T. Ramaswami*, * CLRI, Madras)*

Computer Aided Design of Tunnels

Preliminary design parameters for underground tunnels and caverns are required for initiating underground construction activities. These parameters in spite of being conservative are helpful to install the supports. As the construction progresses the design characteristics are refined using the data from the load cells and the closure meters. Each site provides a case-history. Hence, an attempt is made to study these cases and to develop a suitable model for determining the design parameters. A mathematical model using Block theory was developed to determine three-dimensional wedges which are slid down into the excavated space. This model can help to determine the stability characteristics of these wedges and the optimum design parameters for reinforcement. This model would also be helpful to design parameters for any shape of underground tunnels and caverns. Other theories were also considered to determine the load acting on the supports. Some correlated factors were also developed to suit the Indian conditions. Limitations of this model are also estimated. Development of a software

package with interactive graphics is now in progress. *(A.K. Dube*, V.V.R. Prasad*, A.K. Soni*, A.Swarup*, K.S. Yajnik, N.K. Indira and Sridevi Jade, * CMRI, Roorkee)*

Molecular Modelling for Drug Design

A collaborative programme was initiated by IICT, C-MMACS and Toyahashi University of Technology, Japan to develop a new technique for enhanced conformational sampling for generating all the chemically significant conformations, which is one of the important goals of molecular modelling. The molecule chosen for testing the new technique was 18-Crown-6, which apart from being extensively studied has a moderately large conformational space, yet computationally managable. Several methods have been proposed and they differ in speed and in effectiveness in obtaining all the important conformers. While Molecular Dynamics Simulation, when applied to 18-Crown-6 was not able to generate the experimentally observed conformations, the new program CONFLEX-AMBER (CA) delveloped under this programme was able to do so.

This work has now been extended to handle cyclic peptides. The Arg-Gly-Asp (RGD) sequence, which is a universal cell-recognition site of various extracellular proteins that interact with integrin cell-surface receptors was chosen for study. In order to design low-molecular-mass RGD protein antagonists, the determination of the biologically active conformation is a prerequisite. The CA program is being used to generate all the possible conformers , which will provide a detailed insight into the steric factors that govern the binding of the tripeptide sequence RGD. Since enormous information exists on the adhesion-inhibitory capacity of various RGD containig peptides, the protocol to be used by the CA program for studying cyclic peptides is also being determined.

The research programme has tremendous potential as the CA program can provide the ability to manipulate the specific conformation of peptides, which is an essential feature in the development of novel therapeutic agents and biomaterials. *(B. Jagannadh*, A.C. Kunwar*, R.P. Thangavelu and E. Osawa+, * IICT, Hyderabad, + Toyahashi University, Japan)*