MODELLING APPLICATIONS

1.1 MODELLING PROBLEMS IN BIOLOGY AND CHEMISTRY

MODELLING SELF-ORGANISATION IN LIVING SYSTEMS

A study has been initiated with IICB on modelling self-organisation in living systems. It seeks to investigate the role of oscillatory biochemical reactions in metabolic networks and self-organisation in varied chemical/biochemical pathways in the presence of non-ideal reactions. Since metabolic processes involve many coupled reaction-cycles even in the simplest living cells, a model is selected for two autocatalytic reaction-cycles that are coupled through a common pathway. There are six confirmational or litigation states ($x_1,...x_6$) of an allosteric enzyme with a cofactor Y that may be a proton. In particular, the dynamics of the following seven reactions is studied by differential rate-equations.

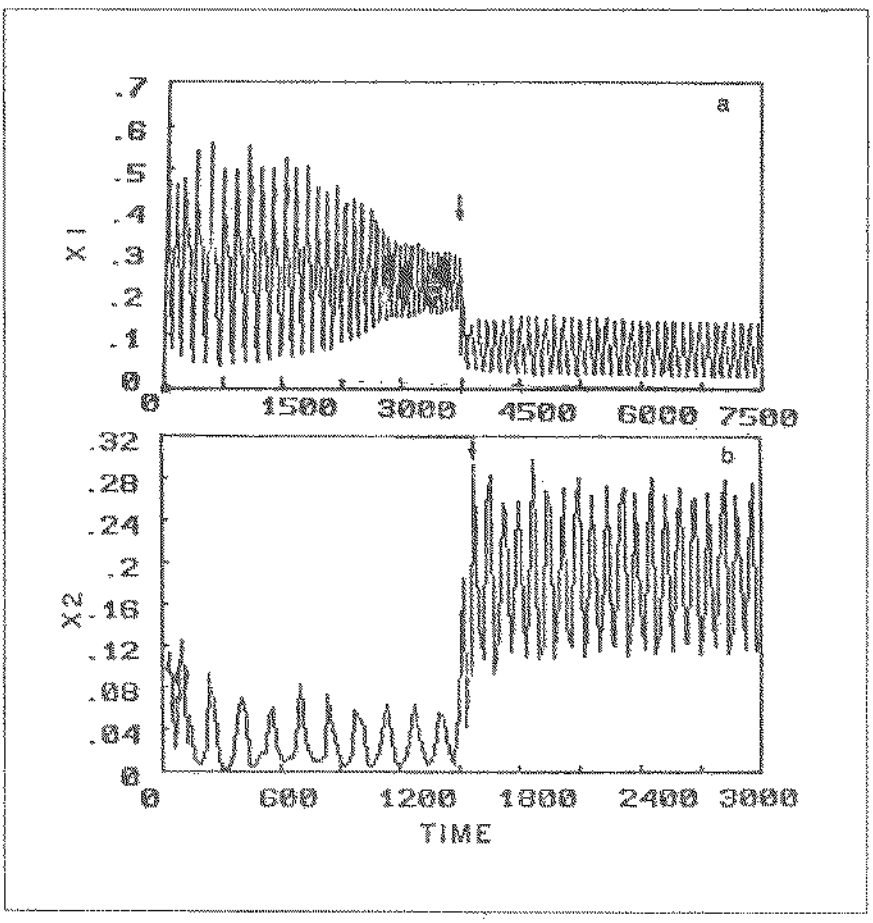
$$X_1 + X_2 + Y \xrightarrow{K_1} 2X_2$$
$$X_2 + X_3 + \xrightarrow{K_2} 2X_3 + Y$$
$$X_3 + X_4 + \xrightarrow{K_3} 2X_4$$
$$X_4 + X_1 + \xrightarrow{K_4} 2X_1$$
$$X_2 + X_5 + \xrightarrow{K_5} 2X_5$$
$$X_5 + X_6 + \xrightarrow{K_6} 2X_6$$
$$X_6 + X_1 + \xrightarrow{K_7} 2X_1 + Y$$

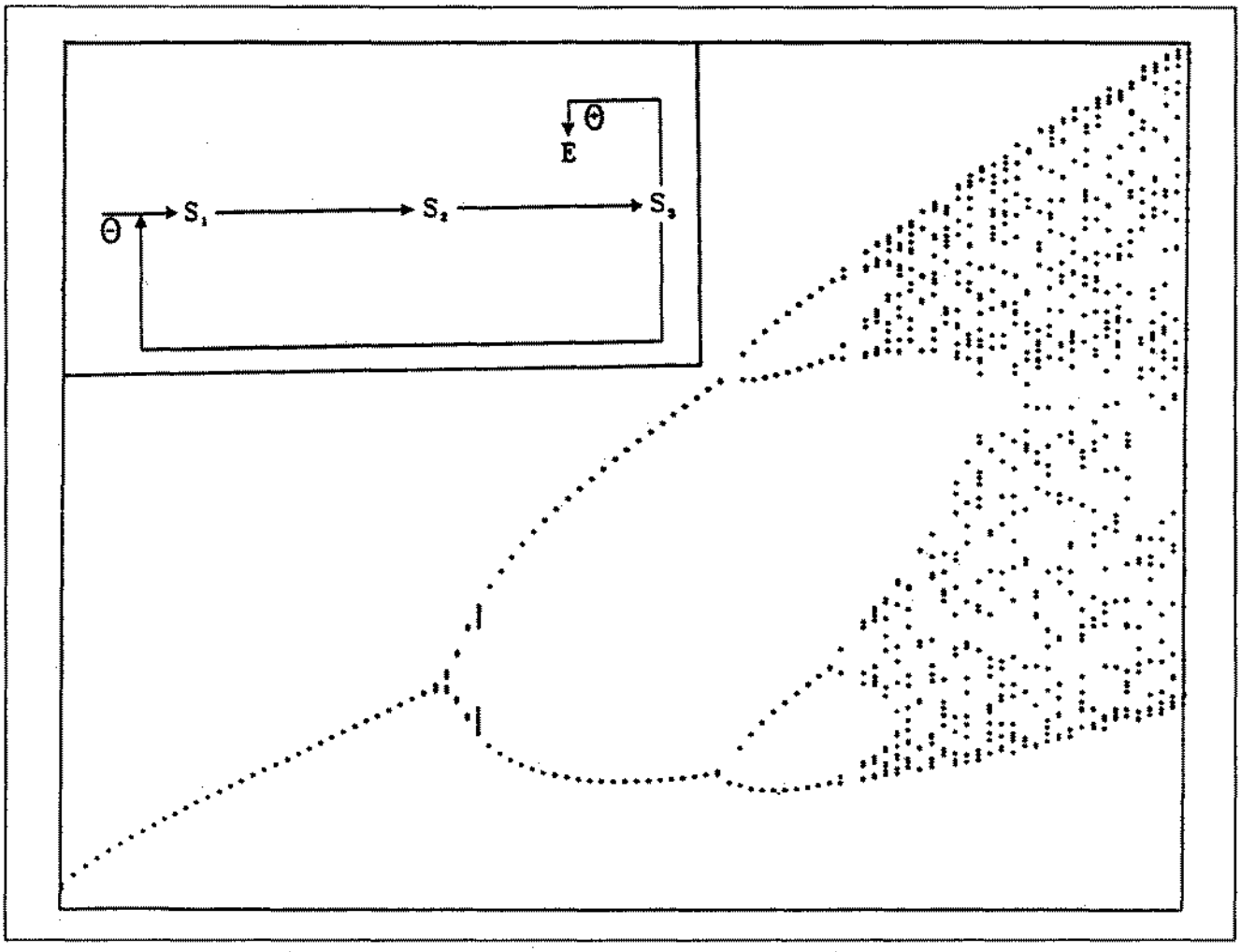
Sensitivity of the dynamical behaviour to parameters like kinetic constants is under study. The model shows a variety of behaviour like complex oscillation and birhythmicity (two periodic or near-periodic states) even when the system is closed to mass flow but open to external free energy sources that drive mass through the network. This behaviour is in contrast to Prigogine's theory that rules out the possibility of any oscillation in mass-closed condition (see *Fig. 1*).

A MODEL OF BIOCHEMICAL REACTION PATHWAYS

The existence of elaborate control mechanisms for the various biochemical processes within living cells is responsible for the coherent behaviour observed in their spatio-tempo-

▼ *Fig. 1 A typical result showing the dependence of the dynamics on the constant K_7*





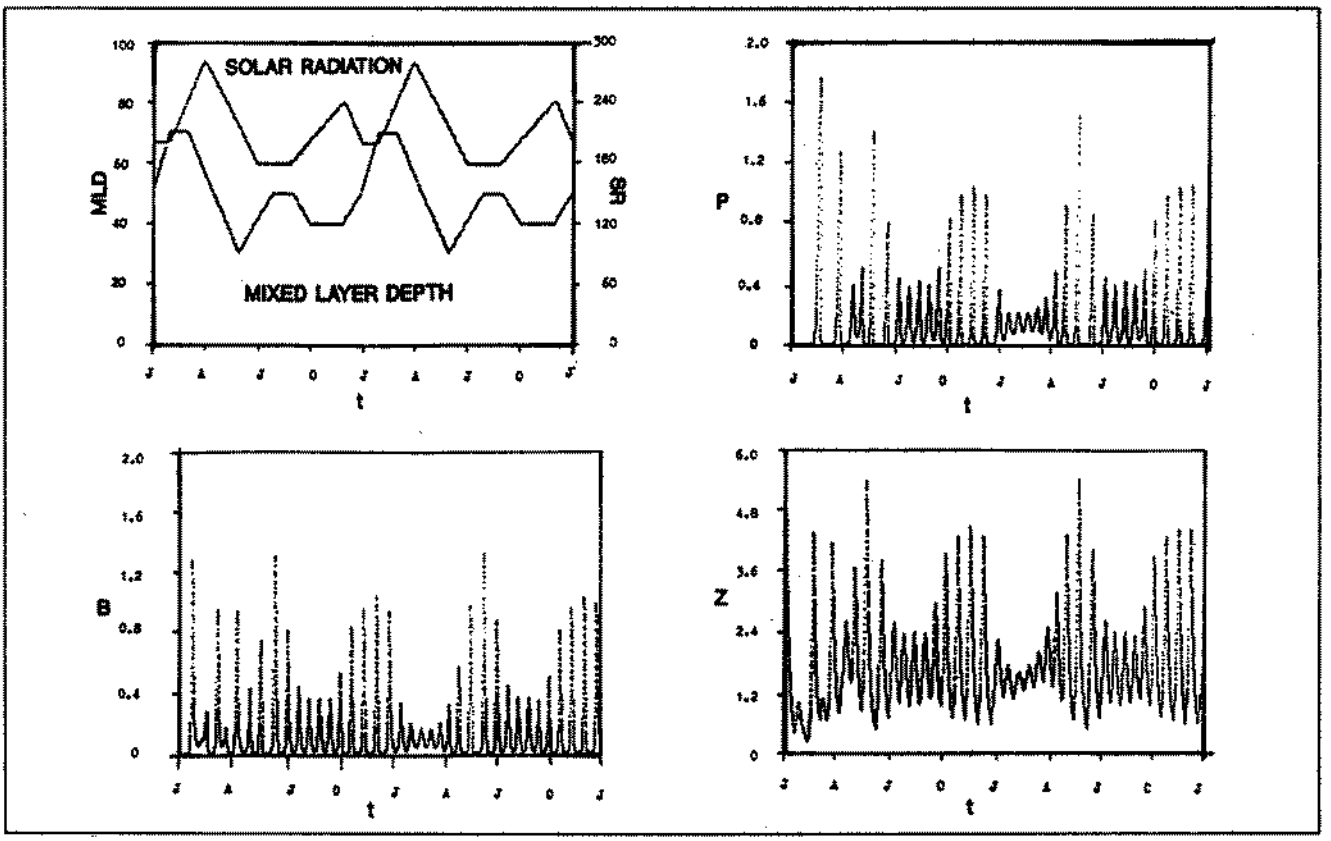
▲ *Fig. 2 The successive maxima of concentration of S_3 plotted against the degradation rate of S_3 in a period doubling bifurcation. The inset shows the model reaction sequence under.*

ral organisation. Stability and sensitivity are both necessary properties of living systems and they are achieved through negative and positive feedback loops. Using a reductionist approach, it has now been possible to know most of the biochemical reactions or pathways in micro-organisms, like the bacteria E. Coli, that control their different functions. Hence a living cell can be considered to a fair approximation as a set of interacting biochemical pathways integrated into an overall reaction network through both enzymatic and genetic control elements.

Since all the processes are essentially governed by the rules of chemical kinetics, it is useful to formulate general models for various processes in the cell having common features and study their dynamical properties. These studies should be able to describe wide ranging properties of living systems to operate in a steady and periodic manner, in basal and alternate conditions (i.e. existence of multiple steady states), show 'switching' behaviour (threshold sensitivity and multistability) and other types of behaviour, some of which may be pathological. A study involving CCMB and C-MMACS aims at delineating some of the dynamical possibilities of one such model of a regulated reaction sequence which incorporates a positive and a negative feedback loop through allosteric activation and end product inhibition mechanisms (see *Fig. 2*). The system of equations have been studied by using analytical and numerical methods. Since the type of behaviour depends on values of the system parameters, the behaviour around the basal values of two of the model parameters was studied keeping the others fixed. The two parameters chosen were the rates at which the concentrations of S_1 and S_3 reduced. The observed types of behaviour are steady state, limit cycle, period doubling bifurcation, chaotic oscillation, reverse bifurcation to simple periods and mixed mode oscillations (mixture of period two and period four etc.). Long lived transients were also noticed in many cases (see /CM 8/).

MODELLING THE BIOLOGICAL PROCESSES IN OCEAN

Modelling of marine ecosystems in coastal regions and in deep ocean has been of interest from several different viewpoints. Carbon flux between the ocean and the atmos-



▲ *Fig. 3 Modelling of the biological processes in the ocean. The figure shows seasonal response of the open system to mixed layer depth and solar radiation variations typical of tropical conditions.*

phere, and the available fish catch depends on the response of the marine ecosystem to the environmental factors like nutrients, photosynthetically active radiation etc. Biological processes in the surface layer influence the net transport of heat by the ocean as a whole. Also, the plankton produce volatile organic compounds such as dimethyl sulphide which help in the formation of clouds. A study of the models of marine ecosystem has been initiated at C-MMACS which can later be incorporated into larger ocean-atmosphere models for climate calculations. As a first step, the dynamics of a 3-component model were studied and the result were reported in last year's report. A nonlinear 7-component model due to Fasham et al (1990) has been studied during the present reporting period. An important feature of this model is the detail in which nitrogen is modelled, as it is often the limiting nutrient. It describes the temporal response of seven components, namely, phytoplankton, zooplankton, bacteria, detritus, nitrate nitrogen, ammonium nitrogen and dissolved organic nitrogen. The model is intrinsically nonlinear as the growth and grazing terms are nonlinear functions of nutrients, solar radiation and population. The dynamics of the model is studied both as an open system (i.e, including the forcing terms describing upwelling, settling, diffusion and variation of mixed layer depth with time) and also as a closed system. Qualitatively different types of large-time behaviour of the closed system such as stable steady state, limit cycle and chaotic state were observed depending on the value of one parameter namely, the zooplankton maximum growth rate. Also, the dependence of amplitude and period of auto-oscillation on the zooplankton maximum growth rate has been studied. Here the system parameters have been selected to correspond to available data on typical tropical conditions (see *Fig. 3* and /CM 9/ for a more detailed description).

1.2 MODELLING PROBLEMS IN EARTH SCIENCES

MODELLING STUDIES IN GEOLOGICAL FLUID MECHANICS

Quantitative understanding of generation and transport of hydrocarbons and ore forming fluids in the evolving sedimentary basins can be achieved through modelling of physico-chemical processes occurring in them in response to their environment. C-MMACS and NGRI, Hyderabad are involved in a collaborative project that seeks to develop general models which include the various basin formation processes like subsidence, sedimentation, uplift/erosion, internal heat generation, surface temperature variation with geological time, magmatic activity, vertical faulting, change in properties with burial etc.. In the present study the effect of subsidence on a thermal model of a basin is analy-

sed. Subsidence occurs due to the cooling of lithosphere and downward movement of lithosphere-asthenosphere boundary (LAB). In earlier studies, the solution was obtained by solving heat conduction equation in a fixed domain. In the present formulation we assume the LAB as a moving interface and include latent heat component in the model. The movement of upper surface of the lithosphere, which constitutes the base of the sedimentary basin is included in the analysis. The resulting nonlinear stiff system is solved using a spectral method and preliminary tests are being carried out to validate the software. Numerical studies are also in progress for a two dimensional model for heat and mass transfer in compacting sediments for a class of basins.

COASTAL CIRCULATION AND MARINE POLLUTION MODELS

The Bombay region is one of four regions on Indian coast identified by the Department of Ocean Development (DOD) for intensive studies of marine pollution. Work on the construction of a suitable hydrodynamical model for the Bombay harbour and Thane creek and a transport model for the pollutants has been undertaken at C-MMACS under DOD sponsorship and in collaboration with NIO, RC, Bombay.

Preliminary results obtained during the last year, reported earlier, were presented to a committee involving local agencies for feedback and guidance. Following the suggestions received, the computational domain was enlarged to include certain parts subjected to pollutant load. Also, extensive bathymetry data supplied by the Hydrographer, Maharashtra State were used to build a digital bathymetry database. It was also decided to concentrate on a periodic boundary condition which corresponds to M2 component of tide, which has the largest energy.

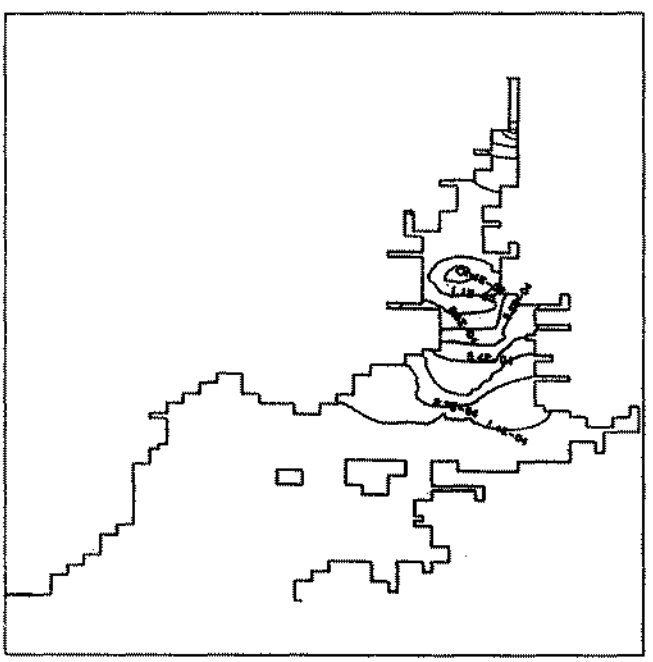
Detailed simulation studies were carried out with a 73x105 grid with horizontal resolution of about 300 m in north-south and east-west direction to show how a periodic state is approached.

Coastal current in the Bay of Bengal is known to vary seasonally in response to monsoon winds and freshwater influx from the Ganga-Brahmaputra system. A reduced gravity model is being developed at C-MMACS and NIO to elucidate the nature of forcing. It is a two-layer model with the shallow upper layer moving in baroclinic mode over the lower layer. A C-MMACS scientist participated in the oceanographic cruise SK70 on board ORV Sagar Kanya during 26 November - 31 December 1991 and assisted in the temperature and salinity measurements off the east coast of India. The data is now being analysed (see *Fig. 4*).

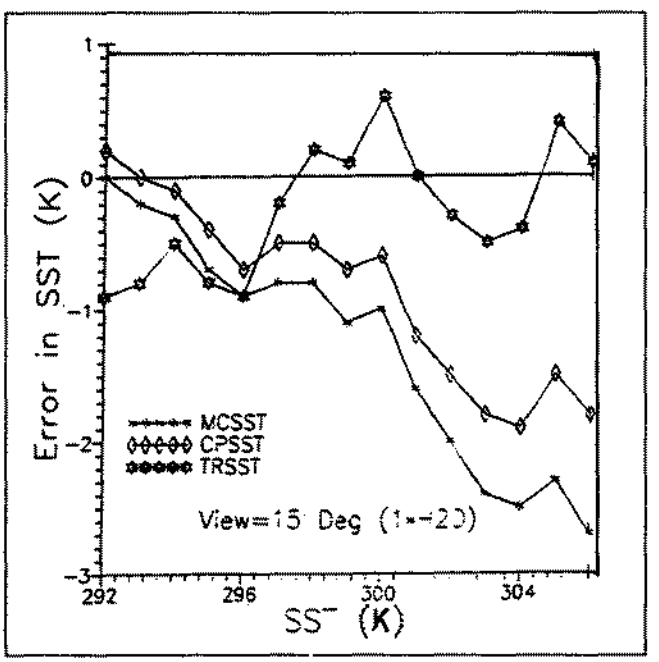
SEA-SURFACE TEMPERATURE IN THE TROPICS

The National Remote Sensing Agency (NRSA) has been disseminating the sea surface temperature (SST) regularly to many users including fisher-

▼ *Fig. 4 The pollutant distribution after 20 tidal cycles when it is introduced near Trombay at a constant rate 0.5 kg/sec, after the flow has become approximately periodic.*



▶▼ *Fig. 5 Error in sea surface temperature (SST) for the SST algorithms. Error is defined as Satellite SST - Actual SST. TRSST (Tropical SST) is the SST algorithm developed at C-MMACS. View angle is the satellite zenith angle. The total water vapour content in these simulations is 3.32 gm/sq.cm. Note that, in the simulated conditions, TRSST gives lower error than MCSST and CPSST.*



men. SST is obtained from radiometric data from the NOAA-11 satellite by using a global MCSST algorithm. A comparison with sea-truth has shown a significant underestimation of SST in the North Indian Ocean, when moisture levels are high. NOAA has recently introduced a new algorithm, the cross product sea-surface temperature (CPSST) which seeks to give better estimates of SST. Under the DOD sponsored project on ocean modelling, C-MMACS, in collaboration with NRSA, has been conducting extensive simulation studies of atmospheric radiative transfer with the aid of LOWTRAN 7, a state-of-the-art software package, to assess the performance of these algorithms and to develop new algorithms, which could be region-specific. Extensive simulations at C-MMACS have brought out conditions when the errors of MCSST are significant. A new algorithm, tropical sea-surface temperature (TRSST) is under development at C-MMACS, which gives improved performance under simulations for typical tropical conditions. Evaluation with satellite data is in progress at NRSA (see *Fig. 5*).

MODELLING STUDIES ON THE ROLE OF THE OCEAN IN CYCLONE DEVELOPMENT

The high frequency of cyclones originating in the Bay of Bengal is generally attributed to relatively high sea surface temperature and consequent energetic air-sea interaction. A study has been initiated at C-MMACS to elucidate the role of warm ocean water in the cyclone formation. A limited area model of NRL type is used. It is a mesoscale quasi-hydrostatic baroclinic model which uses primitive equations. Large scale precipitation and cumulus parameterisation (modified Kue scheme) are used. First tests based on available data near Calcutta during July 1990 are in progress.

1.3 MODELLING IN ENGINEERING

MODELLING OF AN ELECTROMAGNETIC ACTUATOR

Electromagnetic actuators have many applications, which require that their main component, the electromagnet, is able to operate satisfactorily under a variety of circuit conditions. The traditional method of design and development of these actuators usually requires the construction of several prototypes, which are then modified many times by trial and error, until satisfactory performance is obtained. The method is expensive and time consuming. The design process can be significantly improved by using the modelling approach. The engineer can now experiment with a number of configurations and visualise the results without having to build and test prototypes. C-MMACS, in a project sponsored by Larsen and Toubro Ltd., Bombay, has developed a software for simulation of electromagnetic actuators for industrial applications.

The modelling consists of two parts. One deals with the flux distribution of the electromagnet, while the other deals with the nonlinear dynamical behaviour of the electromechanical system.

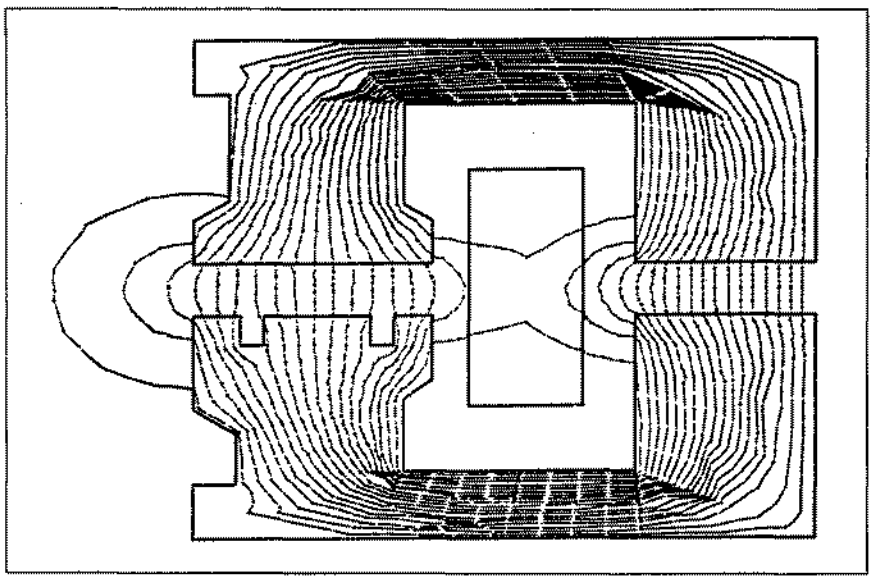
The flux distribution of the electromagnet is modelled in the present work using a two-dimensional, finite element analysis. In this method, the domain of the magnetic field is discretised by a mesh of four-noded quadrilateral elements. Then the field equations are solved to satisfy the given boundary conditions using software developed in C-MMACS. The software is used to map the magnetic flux lines and to calculate the inductance of the coil. Currently, work is in progress to develop a three-dimensional finite element model.

The analysis of the nonlinear dynamical system consists of solving the equations of motion for the electromechanical system, i.e, calculating the time of the desired operation under a variety of initial conditions. The temporal behaviour of electrical and mechanical parameters is also given by the software.

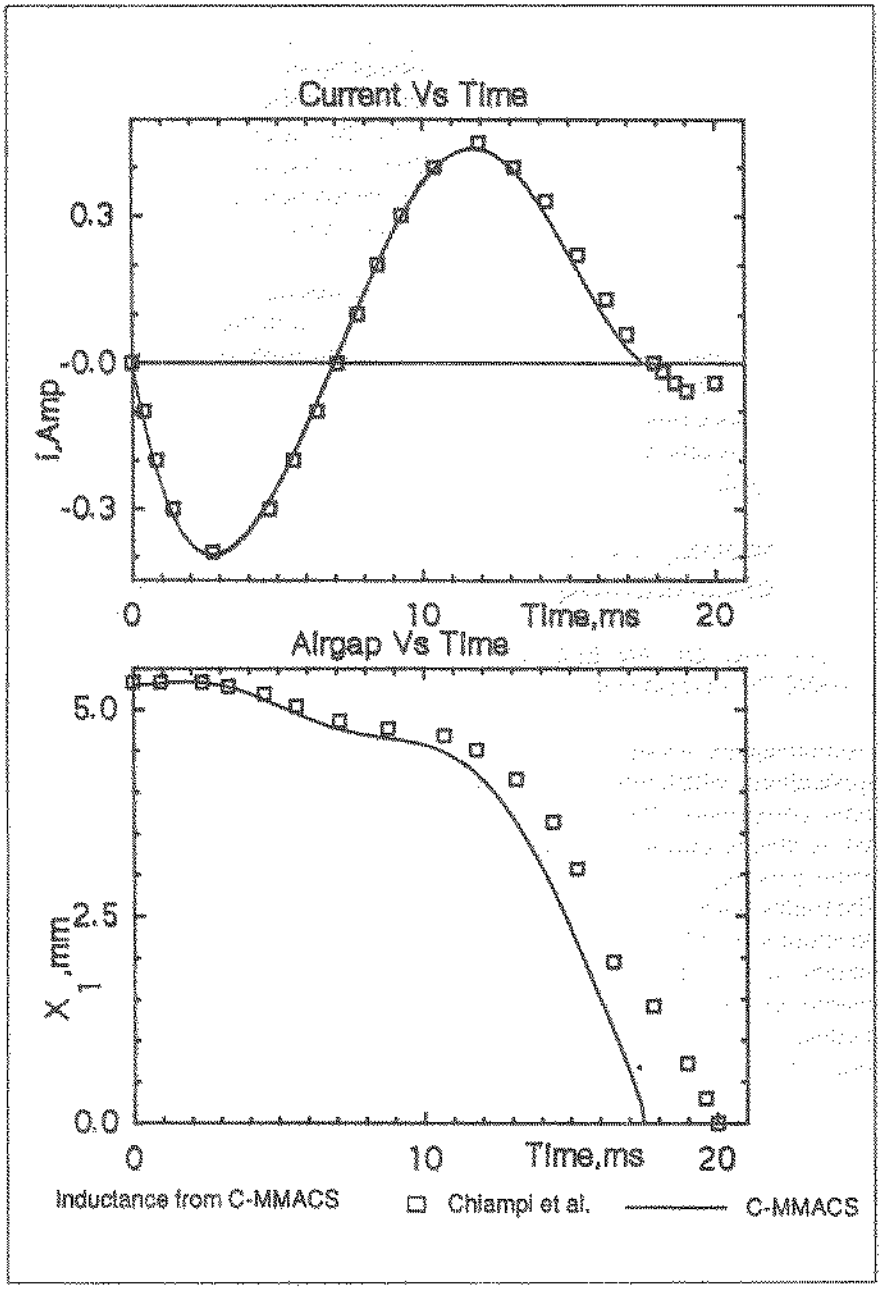
The model has been validated for one test case given in the literature. The *Fig. 6 and 7* give typical results.

GEOMETRICAL MODELLING AND CAD

• The geometrical modelling of the geostationary launch vehicle (GSLV) with its four strap-on booster rockets and the secondary injection thrust vector control rockets was under-

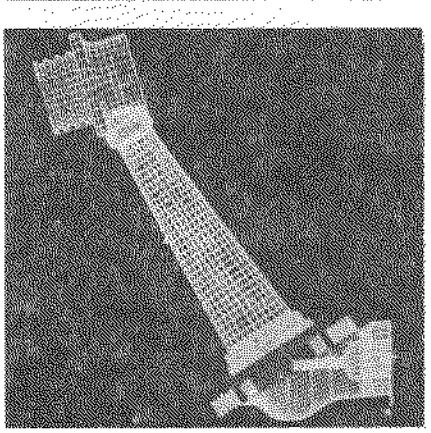


◄ *Fig. 6 Calculated flux lines for an electromagnet.*



◀ *Fig. 7 Calculated dynamic response of an electromagnet.*

▼ *Fig. 8 A view of the airblast atomiser.*



taken in a collaborative project with NAL on the IRIS graphics workstation in C-MMACS using CAD/CAM software. CNC software for machining the asymmetric nose cone of the booster rockets to 1/100th the scale for model testing in the wind tunnel, was developed. Four nose-cones were machined and handed over to NAL's Experimental Aerodynamics Division for wind tunnel tests.

● An air blast atomiser injects a clean spray of atomised fuel into the combustion chamber of an aircraft engine for instant ignition and efficient combustion. Computer aided modelling and machining of an air-blast atomiser leads to the development of technology in carving out the air-blast atomiser out of the stock of material as a single integral piece. Apart from this, precision machining of air-guides and jets is required. One set of production drawings for the fabrication of the air-blast atomiser for the KAVERI engine was completed using the C-MMACS graphics workstation. A precise 3-D model of the air-blast atomiser was built up using this CAD geometry, CNC software for machining the outerbody of the airblast atomiser was developed. The CNC programs were proved by machining the air-blast atomiser in a soft material (see *Fig. 8*).