

PUC

Série: Monografias em Ciência da Computação

Nº 7 / 77

(antiga/formerly: Monographs in Computer
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COMPUTER KINETIC MODELLING OF RADIONUCLIDE
ACCUMULATION IN MARINE ORGANISMS

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Editor: Michael F. Challis

julho 1977

* Work partially sponsored by: FINEP, CNEN, UNIPAN-BID, IAEA
IBM do Brasil and IBM Japan

Accepted in the IFAC Symposium on Environmental Systems Planning Design and Control, Kyoto, Japan, Aug. 1977, to be published by Pergamon Press.

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RESUMO:

CSMP é usado para simular o primeiro estágio da cinética de um radionuclídeo numa cadeia alimentar. Como ilustração foi usado o modelo exponencial de acumulação de água para algas baseado em dados encontrados na literatura. O uso da modelagem computacional como um instrumento para estudos ambientais é discutido em termos das vantagens econômicas e futuras aplicações.

PALAVRAS CHAVE:

acumulação de radionuclídeos, biota aquática, metodologia de modelagem, modelagem computacional cinética, organização de grupos de pesquisa.

ABSTRACT:

Continuous System Modelling Program (CSMP) is used to simulate the first step of the kinetic of a radionuclide in a food chain by using the exponential model of accumulation from water-to-algae based on data found in the literature. The use of computer modeling as a tool for environmental studies is discussed as far as economical advantages and future applications are concerned.

KEY WORDS:

Aquatic biota, computer kinetic modelling, continuous simulation, modelling methodology, radionuclide accumulation, research team organization.

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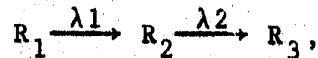
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1 - INTRODUCTION

There is an increasing motivation to study the environmental impact of nuclear power programs. Environmental models which describe the pathways of radionuclides introduced in the biosphere, from source to biological entities, start being widely used. Compartment models with rates of transfer either constants or as functions of time are usually employed.

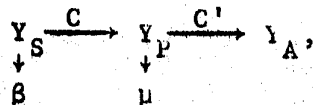
The first order kinetics of transference of radionuclide in a food chain may be represented by differential equations analogous to those describing the radioactive decay series. It is well known that the initial part of a radioactive decay series is represented schematically as follows: - see, for example, Evans (1) -



where R_1 , R_2 , and R_3 are the first radionuclides of the series; and λ_1 , and λ_2 are the decay constants of R_1 and R_2 , respectively.

Accordingly, the first steps of the kinetics of radionuclide in a food chain have been simulated by Eberhard (2), assuming transfer coefficients, from source to plant and from plant to one or two-compartment animals, independent of time. Reichle et al. (3) mention several applications of kinetic models for concentration of radionuclides in food chains.

The present work is a simple application of a modified version of the first step of Eberhard's model, represented as follows:



where Y_S , Y_P , and Y_A are concentrations of a radionuclide, respectively, in the source (i.e., activity concentration in water), plant (for example, phytoplankton), and one compartment animal; β is the loss rate of the radionuclide in the source; $C = Y_P/Y_S$ is the transfer coefficient of the radionuclide from the source to the plant (i.e., the concentration-or de-concentration-factor from water-to-algae as a function of time); μ is the loss rate of the radionuclide in the plant (i.e., the biological decay constant

of the radionuclide from the plant to a one compartment animal (i.e., the concentration or de concentration factor from algaer-to-one compartment animal).

The usual exponential model which describes the concentration factors, $C(t)$ of radionuclides in marine organisms may be represented as.

$$C(t) = C(\infty)(1 - e^{-\lambda t}).$$

where: $C(\infty)$ is the concentration factor after the accumulation process has reached a steady state; λ is the characteristic coefficient of the release process, and t is the time after accumulation started.

The use of this model implies the knowledge of the characteristic coefficient, λ , to fit the experimental data, $C(t)$. The usual procedure to determine λ is to undertake experiments to measure the rate of release of the radionuclide in question. However, this type of procedure is based upon the assumption that the biological mechanism of release is of the same nature as that of accumulation. Besides, when the accumulation rates are suspected to be different for short and long terms, it is necessary to establish two different values of λ if the exponential model is to be used for short as well as long term experimental results.

Polikarpov et al. (4), based on a literature review of the abilities of various marine organisms to accumulate radionuclides in different regions of the world oceans, pointed out that the kinetics of accumulation of radionuclides by marine organisms is not necessarily of an exponential character. According to Polikarpov, the phenomenon of accumulation of radionuclides by aquatic organisms may be better described by the generalized forms of logarithmic and power functions among others. As a matter of fact, short term (less than 200 hours) experiments performed with zooplankton accumulating ^{226}Ra under laboratory conditions (Ref. 5) have shown that both, logarithmic and power functions, can fit limited data taken during the accumulation period.

In any case, simulation can be a helpful tool to determine the best function to describe the accumulation process of a radionuclide by a particular species of marine organisms. Once a

function which describes the process is established, extremely valuable information may be obtained by inserting known parameters.

2 - THE USE OF COMPUTER MODELLING AS AN INSTRUMENT OF RESEARCH

The use of computer modelling is highly recommended in at least three circumstances:

- a) When experiments with the real systems can neither be done directly nor be reproduced under laboratory conditions;
- b) when it is economically less expensive to manipulate a model rather than carry out an experiment with the real system; and
- c) when one wants to test different hypotheses about a certain experiment.

In the specific case of radionuclide accumulation in marine organisms the last two circumstances are important factors that recommend the use of modelling for research in the field. Nevertheless the first circumstance also plays a minor role since it is not always possible to carry out experiments with such systems and when it is possible this is in general an expensive exercise.

In planning one such research project in a traditional manner one would have a hierarchy of activities such as the one shown in Fig. 1 (Next page).

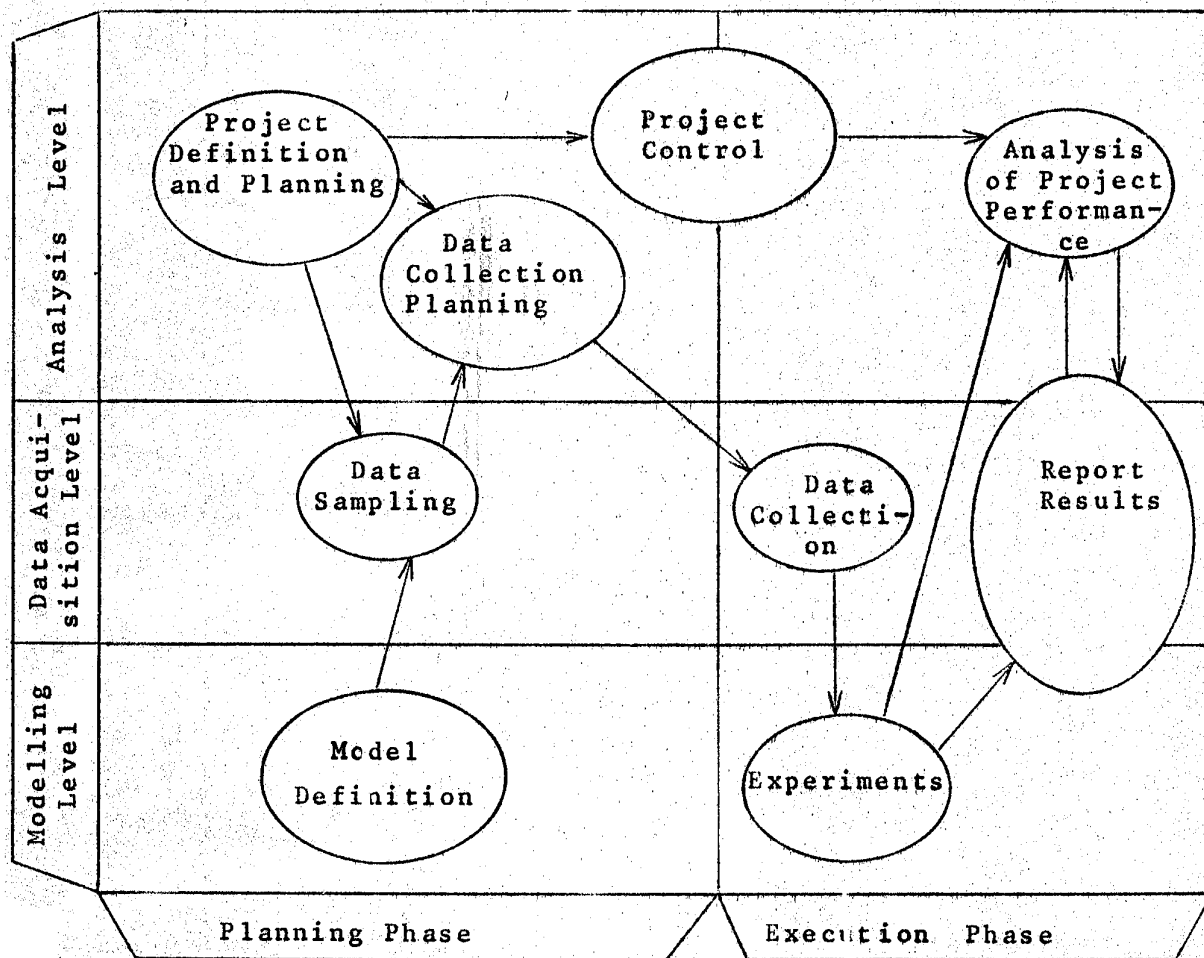


Fig. 1. Levels of hierarchy of activities for a research project.

In Fig. 1 the nodes represent the activities and the edges represent precedence relations. Clearly the "data sampling" activity is a necessity in projects where "data collection" is important. However, in order to reduce costs it is possible (in some cases) to replace real "data sampling" by a simulation exercise and in this manner guide the "data collection" activity and partially subsidize it by saving through simulation.

Amongst the many tools that exist nowadays to aid computer modelling as a research instrument, one of the most important in the field of continuous digital simulation is IBM's CSMP (Continuous Systems Modelling Program) (Refs. 6 to 9).

CSMP is a digital simulator devised to model continuous system by combining analogic functional blocks with logic and algebraic facilities of FORTRAN IV. In this paper a CSMP package for the IBM 370/165 was used as a tool to test the exponential model of accumulation of radionuclides in marine organisms based on data published in the literature (Ref. 10).

A number of integration methods are available in CSMP. The method chosen for use in the present work was the fourth order Runge Kutta with variable integration interval (See appendix A). The simulation exercise reported in this work is based upon a model described by the following differential equation:

$$\frac{dY_P}{dt} + \mu Y_P = \left(\frac{C}{\tau}\right) Y_S$$

where Y_S , Y_P , and μ have the same meaning as in the preceding section; $\tau = 1/\lambda$ is the biological half-life of the radionuclide (^{60}Co) for a particular species of marine organisms; and C is given by the usual exponential model mentioned earlier.

Here it is important to observe that the loss of rate, β , defined earlier, can be considered negligible for radionuclides with long half lives (e.g., ^{60}Co , 5.26 years) when compared to the accumulation time to reach a steady state.

3 - RESULTS AND DISCUSSION

Data taken from Nakahara et al. (10) on the concentration of radioactive cobalt by three species of seaweed (brown algae - Sargassum Thunbergii and Laminaria japonica; and red algae Ahnfeltia paradoxa) are summarized in TABLE 1.

TABLE 1 Data on $C(\infty)$, τ and μ for Co-60 in seaweed taken from Nakahara et al. (10)

	<u>S. Thunbergii</u>	<u>Laminaria</u>	<u>Ahnfeltia</u>
$C(\infty)$	2.6×10^3	1.4×10^2	3.0×10^2
$\tau(\text{day})$	7.5	14	4.3
$\mu(\text{day}^{-1})$	9.3×10^{-2}	2.8×10^{-2}	3.4×10^{-2}

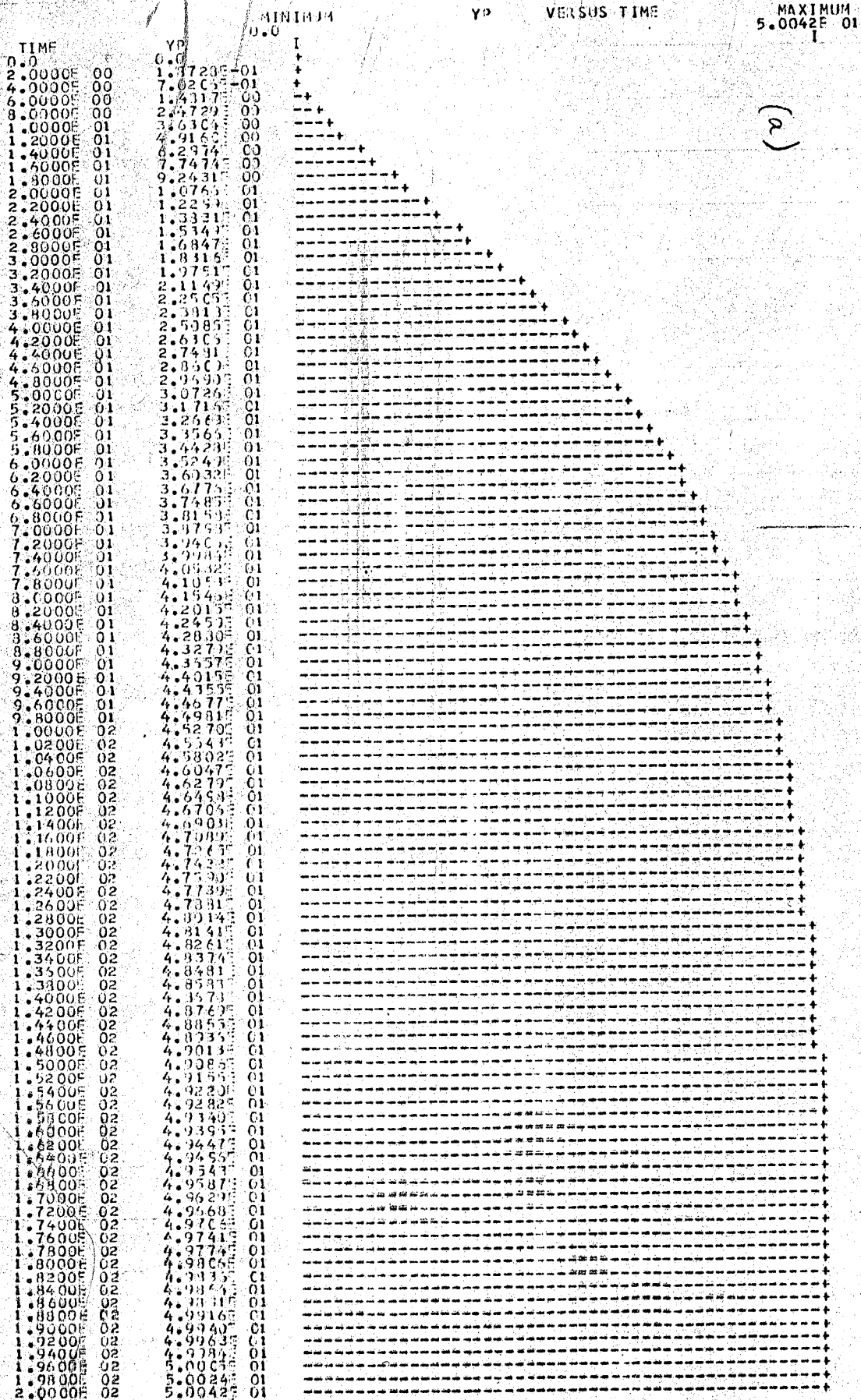


Fig.2. Results of simulation for Yp (cpm/g) for a time-range from zero to 200 days: a) Laminaria

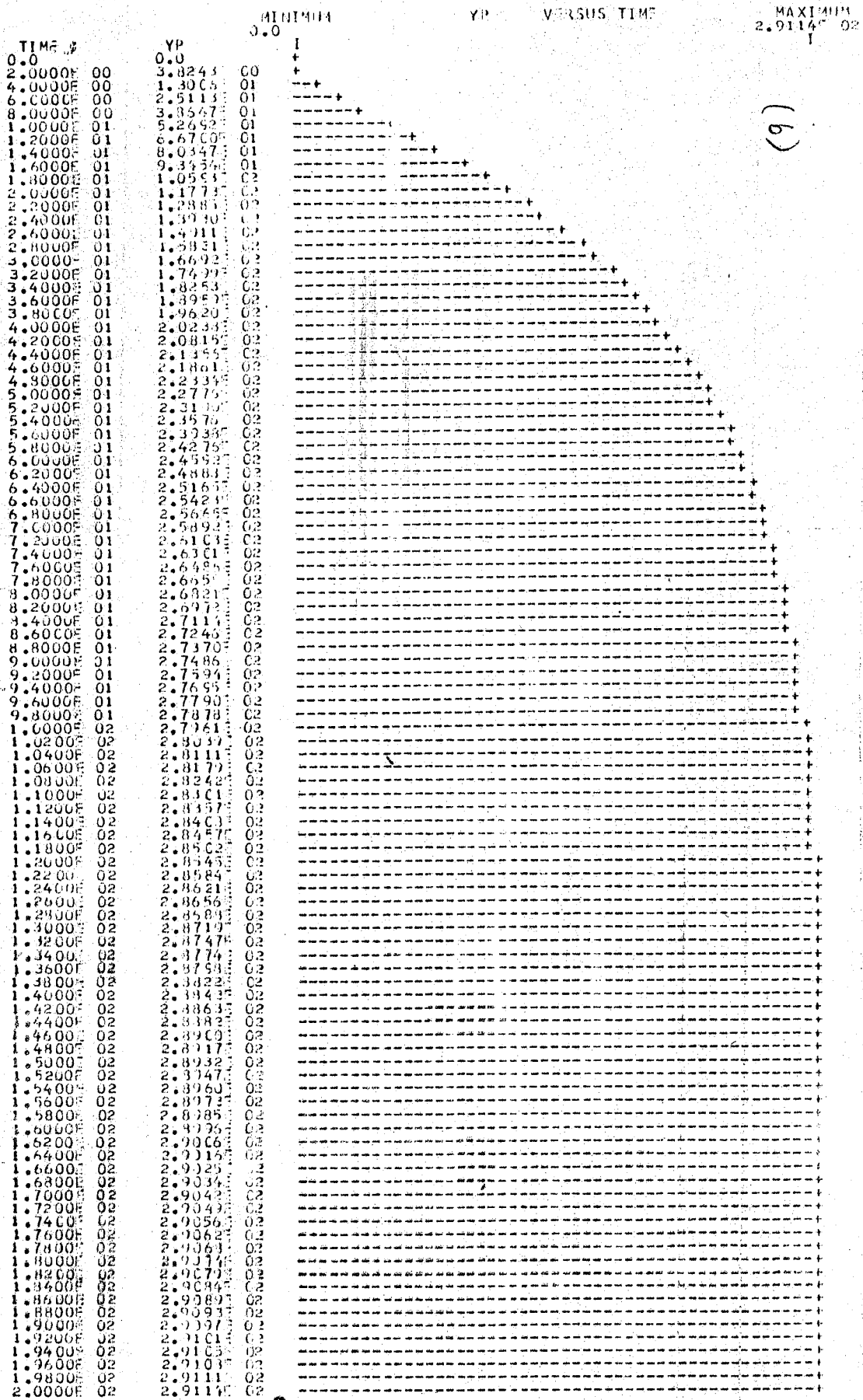


Fig.3. Results of simulation for Yp (cpm/g) for a time-range from zero to 200 days: b) Ahnfeltia

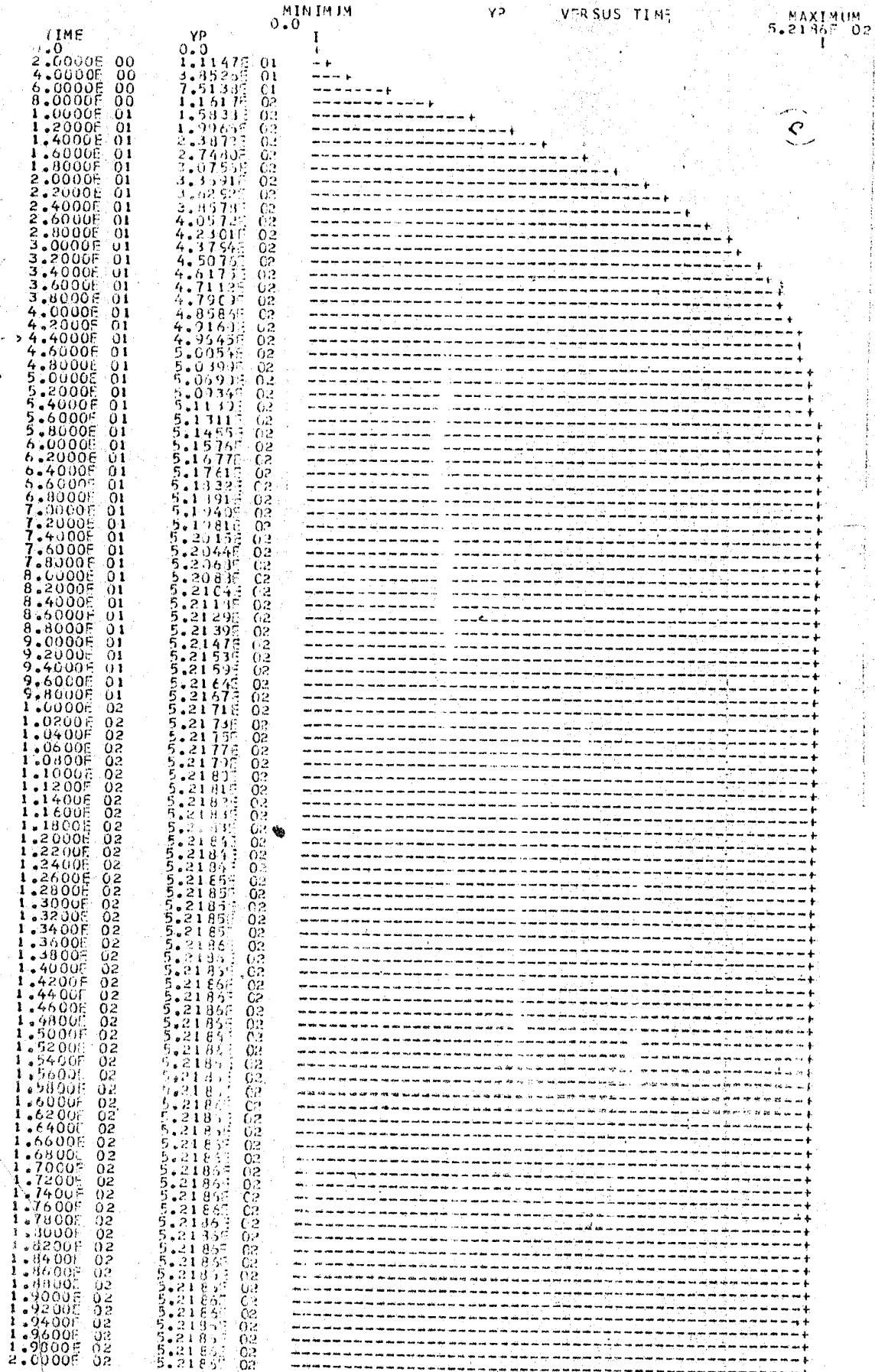


Fig. 4. Results of simulation for Y_p (cpm/g) for a time-range from zero to 200 days : c) S. Thunbergii

The results of simulation for Y_p (in cpm/g), for a time-range between zero and 200 days, based upon the data presented in TABLE 1 and the differential equation written in the preceding section are presented in Fig. 2.

From the results shown in Fig. 2 one can observe that according to the exponential model used for the simulation 95% of the steady state concentration of ^{60}Co in the algae Laminaria, Ahnfeltia, and S. Thunbergii are reached respectively at 122, 93, and 43 days after accumulation started. Such results are entirely consistent with the short term (maximum twenty days) accumulation experiments reported by Nakahara et al. (10).

Thus, laboratory experiments to study the concentrations of ^{60}Co in those species of algae should be extended to time-ranges neither much longer, nor much shorter than the times found to be necessary, by using the exponential model, to accumulate 95% of the steady state concentration of ^{60}Co in the organisms. On the other hand, an optimization of those findings can be achieved by trying models and by using more experimental data.

4 - CONCLUSIONS

Saving Through Simulation

In performing data acquisition for a study of radionuclide accumulation in marine organisms one needs at least the following equipment: sporting or fishing boat (fuel, maintenance), sampling material, storage facilities (tanks, freezers, etc.), and detection systems (γ and α spectrometers).

In most case the lease/hire cost of equipment is approximately the same in "data sampling" and "data collection" activities. The personnel cost may be reduced in "data sampling" activities but not substantially. In TABLE 2 we show minimum estimated costs for "data collection" and "data sampling" in US\$ per week according to Quintella (11).

TABLE 2 Estimated costs in US\$/week prices of May 1976 in Greater Rio area

		with rate of exchange US\$ 1.00 Cr\$ 10,00	
	Number	"Data collection"	Simulation
Personnel	Cost (US\$)	10 1200.00	3 300.00
Equipment		800.00	(10x)10.00

Such results allow as a conclusion that in a research institution that already has access to a computer system it is possible to make substantial savings by the use of computer simulation in projects in which "data collection" is an important phase.

Structuring a Research Team that Uses Modelling as an Instrument

The substance of computer simulation is the indirect study of a process P by investigating a computation process P' similar to P and such that P' models P. One of the many problems here is how to program the process P' and verify its similarity to P. Win-kowsky (12) and Klir (13) propose theoretical solutions to such problems. In practical terms one important result of their theory is that the environmental scientists must have a reliable and easily accessible experimental data bank (EDB) in order to validate computer models and check their correctness.

Consequently, the use of computer modelling to supplement or

replace "data sampling" requires:

- a) easy access to a computer system with appropriate reliable software; and
- b) the existence of a scientific team composed at least of an EDB administrator and a systems modelist to aid the environmental scientist (the systems analyst) in his work.

Future Applications

Much research is still necessary until a comprehensive computer kinetic model of radionuclide accumulation in marine organisms can finally be developed. As the amount of ecological data increases, environmental predictive models should be developed to assess the radioecological consequences of the impact of nuclear power programs for time-intervals well beyond the time-range of an actual experiment. A simple model source-to-plant is nothing but the very first step in the development of a more complex model much needed to describe comprehensively the accumulation of radionuclides by marine organisms.

Pre-operational surveys in the vicinity of nuclear installations should enable a research team, as suggested earlier, to analyze, model and monitor the future behaviour of the radionuclides to be incorporated into the ecosystems surrounding nuclear installations. Unfortunately, ecological information gathered in one place may not be applicable in other places. However, much will be added to the experience with the consequences of radioactivity release from the nuclear power industry, if computer modelling of radionuclide accumulation becomes generally used.

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APPENDIX

Integration Method

CSMP provides several methods of integration:

1. Fixed interval methods:

- 1.a - ADAMS (second order)
- 1.b - RKSPX (fourth order Runge-Kutta)
- 1.c - SIMP (Simpson's rule)
- 1.d - TRAPZ (trapezoidal)
- 1.e - RECT (rectangular-Euler)

2. Variable interval methods:

- 2.a - RKS (fourth order Runge-Kutta and Simpson's rule to estimate the error)
- 2.b - MILNE (fifth order, predictor corrector)

In the present research RKS method was used throughout with satisfactory results. The package also provides the flexibility of accepting methods developed by the user when satisfactory results are not obtained with either of the methods provided.

In the CSMP, the RKS method computes the integral by means of the equation

$$Y_{t+\Delta t} = Y_t + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4),$$

where: $k_1 = \Delta t * f(t, Y_t)$

$$k_2 = \Delta t * f\left(t + \frac{\Delta t}{2}, Y_t + \frac{k_1}{2}\right)$$

$$k_3 = \Delta t * f\left(t + \frac{\Delta t}{2}, Y_t + \frac{k_2}{2}\right)$$

$$k_4 = \Delta t * f(t + \Delta t, Y_t + k_3)$$

The integration interval varies to satisfy the error criterion

$$\frac{|Y_{t+\Delta t} - Y^s|}{a + r|Y_{t+\Delta t}|} \leq 1$$

where Y^S is the term $Y_{t+\Delta t}$ computed by Simpson's rule, a is the absolute error and r is the relative error.