

## Modelling of Marine Productivity

A nonlinear dynamical model was developed at C-MMACS (Annual Report 1994-95) to quantify the physical and biological processes involved in the marine productivity. This model was earlier used for estimating the annual averages of variables (phytoplankton, zooplankton, bacteria, nitrate, ammonium, DON, detritus) of the marine ecosystem in the Arabian Sea. It has now been extended to quantify monthly averages which were required for interpreting JGOFS cruise data on primary productivity and chlorophyll concentrations. The model simulation captures essentially seasonal variations under average climatological conditions. This model is also used to study the sensitivity of monthly averages to six model parameters which affect the grazing by zooplankton, detritus sinking and thermocline mixing at selected stations on the track of Indian JGOFS cruise programme. The ranges of certain observable quantities like chlorophyll and primary productivity for two periods of JGOFS cruises were compared with simulations and the parameter values were selected to give best comparison. Figs. 7 and 8 show the monthly variations of the simulated concentrations of the variables and some of the observable quantities, respectively. At present, various marine ecosystem models (both for mixed layer and for water column) are being studied. In particular, a water column model is being formulated for tropical conditions. (K.S. Yajnik and M.K. Sharada)

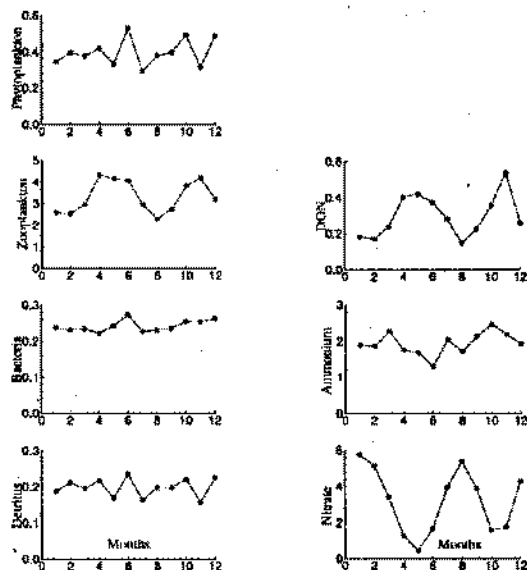


Fig. 7: Model simulations of monthly averages of different variables ( $\text{m Mol N/m}^3$ )

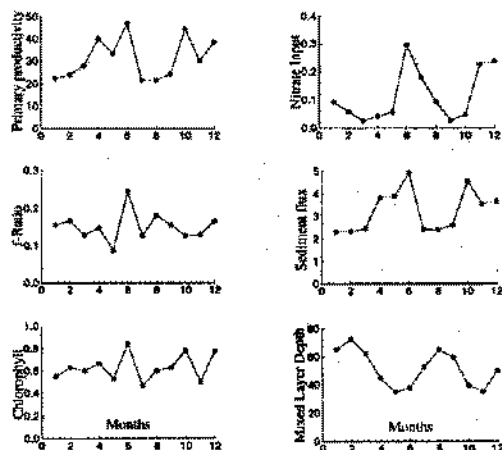


Fig. 8: Model simulation of monthly averages of observable quantities: primary productivity ( $\text{mg C/m}^3/\text{month}$ ), f-Ratio, chlorophyll ( $\text{mg Chl/m}^3$ ), nitrate input ( $\text{m Mol N/m}^3$ ), sediment flux ( $\text{mg C/m}^3/\text{month}$ ), and mixed layer depth (m)

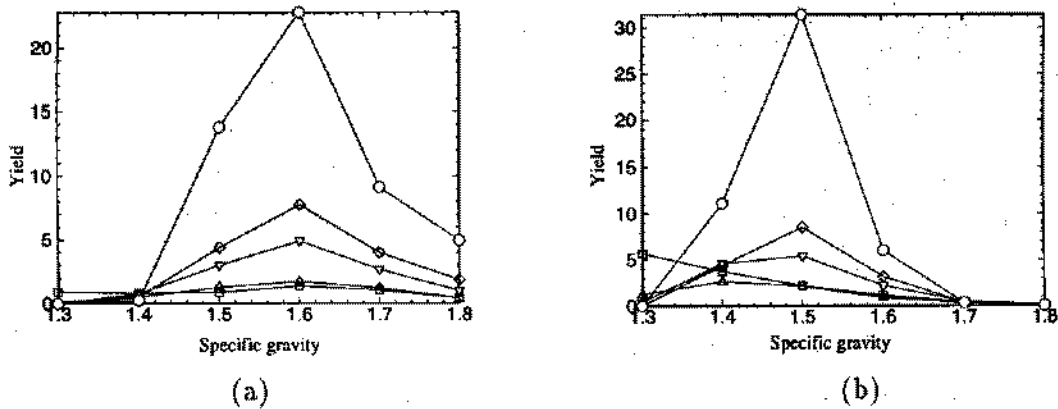


Fig. 9: Effect of  $\rho$  on the coal yield of (a) top and (b) bottom sections of the X seam for different sizes of the crushed coal.  $\square$ , below 3 mm;  $\triangle$ , 3-6mm,  $\nabla$ , 6-13mm,  $\diamond$ , 13-25mm and  $\circ$ , 25-75mm

## Ash Distribution in Indian Coal

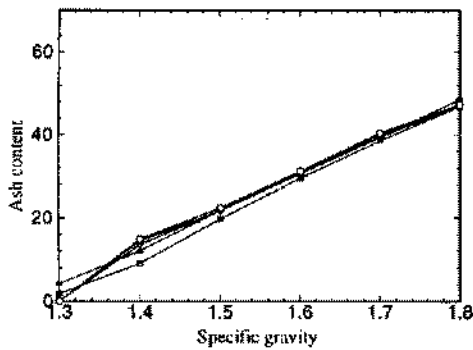
In the thermal plants for power generation it is seen that out of the quantity of coal used, 40% comes out as ash. It therefore becomes essential to reduce the content of ash in coal. The ash content in coal depends on the size of the crushed coal, size of the mesh used and the specific gravity of the processing liquid. Such a data set is available for sections of various seams in collieries. Using this data, a generalised model for ash distribution has been constructed to address this problem.

At CFRI, data on coal yield and ash content are being compiled for Jharia coal field. The data consist of the size of the initial crushed coal, coal yield and ash content when passed through liquids of different specific gravities. The data, which are for several seams and sections in a colliery, have been analysed.

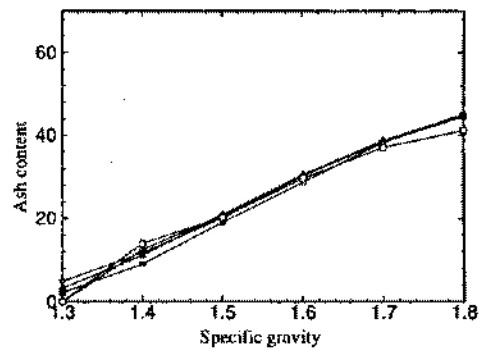
Fig. 9 shows the variation in the yield with different specific gravity  $\rho$  of the processing liquid for the top and bottom sections of the X seam for 75 mm initial crushed coal. Each data point on the figure represents a range of  $\rho$ , and for simplicity we have chosen to represent the range by its upper value; e.g., the data point at  $\rho$  of 1.5 represents the range 1.4 to 1.5. It is seen that the yield is maximum when  $\rho$  is between 1.5 and 1.6 for the top section and

between 1.4 and 1.5 for the bottom section. For another seam, namely the IX seam, both top and bottom sections show maximum yield when  $\rho$  is between 1.4 and 1.5. Analysis of data for other seams also shows that for some cases the yield is maximum when  $\rho$  is between 1.4 and 1.5 and for other when  $\rho$  is between 1.5 and 1.6. Thus the yield is in general maximum when coal is processed in a liquid with  $\rho$  between 1.4 and 1.6.

Fig. 10 shows the variation in the ash content in coal with  $\rho$ . It shows a linear relationship for both top and bottom sections of the X seam. This linear relationship also holds good for other seams and sections. Fig. 10 also provides information about  $\rho$  for an allowable ash content in coal. A similar analysis for yield and ash content on the available data on different sizes of initially crushed coal, viz, 75 mm, 50 mm and 13 mm, were carried out. The results are similar to the ones given above. Analysis of the data for other collieries is in progress. (N.K. Indira, K.S. Yajnik, R. Dasgupta\*, and A. Chowdhary\*. \* CFRI, Dhanbad)



(a)



(b)

Fig. 10: Effect of  $\rho$  on the ash content in coal of (a) top and (b) bottom sections of the X seam for different sizes of the crushed coal. Symbols are as given in Fig. 9

## Thermal Modelling for Mineral Genesis

Mineralisation processes in the crust involve generation of fluids at depth and their transport to the upper levels of the crust. This requires some heat source. Generally this is provided by magma sources rising from greater depths in the earth. The temperatures in the upper levels are also controlled by processes such as uplift and erosion. A mathematical model which combines the complex radiogenic source function and uplift/ erosion rate, both depending on space and time, has been developed. Fig. 11 shows the results of evolution of the temperature field over  $\sim 40Ma$ . It is seen that initially the temperature rises in the upper levels but subsequently falls owing to reduction in the heat source due to uplift/ erosion. The model can be used in relevant geological terrains to constrain the generation of fluids using thermodynamic data of rocks.

Further a one-dimensional mathematical model is developed to describe the effects of the fluid transport on temperature field in the presence of uplift/erosion, and variations in the basal temperature. This model was used for understanding gold mineralisation in Dharwar craton. The essential condition for the mineralisation is that temperature  $\geq 300^\circ C$

should occur at a depth of  $5km$ . Numerical results reveal that in the absence of fluid transport, the temperature of  $300^\circ C$  at a depth of  $5km$  is attained after a time period of  $\simeq 5.8Ma$  with uplift/erosion rate as  $7.5mm/yr$ . For an uplift/erosion rate as  $10mm/yr$  this is achieved only in  $\simeq 2.2Ma$ . In the presence of both processes, i.e. uplift/erosion at a rate of  $7.5mm/yr$  and fluid transport at the rate of  $1mm/yr$  and for  $450^\circ C$  basal temperature, the temperature of  $300^\circ C$  at  $5km$  depth is obtained within  $\simeq 3.8Ma$ . Thus the essential condition for gold mineralisation are met in this region. From these numerical results it is concluded that the uplift/erosion rate, velocity of fluid transport and the state of basal temperature at the moho have significant effect on the evolution of temperature field, which in turn controls the whole process of mineralization. (D.V. Ramana\*, R.N.Singh\*\* and P.S. Swathi, \* NGRI, Hyderabad, + presently at C-MMACS)

## Bioremediation

Current pollution levels demand immediate attention and scientific and technological solutions on an urgent basis. Soil and ground water get contaminated with organic matter in

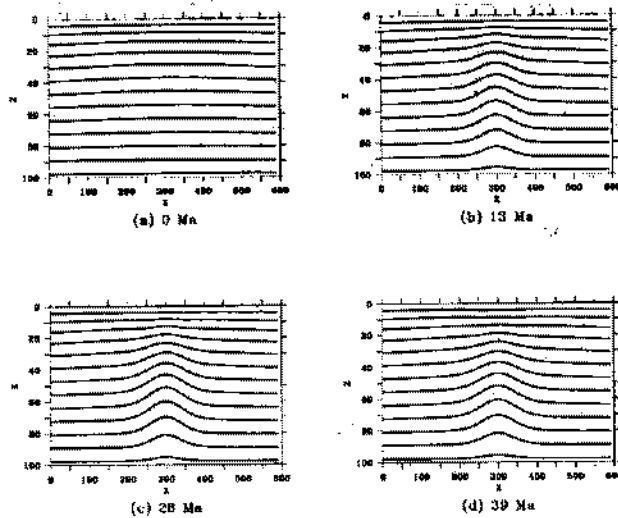


Fig. 11: Time history of the temperature field during the first 40Ma years of uplift and erosion. The basin is 600km wide and 100km deep. Radiogenic heat generation decreases exponentially with depth in the first 10km. Uplift rate varies exponentially laterally as well as with time.

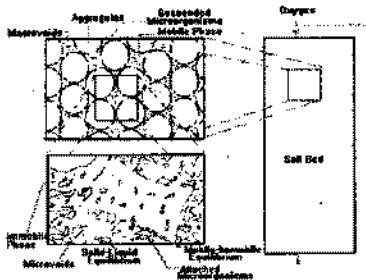


Fig. 12: Schematic of soil aggregates

the process of oil exploration and processing. One method of remediation in such situations, called bioremediation, is by management of the subsurface environment using microorganisms. In a collaborative project with RRL, Jorhat the modelling & simulation studies on bioremediation are being carried out at C-MMACS while laboratory experiments are being carried out at RRL, Jorhat. Since a typical run in the laboratory takes months, simulation studies using mathematical models become an extremely important tool for optimisation of the various parameters that can lead to a viable

process under field conditions.

A schematic representation of the soil bed is shown in Fig. 12. The void in a porous soil medium typically consists of a mobile phase in the macrovoids, and an immobile phase entrapped in the relatively smaller pores, the microvoids. Dispersion and convection dominate the transport in the macrovoids, whereas diffusion dominates the transport in the aggregates. The mathematical model thus has partial differential equations (PDEs) for the latter and ordinary differential equations (ODEs) take care of the macrovoids. This coupled set of PDEs and ODEs is a characteristic feature of the problem. There are three variables in the model, namely, substrate (contaminant), biomass (bacteria) and oxygen. Microorganisms are present at appreciable depths in the subsurface zone. They grow by utilising organic contaminants as carbon and energy source. The availability of oxygen is a critical factor in this process. The contaminants are present in adsorbed state inside the aggregates and the process of biodegradation is accelerated when the oxygen front starts moving into

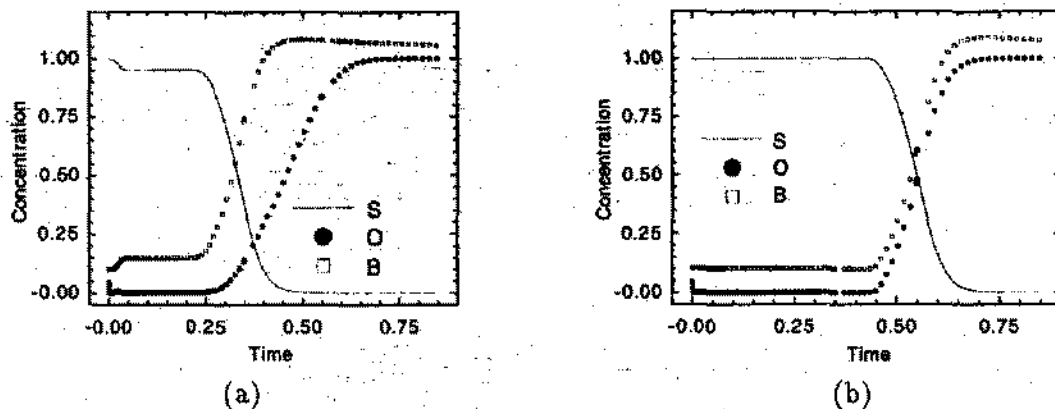


Fig. 13: Time evolution of non-dimensional concentrations of substrate ( $S$ ), Oxygen ( $O$ ) and biomass ( $B$ ) at (a) the centre of the aggregate, and (b) at a radius of 0.5 inside the aggregate

the micropores which makes it possible for the bacteria to start consuming the contaminant.

The results of a typical simulation are shown in Fig. 13. Contaminant concentration is reduced to zero level at half the radial distance inside the aggregate within 0.45 time units (Fig. 13a). At the centre of the aggregate, this occurs only at a later time, at 0.7 time units

(Fig. 13b). The rise in oxygen levels and the concurrent increase in the biomass concentration which facilitates the degradation of substrate is clearly seen in the figures. These typical results were obtained by a software package developed at C-MMACS which has been tested against published results. (T.R. Krishnamohan and K.S. Yajnik)