RADIONUCLIDE PATHWAY ANALYSIS CALCULATIONS USING A SET OF COMPUTER PROGRAMS INTERFACED WITH GASP IV

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ABSTRACT

To assess the radiological impact of nuclear facilities (reactors, storage sites, reprocessing facilities, etc.), it is necessary to consider the movement and eventual fate of radionuclides which may be released. A generalized set of computer programs, interfaced with the GASP IV continuous/discrete simulation system, has been developed to assist in the analysis of the movement of radionuclides through the environment to man.

A nodal approach is used whereby the system to be analyzed is split up into parts or nodes within which the distribution of nuclides may be taken to be homogeneous. Radioactive decay is accounted for implicitly. Pathways are defined between nodes, and appropriate transfer coefficients are input or generated.

Output includes the time-dependent contents of the nodes, and radiation dose rates and dose commitments where required.

INTRODUCTION

All facilities handling radioactive material must meet certain standards with respect to limiting radiation dose to people. Proposed facilities must be assessed to demonstrate to the satisfaction of some regulatory agency that the proposed mode of operation will not result in sufficient release of radionuclides that an unacceptable radiation dose would be received by the surrounding population. Such an assessment requires prediction of the releases from the facility and of the subsequent movement through the environment to man of the released radionuclides.

Figure 1 shows the major pathways which can lead to intake (either inhalation or ingestion) of radionuclides by people. Figure 2 illustrates the modes of external irradiation due to released radionuclides. Clearly there is a great variety of types of pathways to be considered. For initial studies it would be very useful to be able to model a reasonable representation of the total system. This would identify important pathways or sections of pathways and radionuclides. More detailed models could then be made of these sensitive areas, to be used either by themselves or in conjunction with the first 'reasonable representation'. The system of computer programs described here was developed with the objective of providing a generalised capability for modelling that 'reasonable representation' of the total system.

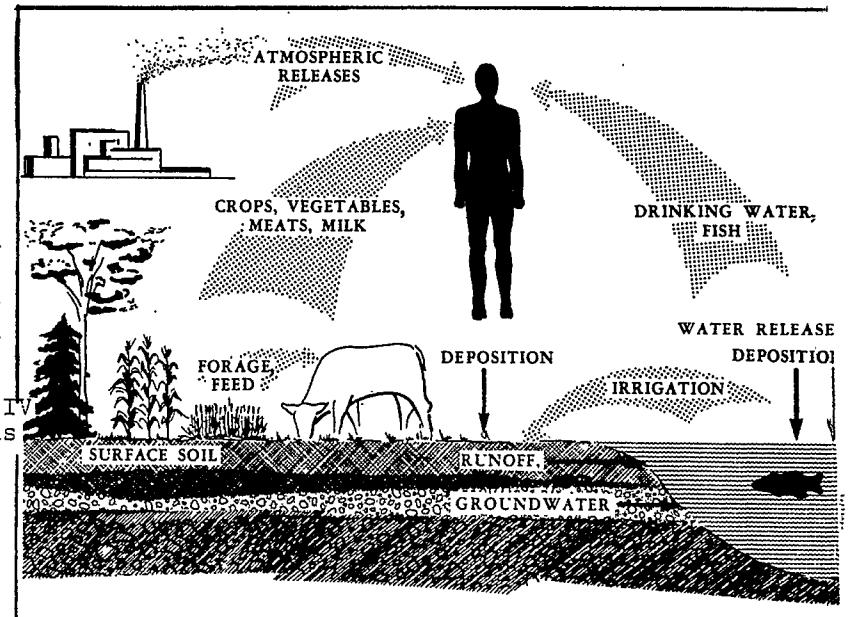


FIGURE 1 PATHWAYS LEADING TO INTERNAL EXPOSURE OF MAN

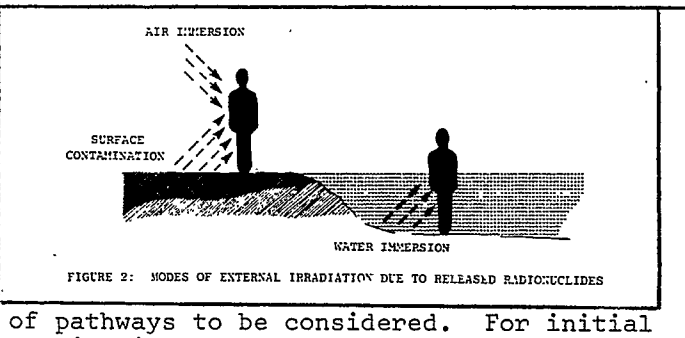


FIGURE 2: MODES OF EXTERNAL IRRADIATION DUE TO RELEASED RADIONUCLIDES

MODELLING PROCEDURE

The GASP IV continuous/discrete simulation language (1) provides an excellent vehicle for the preparation of the models

of interest in pathway analysis. The extra programs essentially comprise a 'pre-compiler' which will accept input in terms suited to the description of the physical model and which will then fill the appropriate GASP IV arrays and pass control to GASP IV. No changes have been made to GASP IV itself other than the usual changes associated with different computers, (random number generator, for example, and changes in some array dimensions). The combined system has been designated RAMM (Radioactive Materials Management) (2).

A nodal approach is used to convert a concept of the physical model to the computer model. This is illustrated by the following simple example. Consider the physical model (Figure 3) of a facility

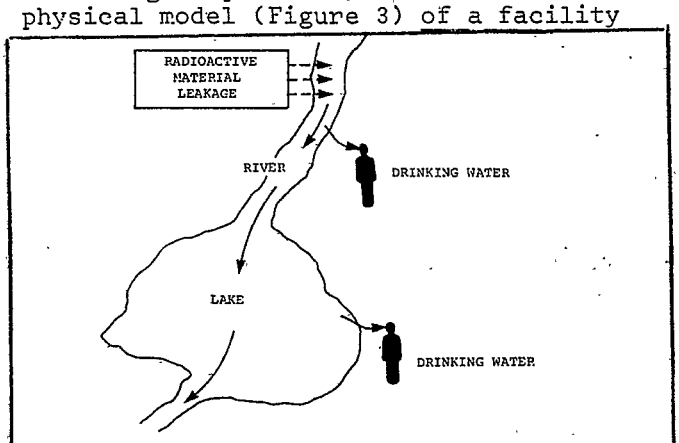


FIGURE 3 PHYSICAL MODEL

releasing radioactive material to a river which leads to a lake. People are assumed to be taking drinking water from two locations - the river and the lake. The first step is to convert the components of the physical model to nodes or compartments as shown in Figure 4. Nodes are chosen such

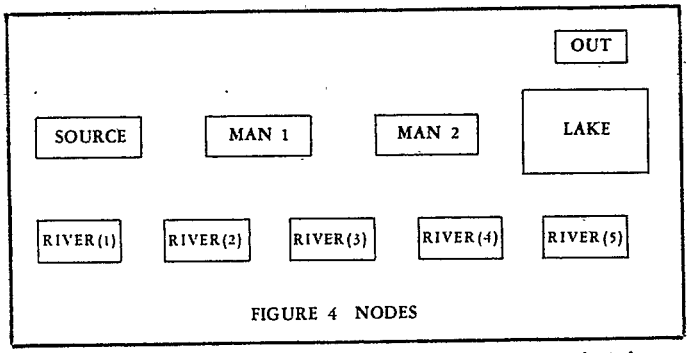


FIGURE 4 NODES

that the distribution of nuclides within a node may be taken to be homogeneous. They are general 'containers of nuclides' and may be volumes, such as a volume of water or a body organ, or surfaces such as a square metre of land surface. In this case the lake is considered to be a perfectly mixed node and the river is split into five nodes. This set of nodes is then interconnected by the appropriate pathways, 'flow' and 'diffusional', as shown in Figure 5. This 'pathway' approach, while

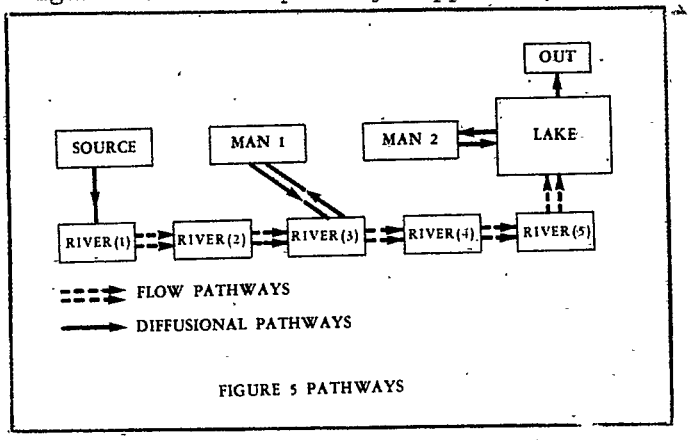


FIGURE 5 PATHWAYS

simple, is an important feature of the system. Every pathway has a beginning and an end, and only the required pathways are defined. This could be contrasted with an approach oriented towards nodes where a generalized node might have a number of available inputs and outputs of which only some would be used in most cases. The general mathematical model used in solving such node/pathway models is shown in Figure 6.

The differential equation defines the radionuclide balance in time for each node, i, and nuclide, j. Gains and losses of radionuclides are as follows:

1) Loss due to radioactive decay and gain from radioactive decay of precursor, or parent, nuclide.

2) 'Diffusional' transfer whereby the rate of transfer from a source node to a receiving node is proportional to the amount present in the source node, with the proportionality factor called a 'transfer coefficient'.

The transfer coefficients, $\alpha_j^{\ell i}$, etc., may vary with time, and various models may be incorporated for their computation. The approach taken is independent of the geometry of the situation, requiring only the definition of nodes and the paths between. Detailed finite difference or finite-element calculations may be required in some cases to derive appropriate transfer coefficients.

3) 'Leakage' transfer whereby the rate of transfer is not dependent on the quantity in the source node and is generally constant to simulate a constant leak rate, say from a tank containing radioactive solution.

$$\frac{dN_j^i}{dt} = -\lambda_j N_j^i + \lambda_{k_j} N_k^i - \sum_\ell \alpha_j^{i\ell} N_j^i +$$

$$\sum_\ell \alpha_j^{\ell i} N_j^\ell - \sum_\ell A_j^{i\ell} + \sum_\ell A_j^{\ell i}$$

+ INFLOW - OUTFLOW

where N_j^i = number of atoms of nuclide j in node i

$\lambda_j N_j^i$ = loss of atoms of nuclide j in node i due to decay

$\lambda_{k_j} N_k^i$ = gain of atoms of nuclide j from precursor k

$\sum_\ell \alpha_j^{i\ell} N_j^i$ = total 'diffusional' transfer of nuclide j from node i to nodes ℓ

$\sum_\ell \alpha_j^{\ell i} N_j^\ell$ = total 'diffusional' transfer of nuclide j from nodes ℓ to i

$\sum_\ell A_j^{i\ell}$ = total 'leakage' transfer of nuclide j from node i to node ℓ

$\sum_\ell A_j^{\ell i}$ = total 'leakage' transfer of nuclide j from nodes ℓ to i

INFLOW
OUTFLOW = Stream flow transfer

FIGURE 6: GENERAL MATHEMATICAL MODEL

4) Stream flow transfer, in which a set of nodes may be defined as belonging to a stream. The length and velocity of the stream are given, and a 'shifting time' is calculated as (length of one node in the stream/velocity). Every shifting time unit, the contents of the stream are moved down one node as shown in Figure 7. The shaded areas represent the radionuclide content of the nodes. In the 'slug' model the quantity shifted from node I to node I+1 is equal to the quantity in node I.

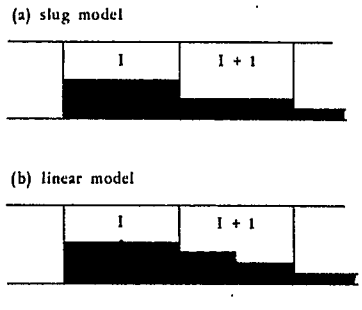


FIGURE 7 MODELS FOR STREAM FLOW

The contents of the last node in the stream are discharged to a 'dump' node (which may be a lake or another stream, etc.). Stream nodes are otherwise treated just as normal nodes are, and may interchange nuclides continuously. The velocity may vary in time and may reverse. In circumstances where there is a significant deposition from the stream, or chemical interaction with soil or rock, this 'slug' model tends to overestimate the nuclide transport along the stream. For such calculations, an alternative 'linear model' is provided which uses a linear interpolation between adjacent nodes to estimate the transfer due to water flow. In this case the quantity shifted from node I to node I+1 is the average of the contents of the two nodes. This approximates transfer of solution with a concentration equal to the concentration at the boundary between the nodes.

The total number of atoms entering a node can be computed by use of an input parameter which prevents radioactive decay computation for specified nodes. This enables calculation of overall transfer coefficients which can be used in subsequent larger-scale models.

Radioactive dose calculations may be carried out for any node. These are of two types, dose commitment and dose rate. In the dose commitment calculation for a node, the lifetime dose commitment due to the reception of nuclides is accumulated. As an atom enters a node it contributes to the dose commitment. The dose commitment per atom entering the node is based on biological and radioactive half-lives, rem (a measure of dose) per disintegration, and expected lifetime of the individual, and is provided on input. Dose rates for a node are based on rem per atom present in the node and also on rem to this node per atom present in up to four other nodes (to take account of external irradiation). Integration of the dose rates for a node provides the value for doses integrated over the time span of the simulation.

Provision is made for the inclusion of subroutines to calculate transfer coefficients both at the start of and during the calculation. It is intended that a library of appropriate subroutines and data sets will be developed for the calculation of transfer coefficients.

A general principle in terms of maintaining sensible computer times is that the sections of pathways should be 'well balanced' in terms of time constants where possible. For example, if the model includes a pathway through soil, taking many hundred of years, followed by transfer down a river, taking a few hours, it is impractical (and should be unnecessary) to model the transfer down the river in detail in the total calculation. In this case, the spatial distribution due to river dispersion

could be derived in a separate calculation, followed by the total calculation in which the river transfer would be assumed to reach its predicted spatial distribution instantaneously.

In some situations, an equilibrium exists between nodes. For example, a chemical equilibrium may be set up between soil and groundwater whereby the rate of transfer of a nuclide from soil to water eventually equals the rate of transfer of the nuclide from the water to soil. Often the equilibrium is very rapidly approached, compared to the rate of other processes, such as groundwater movement. In such circumstances, the quantity in the water divided by the quantity on the soil can be regarded as constant and equal to the partition coefficient multiplied by some constant to convert concentrations to quantities.

One way of modelling this situation is to put in the forward and reverse pathways between the two nodes, with their appropriate transfer coefficients, and equilibrium will be naturally approached. However, this presents two difficulties. First, if equilibrium is rapidly approached, then the transfer coefficients must each be large. The calculation will thus require short time steps. Second, the only information available in such situations is usually the partition coefficient, which is equal to the ratio of the two transfer coefficients. It would be possible to assign a high value to one of the transfer coefficients and derive the other such that the correct equilibrium is rapidly attained but this introduces an uncertainty and increases computer time. The situation can easily be resolved, however, by adopting the following procedure: consider nodes A and B and a value β derived from the partition coefficient between A and B, such that we expect, at equilibrium, the content of A = β x the content of B for the nuclide concerned. In RAMM, use a single node called, say, AB, which contains all the atoms expected to be in both A and B. For transfer from node A to another node C for which a transfer coefficient αAC has been derived, use instead a transfer coefficient $\alpha = \alpha AC\beta$ since a fraction of β of the atoms in AB is in A. The transfer coefficient α thus defines transfer from the combined node AB to the node C. A similar procedure should be used for streams when each moving node is considered to be always in equilibrium with a stationary node. In this case, provision is made in the input data for defining a value of β to be used for each combined node in the stream with values input separately for each nuclide. When shifting occurs, the number of atoms shifted is β multiplied by the number that would otherwise be shifted.

There are many features of GASP IV which could be of use in analyzing radiological impact (such as sampling from standard distributions to model random sequences of accidents associated with appropriate weather patterns, also sampled from appropriate distributions), however, the major features used are the numerical integration capability, used to solve simultaneous differential equations, and the event scheduling capability. The user provides the subroutine EVNTS in which various types of events can be coded. An EVNTS subroutine is provided in the RAMM codes which includes output events, stream shifting and transfer coefficient modifying events. In addition, the following subroutines are provided in RAMM to interface with GASP IV.

Main Program - Assigns units, reads and prints title card, and calls appropriate subroutines.

Subroutine PLOTP - Writes files for plotting. A generalized plotting system is available to access the written files.

Subroutine INPATH - Reads the input data, carries out extensive error checking, and sets up the arrays needed for the integration routine.

Subroutine PATHWAY - Computes the differential coefficients of the differential equations.

Subroutine NOUT - Prints out the model structure and description, including a formatted output of all the input data.

Subroutine POUT - Prints out the current status - the nodes and their contents and the dose data for appropriate nodes.

Subroutine STRE - Carries out the stepping function for streams.

Subroutines ATOSS, SSTOA, DTODD - Convert differential equation data from GASP IV arrays to RAMM arrays and vice versa.

Subroutine CALTR - Within which models may be coded for the computation of transfer coefficients.

One GASP capability not yet significantly utilized but which could be of great interest for modelling long-term radioactive material movement is that of altering the model itself as the simulation pro-

gresses. To take a simple example, for nuclides travelling along a soil/groundwater column, nodes could be progressively added at the front of the column and deleted at the back. Similarly, if a model of surface run-off is developed, the effects of erosion on the system under consideration could be taken into account.

APPLICATION

One application of this system was to analyse the consequences of the release of a mixture of radionuclides from the Whiteshell Nuclear Research Establishment (WNRE) to the Winnipeg River System (Figure 8).

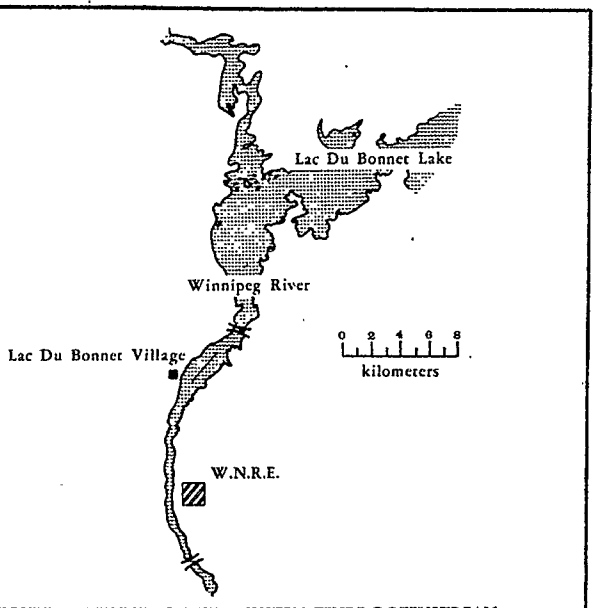


FIGURE 8 WINNIPEG RIVER SYSTEM WNRE DOWNSTREAM

Populations that might be affected by such a release are located at Lac du Bonnet village, about 8 km downstream from WNRE, and on the shores of Lac du Bonnet Lake, about 2 km further downstream.

Figure 9 shows the model used for the transport of nuclides from WNRE as far as the outlet of Lac du Bonnet Lake. The model contains the following sets of nodes:

Source node - WNRE

Population nodes - Four 'reference' men eating fish and drinking water at Lac du Bonnet village and at Lac du Bonnet Lake.

Stream nodes - Four streams linking the source node with Lac du Bonnet village and discharging into the lake. Four are necessary to model the dispersion of nuclides across the river since the concentration in the Lac du Bonnet village drinking water is sensitive to this transfer.

Lake nodes - Lac du Bonnet Lake is modelled with a water node, a sediment node, which interchanges with an interstitial water node, a fixed sediment node, and an exit node to allow for flushing of the lake.

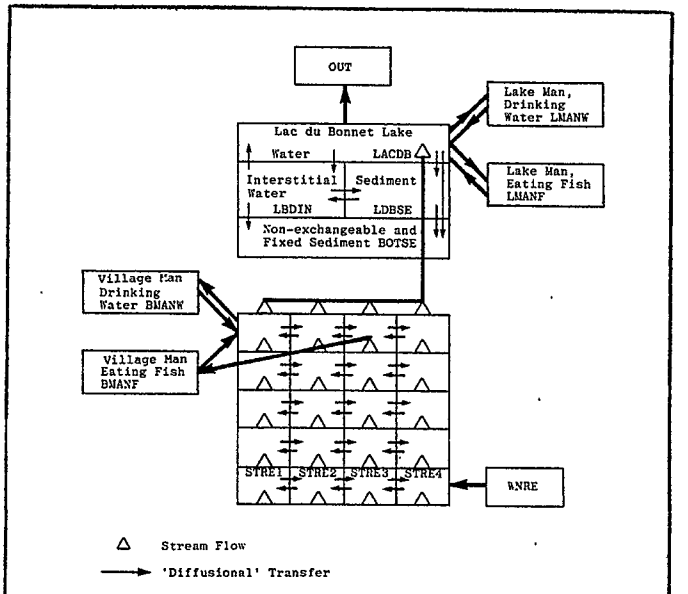


FIGURE 9 MODEL TO OUTLET OF LAC DU BONNET

Transfer coefficients were derived as follows:

a) Stream transfer coefficients.

Dye injection experiments (3) provided the data necessary to model the flow along and across the river. The transfer coefficients across the river and the relative flows in the four streams were all tuned to give agreement with measurements of dye concentrations along the river and at the Lac du Bonnet Village water intake for a pulse of dye released into the WNRE effluent.

b) Lake transfer coefficients.

Transfer coefficients between the lake water, the interstitial water and the various sediments were derived using method and data from Booth (4). Factors taken into account include partition coefficients between sediments and water, settling velocities and packing rates of bottom sediments. The flushing transfer coefficient from the lake water was simply the ratio (volume flow out of the lake/volume in the lake).

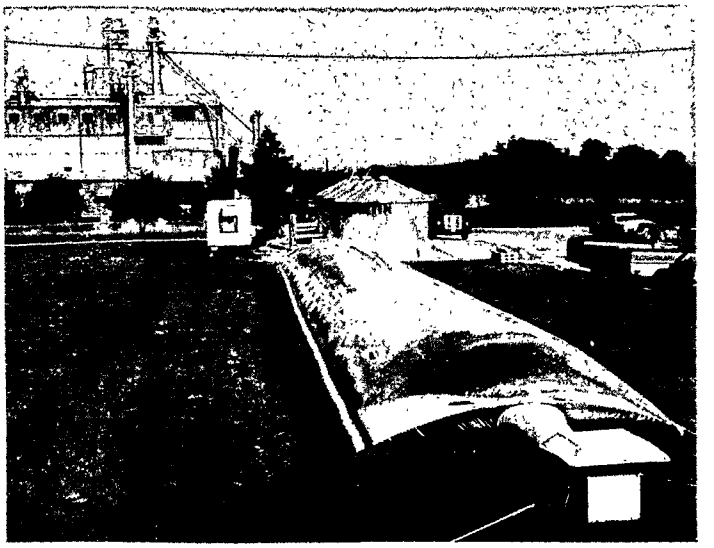
c) Transfer coefficients to man.

The drinking transfer coefficients were taken as the ratio (water volume drinking rate/volume of the node from which the water was being taken), and the eating-fish transfer coefficients as the ratio (fish eating rate x fish concentration factor/volume of the node inhabited

by the fish). The fish concentration factor is the ratio (concentration in fish/ concentration in water).

Details of the input and output data for the case described are available, but are not presented in this paper (Ref. 2 should be consulted for instructions on preparing the input data and running the program).

Other studies for which RAMM/GASP has been used include the analysis of the atmospheric transport of radionuclides from WNRE with subsequent deposition and transfer through plants and animals to man. It is expected that these computer programs will continue to provide a capability of modelling 'reasonable representations' of the release and transport of radionuclides from various nuclear facilities, through the surrounding ecosystems to man.



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