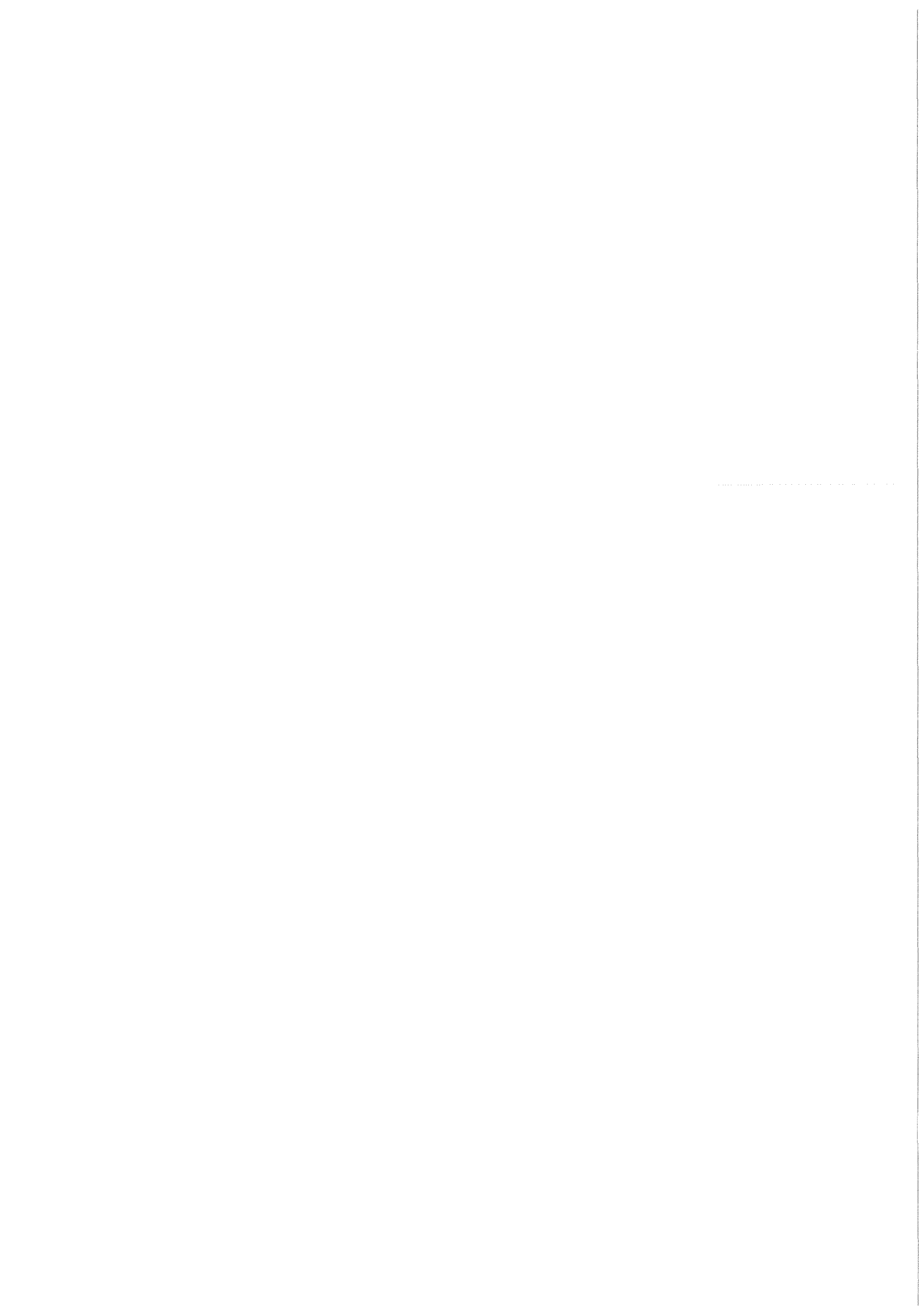


KfK 4853
März 1991

**User Guide for UFOTRI:
a Program for Assessing
the Off-Site Consequences
from Accidental Tritium
Releases**

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Kernforschungszentrum Karlsruhe GmbH
Postfach 3640, 7500 Karlsruhe 1

ISSN 0303-4003

Abstract

The computer program UFOTRI for assessing the consequences of accidental tritium releases from fusion facilities has been developed; its first version is now being released. Processes such as the conversion of tritium gas (HT) into tritiated water (HTO) in the soil, reemission after deposition and the conversion of HTO into organically bound tritium are considered. During a time period of some days, all the relevant transfer processes between the compartments of the biosphere (atmosphere, soil plants, animals) are described dynamically. A first order compartment model calculates the longer term pathway of tritium in the foodchains. Additionally, UFOTRI allows probabilistic assessments of the tritium impact in the environment. This report contains a description of the main processes which are important for the understanding of the input parameter list, as well as a detailed listing of the input parameters which can be changed by the user. Additionally, an input and output description with examples completes the report.

Benutzerhandbuch für UFOTRI: Ein Programm zur Abschätzung der radiologischen Folgen nach einer unfallbedingten Freisetzung von Tritium

Zusammenfassung

Um die radiologische Belastung der Bevölkerung nach einer unfallbedingten Freisetzung von Tritium abzuschätzen, wurde das Computerprogramm UFOTRI entwickelt, das inzwischen in einer ersten Version veröffentlicht ist. Bei einer Freisetzung von Tritium in die Atmosphäre müssen Prozesse wie die Umwandlung von HT in HTO im Boden, die Reemission des HTO nach der Ablagerung und die Umwandlung von HTO in organisch gebundenes Tritium mit berücksichtigt werden. Alle relevanten Transferpfade zwischen den einzelnen Teilbereichen der Biosphäre wie Atmosphäre, Boden, Pflanzen und Weidetiere, können jetzt innerhalb der ersten Tage dynamisch beschrieben werden. Der weitere Weg des Tritiums innerhalb des Ingestionspfades wird mit Hilfe eines Kompartimentmodelles erster Ordnung beschrieben. Eine probabilistische Abschätzung der zu erwartenden radiologischen Belastung ist ebenfalls möglich. Dieser Bericht enthält neben einer kurzen Modellbeschreibung eine ausführliche Beschreibung der verschiedenen Eingabeparameter, die vom Benutzer frei gewählt werden können. Eine zusätzliche Beschreibung der Ein- und Ausgabefelder sowie Beispiele einer Eingabeliste vervollständigen die Programmbeschreibung.

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1. Introduction

While the exposures (and thus risk) occurring during normal operation can be estimated deterministically, those from postulated accidents can only be estimated probabilistically. The consequences of a postulated release of radioactive material will vary considerably with the conditions pertaining at the time, in particular with the prevailing meteorological conditions, the season, the location and habits of population. For any given release, therefore, there will be a spectrum of possible consequences, each having different probabilities of occurrence determined by the environmental characteristics of the release location and its surroundings.

To estimate the spectrum of consequences, accident consequence assessment (ACA) models have been developed in different countries. The recently released program package COSYMA /9/ (COde SYstem from MARIA) has been developed within the MARIA project (Methods for Assessing the Radiological Impact of Accidents) which is supported by the Commission of the European Communities within its Radiation Protection Programme.

Within the code system COSYMA a model will be provided, which describes the behaviour of tritium in the environment, taking into account all relevant interactions of the different chemical forms of tritium with the ecosphere. Because of the dynamical properties of these processes, such as dispersion, deposition, re-emission, conversion of tritium gas (HT) into HTO and conversion of HTO into organically bound tritium (OBT), the model must be able to cope with all relevant time-dependencies. The processes mentioned above necessitates special modelling for a realistic description of the behaviour of tritium released during a nuclear accident. An atmospheric dispersion module which describes the atmospheric transport and deposition processes (dispersion, deposition and re-emission) and which considers of all relevant transfer processes in the environment (soil, plant and animal) for approximately 100 hours after the release event (during which the atmospheric transport plays the dominant role), was coupled to a first order compartment module /14/, which allows a dynamic description of the longer-term behaviour of the two different chemical forms of tritium in the food chains. As a result, the computer program UFOTRI emerged after extensive tests, sensitivity analyses and comparative calculations.

The physical and mathematical basis of UFOTRI is described in /12/. In this User Guide, only a short description of the main processes which are important, for the understanding of the input parameter list will be described. Therefore, the main report of UFOTRI is recommended to become familiar with the model and its main features.

The user guide is subdivided into 3 parts:

- a short model description
- a listing of the input parameters

- an input and output description with examples

A user familiar with the main report of UFOTRI may skip the next chapter and may continue with the chapters 3 to 5.

The model described here is a stand alone version but its input characteristics are approximately identical with those from the program package COSYMA. Thus a user who has experience with COSYMA should have little problems with the structure of the input list of UFOTRI.

2. Model description

The model UFOTRI for assessing the radiological consequences of accidental tritium releases describes the behaviour of tritium in the biosphere and calculates the radiological impact on individuals and the population due to inhalation, skin absorption and incorporation of contaminated foodstuffs. The present version is based on the Gaussian trajectory model MUSEMET /16/ which was slightly modified for describing the behaviour of tritium in the environment in both chemical forms gaseous tritium and tritiated water vapour. The importance of the re-emission process necessitates dual modelling of the atmospheric dispersion. Primarily, MUSEMET calculates the dispersion after a single release event and the subsequent deposition on soil and plants. In a second step, the re-emission of tritium after deposition from soil (evaporation) and plants (transpiration) is taken into account by an area source model specially developed for that purpose and combined with the original model. The exact solution of the Gaussian algorithm of such an area source model - a double integral - would require a large amount of computing time. Therefore a simplified assumption which replaces the area source by a single source point in the centre of the area, with a given initial widening of the plume, is used in UFOTRI /17/.

All processes, which may modify the total balance of the available HT or HTO such as the conversion of tritium gas into tritiated water (HT into HTO), the transport of tritium into deeper soil layers, the uptake of tritium by the plant root system, and the conversion of HTO into OBT are taken into account in the atmospheric dispersion module (Fig. 1), together with the foodchain pathways such as the production of milk, milk products and beef.

2.1 *Plant/Atmosphere exchange processes*

The exchange reaction of the plant with the atmospheric tritium takes place via the water circulation in the leaves. This process of direct uptake is negligible in case of an HT release /15/. The mechanisms of the plant/atmosphere exchange are described according to the model of Belot /2/. There, the temperature, the anorganic content of plant matter and the transfer resistances (aerodynamic, boundary layer and stomata resistance) determine the uptake of tritium in the vegetation as well as the loss of tritium from the vegetation. Both processes show an exponential decay which is considered in UFOTRI. The dominating factor is the total transfer resistance. The formulae for the calculation of the single resistances are taken from the literature, especially /10/, /1/ and /8/.

The aerodynamic resistance characterizes the transfer from the free atmosphere to the surroundings of the leaf, whereas the boundary layer resistance describes the mass

transfer through the quasi laminar air layer directly connected to the surface. The main parameters influencing both resistances are the atmospheric stability, the wind speed and the characteristics of the vegetation properties. The stomata resistance is dependent on the type of plant, the temperature, the photosynthetically active radiation, the humidity of the air and the water content in the soil. In the actual version of UFOTRI two possibilities of calculating the stomata resistance are offered. The simple one uses only the parameters water content in the soil and solar insolation, the second one simply by dividing the day in a daylight and nighttime period. The extended plant model considers additionally air temperature, photosynthetic active radiation and relative humidity. The diurnal cycle is replaced by the actual solar radiation balance.

At night, the plant stomata, in which over 90% of the water vapour exchange takes place, are usually closed, and exchange takes place only via the plant epidermis whose resistance is higher by at least a factor of 10 than the stomata resistance /13/. In case of precipitation, it is assumed that the stomata resistance goes towards 0 and only the atmospheric resistance is relevant. At night, when the stomata are closed, the leaf resistance (now: epidermal resistance) remains constant also in case of rain.

The influence of the soil water content on the diffusion resistance can be characterized by a step function /3/: if the water content in soil falls below a defined threshold, the diffusive resistance will increase rapidly to a second value which is nearly independent of the further decreasing water content.

Because vegetation occurs always as a plant population (fields, forests, etc.), an effective stomata resistance (now canopy resistance) has to be calculated. This is done by dividing the stomata resistance of a single plant by the leaf area index which describes the area of all leaves of the vegetation normalized to one square meter.

UFOTRI considers two different plant species, namely nutriment plants and pasture grass. Because of the plant specific parameters describing the exchange processes plant/environment, the model has to account for two different areas, one covered with the nutriment plants and one for the pasture grass. Due to missing land-use data, at present it is not possible in the model to consider a site specific distribution of the two areas. So it is assumed that each grid point which is representative of a certain grid area contains pasture grass as well as cultivation fields for nutriment plants with percentage contributions selected by the user.

2.2 Soilatmosphere exchange processes and transport in soil

The deposition process of HT and HTO to the soil is expressed in the form of a deposition velocity. The HT deposition rate depends on the type of soil and on the soil moisture. Once deposited, HT is transformed into HTO very quickly as a result of microorganism activity. Only the transformed part of HT remains in the soil. The process of transforma-

tion is assumed to take place very rapidly. In UFOTRI a value with a seasonal variation was chosen for the deposition rate (with a lower value for the winter season in order to take account of the smaller number of active microorganisms). The deposition rate of HTO is assumed to remain constant throughout the year.

The re-emission processes are modelled by coupling the re-emission of HTO to the evaporation of water from soil. Only the water content in the top five centimetres of soil is taken into account /4/. The water content in the soil will increase in case of rain and will decrease as a result of evapotranspiration of plants and soil. As for the plants, for the soil two different soil-water transfer models are eligible. In the simple version, water transport will occur only if the influx from precipitation exceeds the maximum water uptake capacity. In the more complex version, transport of water between each layer due to matrix forces is considered. Therefore the hydraulic conductivity and the suction tension of the soil (the soil parameters should be representative of the whole area, if possible) will be calculated.

The process of water loss from the top layer by evapotranspiration is subdivided into two separate processes, i.e. evaporation from soil on the one hand and transpiration of plants on the other hand. The re-emission rate of HTO is assessed on the basis of the soil evaporation, and the plant transpiration determines the amount of water which must be transported from the root system to the plant in order to balance the loss of water. Together with the water, also a given amount of tritium is taken up by the plant root system.

The potential evapotranspiration is derived using Penman's empirical equation /11/, which combines the radiation balance with the wind effects. The potential evaporation of soil is calculated by this equation with an additional modification based on the shading effect of leaves on the soil. The difference between potential evapotranspiration and soil evaporation gives then the plant transpiration. From the potential evapotranspiration an actual value is calculated which is depending on the soil water content.

The re-emission rate is coupled to the soil evapotranspiration rate by an additional conversion factor which describes the differences of tritium and water behaviour. The re-emission rate for conditions without insolation (nighttime) was determined by comparisons with field experiments. The resulting re-emission rate decreases with the time after release (this is to account for the variation in the concentration difference between atmosphere and soil).

2.3 Uptake of HTO by the plant root system

The uptake of HTO by the plant root system depends on the actual transpiration of the plant. To compensate the loss of water due to evaporation in the atmosphere the roots

of agricultural plants take up water, and thus also HTO, from soil layers up to a depth of 30 cm. For the model, it is assumed that 20% of the water taken up by the plant contains HTO with the specific concentration of the top 5 cm of soil. The remainder of the water (80%) taken up by the plant is assumed to have a specific HTO concentration of deeper soil layers.

2.4 Exchangeable and non-exchangeable tritium

Plants exposed to a tritium atmosphere contain HTO not only in the plant water, but tritium atoms are also incorporated in the organic matter of the plant. Tritium atoms in compounds with oxygen, sulphur, or nitrogen (exchangeable OBT) can be separated easily and are in equilibrium with the free HTO in the plant water.

In case of non-exchangeable OBT, the tritium atom is permanently bound to a carbon atom by two different processes: on the one hand, stable incorporation of tritium into the organic matter may take place via a process of photosynthesis; on the other hand, tritium may be incorporated into the organic matter of the plant via a reaction between exchangeable organic hydrogen and free HTO molecules. The first-mentioned process is about three times more efficient than the second one /6/.

In the model, the uptake rate will be divided into an increased daytime (photosynthesis) and a reduced nighttime value. A loss out of the organic tritium compartment is observed as well. Assuming an exponential concentration decrease in the OBT compartment, a mean loss rate of some tenths percent per hour is assumed in the model.

2.5 Cow compartment

In the atmospheric part of UFOTRI, all exchange processes cow/atmosphere, cow/plant and cow/soil, which are important for the ingestion pathways via milk, beef and dairy products, are also considered. The transfer rates are in general the same for the ingestion module of UFOTRI (see below), which were derived on the basis of a constant daily rate, but now converted to an hourly value. This shortening of the time step allows to model some processes more accurately. So the cows ingest their pasture grass only during the daytime. Further on the cows do not produce milk continuously but they are usually milked two times a day in the morning and in the evening.

2.6 The ingestion module of UFOTRI

In this part of the model, the long term behaviour of tritium in the environment and the assessment of the long term doses of the population from the consumption of tritium contaminated foodstuffs in the vicinity of a site up to about 50 km are described. To that purpose, the model calculates the time integrated tritium concentrations in vegetables, meat and milk products. The dose resulting from the uptake of drinking water is negligibly small because of the dilution processes of tritium in rivers, lakes and ground water, before it may be used for consumption.

To consider all relevant components of the foodchains and their link to the dispersion module, it was again necessary to subdivide the whole complex into two parts, corresponding to the production of nutriment plants only and for production of milk products and meat, respectively. The complicated exchange processes between plant soil and atmosphere and the great variability of plant species do not allow to consider them all in detail, in particular with regard to the unacceptable computer time required by such a model.

To describe the transport processes mathematically, the areas in the environment where tritium may appear are divided into different compartments as shown in Fig. 2. A compartment is an idealized range of the environment in which specific material can be enriched or diluted by exchange processes. The transfer rates which quantify the transfer processes are averaged values valid for longer periods and calculated assuming equilibrium conditions. The exchange processes between the individual compartments are treated by first order differential equations which describe linear dependencies of tritium concentrations or concentration differences. The system of differential equations resulting from many compartments of the foodchain models cannot be solved analytically. According to this, the computer model COMA (Compartment Model Analysis) developed at NRPB (National Radiological Protection Board), UK, was chosen to solve the problem numerically /5/ .

3. Description of the input data defined by the user

3.1 General remarks

For most of the steering parameters defining the run and adapting the models to the user's needs, default values are given in UFOTRI. The input data are subdivided in several groups, identified by a title card. Only the input group TRIDAT has no title card. The group title cards have to be left justified. One part of the groups must always appear in the input data (obligatory input groups), the other part only if changes in the default values are wanted (optional input groups). The obligatory groups are entered in strict format, as described below. The optional groups are input using a FORTRAN NAMELIST. The ways in which NAMELISTs can be used are described in chapter 5.

The GROUP and NAMELIST names are:

GROUP	NAMELIST
Obligatory	
METEOZON	----
SOURCE	----
END	----
Optional	
PRINTOUT	OUTPAR
POLGRID	GRDPAR
ISOTOPE	ISOPAR
METEOROL	METPAR
----	TRIDAT

Obligatory input groups

- **METEOZON** data for the meteorological zone considered for the atmospheric dispersion calculation, the sampling of the weather sequences and the sites with their population data
- **SOURCE** data defining the release (thermal energy, release height, timing, etc.)
- **END** card at the end of the UFOTRI-specific input data

Optional input groups

- **PRINTOUT** options defining the paper output to be produced
- **POLGRID** definition of the polar grid
- **ISOTOPE** specifications of the nuclides considered, the activity inventory, washout coefficient, deposition parameters
- **METEOROL** parameters for the atmospheric dispersion module (mixing layer height, wind profile, σ -parameters etc.) and the conditions for one single weather sequence chosen by the user (if METIN \neq 0)
- **TRIDAT** Tritium-specific input data for the atmospheric dispersion module and the longer term ingestion module

For the order of the input groups the following rules must be considered:

1. The group ISOTOPE must precede the group SOURCE.
2. The group POLGRID must precede the group METEOZON.
3. The group PRINTOUT must precede the group POLGRID.
4. The last group of the UFOTRI-specific input must be END.
5. If the NAMELIST TRIDAT is used, this card must appear after the group END.

The program unit INDAT gives a printout of the options and input data used for the run. In the following the input parameters of the NAMELIST groups are described. K means one or more input cards; S is a label for branching.

The type of the variables and arrays is given by the implicit FORTRAN type declaration; otherwise it is mentioned below.

Most of the arrays used have a dimension declarator defined by the PARAMETER statement. The maximum dimensions currently used in UFOTRI are shown in the table below. The statements are given in the member PARAM and are input to the code by the INCLUDE statement.

PARAMETER (NSITMX = 5, LWMAX = 144, NPHSMX = 17)

PARAMETER (NTYPMX = 2, NUCMAX = 2)

PARAMETER (NRMAX = 20, NPHIMX = 72)

```
*
* NSITMX      : MAX. NO. OF SITES           : = 5      *
* LWMAX       : MAX. NO. OF WEATHER SEQUENCES : = 144    *
* NPHSMX      : MAX. NO. OF RELEASE PHASES   : = 17     *
* NRMAX       : MAX. NO. OF RADIAL DISTANCES : = 20     *
* NPHIMX      : MAX. NO. OF ANGULAR SEGMENTS : = 72     *
* NTYPMX      : MAX. NO. OF TYPE OF NUCLIDES : = 2      *
*              WITH DIFFERENT DEPOSITION    *
*              CHARACTERISTICS              *
* NUCMAX      : MAX. NO. OF NUCLIDES         : = 2      *
*
```

3.2 Obligatory input groups

3.2.1 Input group METEOZON

The input group METEOZON specifies the selected meteorological zone and defines the data of the sites and of the weather sequences chosen for this zone.

The user can choose his own met-sampling program to generate site-specific weather sequences (read from NUNITS(13)) and similarly his own site-specific population grid (read from NUNITS(31), or he can use the default options, for example cyclic sampling of weather sequences or a uniform population distribution.

- * If the grid differs from the default values the input
- * group POLGRID must precede the input of METEOZON

- K1.1 title card METEOZON
(FORMAT A8)
- METEOZON name of identification (left-justified)
- K1.2 Card of the selected meteorological zone
(FORMAT 1x, A8, 1X, 2110, 515)
- ZONNAM name of the meteorological zone
- LMAX number of weather sequences (max. LWMAX)
- NSTMAX number of sites (max. NSITMX)
- LPOPT option for specifying the probabilities PWET of the weather sequences
= 0 uniform distribution, i.e. $PWET = 1/LMAX$
≠ 0 PWET is defined by
= 1 the input list K1.4
= 2 the weather sequence data file (NUNITS(13))
- LWOPT option for specifying the starting times LWET of the weather sequences
= 0 cyclic sampling
≠ 0 LWET is defined by
= 1 the input list K1.3
= 2 the weather sequence data file (NUNITS(13))

PSTO(NS) probability of the site; in general:
PSTO = number of reactor blocks at the site/
 number of reactor blocks in the zone
the sum over NS must be equal 1

If NSTOPT(NS) = 1 continue with S3
If NSTOPT(NS) = 3 continue with S4

K1.6 Card of the uniform population distribution
(FORMAT E10.2, I10)

POPDIC uniform population density in people/km²

IEIN index of the distance band up to which the
 population distribution is read from K1.7
 (only required if NSTOPT(NS) = 2).

S3 For each angular segment J (J = 1,...JMAX) K1.7 is required.

K1.7 Card of the population distribution
(FORMAT 8I10, as many cards as needed)

IPOP(J,I) population in each distance band I (I = 1,...,IMAX)
 for the angular segment J (see input group POLGRID).
 The middle of the first segment (J = 1) is 0 degree
 (order of the segments clockwise)

S4 End of input group METEOZON

3.2.2 Input group SOURCE

This input group defines the release and its phases. Data relating to the start and duration of the release and reactor building dimensions have to be entered in strict column format.

K2.1 title card SOURCE
(FORMAT A8)

SOURCE name of identification (left-justified)

K2.2 Card of the source term
(FORMAT A8, 2X, 3I10, F10.2)

UNFNAM name of the source term

NPHMAX number of release phases (max. NPHSMX)

IPZ shift of the beginning of all weather sequences
relative to the chosen starting times

For each release phase NP (NP=1,...,NPHMAX) K2.3 (and resp. K2.4) are required.

K2.3 Card of the release parameters for phase NP
(FORMAT 2I10, 3E10.3)

IPHASE(NP) time in whole hours between the end of the chain
reactions and the start of each release phase

IHO(NP) height of the release in meters

QH(NP) thermal energy of the release in cal/sec

BR(NP) width of the reactor building in meters

HOE(NP) height of the reactor building in meters

S5 End of input group SOURCE

3.2.3 Input group END

The input group END consists only of the card K3.1 and shows the end of the input data. If there is no mistake, the following message appears:

"END OF INPUT WITHOUT ERRORS"

K3.1 title card END
(FORMAT A8)

END name of identification (left-justified)

3.3 Optional input groups

3.3.1 Input group PRINTOUT

It is up to the user to define the amount of paper output to be produced (results and control output of input data) for general controll parameters. The line printer output is assigned to unit NAUS (=6) for the control output of module INDAT and to unit NUNITS(6) (=6) for the result output. Even with the output set at a minimum, the amount of output is still quite large.

To get paper output of single values (i.e. all grid points for one weather sequence), the parameters named NOO... should be used. If they are set to 1, results are printed for ALL weather sequences. A value of 2 prints the results of the weather sequences selected by LKZ. LKZ is the index of the weather sequences that you can choose to be shown as output. It allows up to 20 to be chosen, but when choosing fewer, the remaining LKZ must be set to zero, e.g. if there are 30 weather sequences, in order to choose numbers 4, 7 and 23, LKZ = 4,7,23,17*0. IACT will show output of radii dependent results so the number of IACT equals IMAX. If R = 1000, 3500, 7500, and RA = 2000, 5000, 10000, to show results out to 2km, IACT = 1,2*0.

The title card of PRINTOUT is followed by the NAMELIST OUTPAR.

K5.1 title card PRINTOUT
(FORMAT A8)

PRINTOUT name of identification (left-justified)

K5.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST OUTPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----
IBVOUT	1	option for printout of the population distribution ≠ 0 : printout for all sites = 0 : no printout
NOOTMT	0	option for printout of information about meteorological and trajectory data ≤ 0 no printout = 1 printout for all weather sequences = 2 printout for the weather sequences defined by LKZ

NOOTKZ	0	option for printout of concentrations for the radii defined by IACT, each sector and the nuclide group INUKL ≤ 0 no printout = 1 printout for all weather sequences = 2 printout for the weather sequences defined by LKZ
LKZ(L1) (20 values)	1,7,50, 75,90, 115, 14*0	gives the index of the weather sequences, for which a printout of nuclide concentrations is wanted (if less than 20 weather sequences are chosen, the remaining indices must be set to zero)
IACT(I) (20 values)	20*1	specifies whether a printout of radii dependent results is wanted for the distance band I = 0 no printout for distance I ≠ 0 printout for distance I

3.3.2 Input group POLGRID

In the input group POLGRID the user defines the grid for the population, agricultural production and land-sea distribution data and for the calculations of concentrations and individual doses and risks. It must precede the input group METEOZON. The title card is followed by the NAMELIST GRDPAR.

The grid consists of a polar coordinate system with the centre point at the location of the nuclear facility. The concentrations and individual doses and risks are calculated for a grid point representing the whole grid element. If you change the default values, you had to be sure to create new distance bands which are nearly representative for a square, in the view of the modelling of the re-emission part (see also physical description part UFOTRI /12/)

IMAX and JMAX are the number of radii and sectors respectively. RA is the outer radius of each radial band. IMAX, JMAX and RA must be identical to the parameters chosen when calculating the polar population distribution around the site. R is the reference point in the grid element chosen to represent the element as a whole, e.g. it could be half way between two values of RA. UFOTRI refers to each distance band by its referenced point (centre), e.g. if RA=2000, 5000, 10000 and R=1000, 3500 and 7500, then doses for example given at 3500 m would be representative of the doses in the band from 2 to 5 km.

K6.1 title card POLGRID
(FORMAT A8)

POLGRID name of identification (left-justified)

K6.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST GRDPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----

IMAX	20	number of radial distances (max. NRMAX)
------	----	---

JMAX	72	number of angular segments (max. NPHIMX)
------	----	--

R(I) (20 values)		radial grid; distance of the radii R(I), (I = 1,...IMAX) in meters, completed with dummy values to NRMAX values
---------------------	--	---

65.,	100.,	145.,	210.,	320.,
460.,	680.,	1000.,	1500.,	2100.,
3200.,	4600.,	6800.,	10000.,	15000.,
21000.,	32000.,	46000.,	68000.,	100000.

RA(I) outer radius of the distance bands I
(20 values) (I = 1,...IMAX) in meters, completed with
 dummy values to NRMAX values

80., 120., 170., 260., 390.,
570., 840., 1250., 1750., 2600.,
3900., 5700., 8400., 12500., 17500.,
26000., 39000., 57000., 84000., 125000.

The values of the radii RA(I) and the angular segments must be identical with those used in the preprocessing program GRIDS (not included in this UFOTRI package) to calculate the population distribution.

3.3.3 Input group ISOTOPE

In the input group ISOTOPE the user has to define the physical characteristics of the NTPMX nuclide groups NN. The sequence of the nuclides is **obligatory**

- 1. nuclide HT
- 2. nuclide HTO

The title card is followed by the NAMELIST ISOPAR.

K7.1 title card ISOTOPE
(FORMAT A8)

ISOTOPE name of identification (left-justified)

K7.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST ISOPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----
NABL	2	number of type of nuclides with different deposition characteristics (max. NTPMX) NOTE had to be set to 2 NOTE: sequence is obligatory (HT before HTO)
CORRVA(NN) (2 values)	2*1.0	correction factor for deposition velocity
VA(NN) (2 values)	0.0005 0.005	deposition velocity in m/sec for the nuclide group NN; NOTE: sequence is obligatory - NN = 1: HT-gas - NN = 2: HTO-vapour
IWASH	0	option for calculation of washout coefficient IWASH = 0: the washout coefficients and the mean relative duration of precipitation are precalculated for the nuclide groups NN and the precipitation intensity class IR IWASH = 1: the washout coefficients will be calculated according to the power law $XLAM(NN) = AWASH(NN) * (I^{**}BWASH(NN))$ for the nuclide groups NN, where I denotes the precipitation intensity in mm/h; a relative duration of rainfall can also be chosen, independently of the type of nuclide; for noble gases (NN=1) XLAM(1) will be set to 0.

If IWASH = 0 the following variables will be used:

IREGGR(IR1)	100,300	boundaries of the rain intensity classes IR in 0.01 mm/h
(2 values)		- IR = 1: rain intensity IREGGR(1)
		- IR = 2: rain intensity between IREGGR(1) and IREGGR(2)
		- IR = 3: rain intensity \geq IREGGR(2)
AMDA(NN,IR)		washout coefficient in 1/sec for the rain intensity class IR and the nuclide group NN
(6 values)		for IR = 1:
		0.,0.00006,
		for IR = 2:
		0.,0.00010,
		for IR = 3:
		0.,0.00040,
REGTIM(NN,IR)		mean duration of precipitation for the rain class IR and the nuclide group NN
(6 values)		for IR = 1: 1., 1.0
		for IR = 2: 1., 1.0
		for IR = 3: 1., 1.0

If IWASH = 1 the following variables will be used:

AWASH(NN)	0.0, 9.E-5	coefficient in power law for calculation of washout coefficient;
(2 values)		
BWASH(NN)	0.0, 0.6,	exponent in power law for calculation of washout coefficient, dependent on the nuclide group NN
(2 values)		
REGTIM(NN,1)	see above	mean duration of precipitation for the nuclide group NN, independent of any precipitation intensity class
(2 values)		

3.3.4 Input group METEOROL

The input group METEOROL defines the parameters for the atmospheric dispersion part of UFOTRI. If desired (METIN \neq 0) the user can supply weather conditions for a single weather sequence with straight-line Gaussian modelling consisting of one phase. The title card is followed by the NAMELIST METPAR.

K8.1 title card METEOROL
(FORMAT A8)

METEOROL name of identification (left-justified)

K8.2 DATA CARD (NAMELIST-FORMAT)
NAMELIST METPAR

NAME	DEFAULT	DESCRIPTION
----	-----	-----
METIN	0	option to start one single straight-line Gaussian calculation without changing weather situations \neq 0: the data of the atmospheric dispersion and deposition parameters are supplied by the user in the NAMELIST METPAR (IWNR, IWNG, IDIKAT, IREGN and MIXLH must be given there; additional parameters had to be set in the NAMELIST TRIDAT, see later on)
NOSHFT	2	option for the treatment of changes in wind direction during dispersion: = 0 straight-line dispersion model; all release phases are transported in the same direction = 1 straight-line dispersion; each release phase is transported in the direction of the wind at its beginning = 2 for each release phase hourly changes in wind direction are considered
IWNR	360	wind direction in degrees
IWNG	500	wind speed in 1/100 m/sec
IDIKAT	4	diffusion category (1 through 6, representing the categories A through F)
IREGN	0	rain rate in 1/100 mm/h
HGHT(IH) (IH=1,3)	50.,100.,180.	height for the σ -parameters in meters
MIXLH(ISK) (ISK=1,6)	1600,1200,800, 560, 320,200	height of the mixing layer in meters for each diffusion category ISK; (ISK = 1,...,6 represents the diffusion categories A through F)

WPE(ISK)	0.07,0.13,	wind profile exponent for the diffusion
(ISK=1,6)	0.21,0.34,	categories ISK (ISK = 1,...,6 represents the
	0.44,0.44	categories A through F)

The horizontal and vertical dispersion parameters are calculated as a function of distance x assuming the following power law (see KfK-4332)

$$\sigma_y = PY1 \cdot x^{QY1}$$

$$\sigma_z = PZ1 \cdot x^{QZ1}$$

The downwind diffusion is modelled in UFOTRI by the dispersion parameter σ_x ; as long as $\sigma_x < \sigma_y$, it is calculated due to

$$\sigma_x = \frac{2}{3} x \tan STETA1;$$

for $\sigma_x \geq \sigma_y$, it is assumed that $\sigma_x = \sigma_y$ (see KfK-4332, p. 15 - 17).

PZ1(ISK, IH, IRH)	linear term of the formula to calculate σ_z for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	1.321,0.950,0.700,0.520,0.382,0.311,
	1.321,0.950,0.700,0.520,0.382,0.311,
	1.321,0.950,0.700,0.520,0.382,0.311,
	0.151,0.127,0.165,0.215,0.264,0.241,
	0.051,0.070,0.137,0.265,0.487,0.717,
	0.025,0.033,0.104,0.307,0.546,0.485

QZ1(ISK, IH, IRH)	exponential term of the formula to calculate σ_z for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	6*0.711,6*0.711,6*0.711,
	1.219,1.108,0.996,0.885,0.774,0.662,
	1.317,1.151,0.985,0.818,0.652,0.486,
	1.500,1.320,0.997,0.734,0.557,0.500

PY1(ISK, IH, IRH)	linear term of the formula to calculate σ_y for:
(6*3*2 values)	- 6 diffusion categories ISK
	- 3 classes of height IH
	- 2 classes of roughness IRH
	(IRH = 1 : roughness IRAU = 2
	IRH = 2 : roughness IRAU = 3)
	0.946,0.826,0.586,0.418,0.297,0.235,
	0.946,0.826,0.586,0.418,0.297,0.235,
	0.946,0.826,0.586,0.418,0.297,0.235,

1.503,0.876,0.659,0.640,0.801,1.294,
0.170,0.324,0.466,0.504,0.411,0.253,
0.671,0.415,0.232,0.208,0.345,0.671

QY1(ISK,IH,IRH)
(6*3*2 values)

exponential term of the formula to calculate σ_y for:

- 6 diffusion categories ISK
- 3 classes of height IH
- 2 classes of roughness IRH
(IRH = 1 : roughness IRAU = 2
IRH = 2 : roughness IRAU = 3)

6*0.796,6*0.796,6*0.796,
0.833,0.823,0.807,0.784,0.754,0.718,
1.296,1.025,0.866,0.818,0.882,1.057,
0.903,0.903,0.903,0.903,0.903,0.903

STETA1(ISK,IH,IRH)
(6*3*2 values)

horizontal standard-deviation (in degree) of wind
direction for:

- 6 diffusion categories ISK
- 3 classes of height IH
- 2 classes of roughness IRH
(IRH = 1 : roughness IRAU = 2
IRH = 2 : roughness IRAU = 3)

20.5,13.9,10.1,6.9,4.,2.,
20.5,13.9,10.1,6.9,4.,2.,
20.5,13.9,10.1,6.9,4.,2.,
23.8,18.9,15.3,12.6,10.2,8.6,
20.5,13.9,10.1,6.9,4.,2.,
20.5,13.9,10.1,6.9,4.,2.

3.4 Parameters controlling the model part with an hourly timestep for atmospheric dispersion and the longer term ingestion pathways

The input parameters which are listed in this chapter belong to one single input group called 'TRIDAT'.

3.4.1 General control parameters

In this part of the input group TRIDAT general control parameters will be specified. Of special interest for the user may be four parameters which will be described in the following.

Q determines the relative amount of each of both chemical forms HT and HTO of the source term and Q1 contains the absolute amount of the source term in Bq per timestep and phase. BODFAK determines the minimum source strength of a secondary area source of HTO from the soil and the vegetation, which will be considered in the re-emission dispersion part. The minimal source strength will be calculated as

$$\text{minimal source strength} = \text{maximal soil concentration} \times \text{BODFAK}$$

The smaller the minimal source strength, the more computing time will be needed. The below listed values for BODFAK are useful:

BODFAK	release case
1	HT-release
100	HTO-release
10	HTO-release with building wake effects
0.1	HT-release with building wake effects

The fourth important parameter NSTOP controls the minimal duration of the atmospheric dispersion part with its more accurate modelling of all transfer processes. But the greater NSTOP is, the more computing time will be needed, however the results will be more defensible. Test calculations with the model have shown, that values of NSTOP greater than 170 hours give no significant changes in the resulting dose, because the dispersion of tritium due to atmospheric processes are no longer important.

BODFAK = A factor which will be multiplied by the maximum air concentration for defining the minimum source strength of an area source which will be considered in the re-emission dispersion part
(DEFAULT = 100.)

- NSTOP** = Minimal duration of the re-emission process in hours; the re-emission program stops after **NSTOP** hours and the amount of activity in the soil is reduced to the third part of the tritium content after the re-emission routine has started
(DEFAULT = 70)
- IZFREI** = Duration of the release of the primary plume in seconds; is only important for line printer output of concentrations in air
 $0 < \text{IZFREI} < 3600$
(DEFAULT = 3600)
- IFLENG** = Flag to define the area source geometry for the re-emission algorithm
= 1 narrow area source with 6 grid points
Notice if the narrow area source geometry is selected, a special radial grid has to be considered, which is different from the normally used one
= 0 normal area source with 14 grid points
(DEFAULT = 0)
- Q(NN,J)** = Relative source strength of the nuclide type NN in the phase J
 $0. \leq Q \leq 1.$
(DEFAULT = $17 * 0.$, $17 * 1.$)
- Q1(J)** = Absolute source strength in the phase J
(DEFAULT = $17 * 1.$)
- ZEIT** = Time interval between meteorological recordings
NOTE had to be 3600.
(DEFAULT = 3600.)
- CHIMAX** = Minimum value of the time integrated air concentration (cut-off value in Bq s / m³)
(DEFAULT = 1.E-15)
- NUKL(NN)** = names of chemical forms of tritium considered in UFOTRI
(DEFAULT NN = 1 : 'HT GAS '
NN = 2 : 'HTO VAP.')
- NJAHRE** = Number of years with meteorological data
 $\text{NJAHRE} \geq 1$
(DEFAULT = 1)

3.4.2 Plant parameters

In this part of the input group TRIDAT two different plant specific parameter sets will be defined. Two parameters (for each plant species) determine the fraction of organic and anorganic matter content of the vegetation (dependent on the type of plant). At least two additional parameters are necessary to calculate the stomata resistance which is needed for calculation of the exchange velocity plant-atmosphere (model of Belot). If the extended model for calculating the stomata resistance is recommended (IMODEL = 1), a value has to be assigned to five further parameters.

- ISTRGR** = If the solar radiation has greater values than ISTRGR, water stress will occur. **Note** the dimension is $\text{Watt/m}^2 \times 0.357 \times 0.8$
(DEFAULT = 1000)
- IMODEL** = Choice of the model for calculating the plant resistance
= 1 extended model will be used considering:
radiation balance, air temperature, air humidity, water content of soil, water stress from high solar radiation
= 0 simple model will be used considering:
day/night cycle, water content of soil, water stress from high solar radiation
(DEFAULT = 1)
- RCMIN** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, **for area 1**
(DEFAULT = 4.0)
- BEWG** = Weight of vegetation water in g / m^2 **for area 1**
(DEFAULT = 400.0)
- BEWGZ** = Mass content of the organic parts of the plant in g / m^2 **for area 1**
(DEFAULT = 100.0)
- LEAF** = Leaf area index in m^2 / m^2 **for area 1**
(DEFAULT = 3.0)
- RCPARA** = Constant equal to the photosynthetic radiation flux density measured at a stomata resistance two times higher than the minimum value **for area 1; if IMODEL = 1**
(DEFAULT = 20.0)
- VPDA** = Constant related to the vapour pressure deficit **for area 1; if IMODEL = 1**
(DEFAULT = 0.2)

- TMINA** = Minimum temperature at which stomata closure occurs in °C **for area 1; if IMODEL = 1**
(DEFAULT = 0.0)
- TMAXA** = Maximum temperature at which stomata closure occurs in °C **for area 1;**
(DEFAULT = 45.0)
- TOPTA** = Optimum temperature for photosynthesis in °C **for area 1;**
if IMODEL = 1
(DEFAULT = 25.0)
- RCMIN2** = Minimal stomata diffusion resistance normalized to a leaf area index of 1, **for area 2**
(DEFAULT = 4.0)
- BEWG2** = Weight of vegetation water in g / m² **for area 2**
(DEFAULT = 400.0)
- BEWGZ2** = Mass content of the organic parts of the plant in g / m² **for area 2**
(DEFAULT = 100.0)
- LEAF2** = Leaf area index in m² / m² **for area 2**
(DEFAULT = 3.0)
- RCPARG** = Constant equal to the photosynthetic radiation flux density measured at a stomata resistance two times higher than the minimum value **for area 2; if IMODEL = 1**
(DEFAULT = 20.0)
- VPDG** = Constant related to the vapour pressure deficit **for area 2;**
if IMODEL = 1
(DEFAULT = 0.2)
- TMING** = Minimum temperature at which stomata closure occurs in °C **for area 2; if IMODEL = 1**
(DEFAULT = 0.0)
- TMAXG** = Maximum temperature at which stomata closure occurs in °C **for area 2; if IMODEL = 1**
(DEFAULT = 45.0)
- TOPTG** = Optimum temperature for photosynthesis in °C **for area 2;**
if IMODEL = 1
(DEFAULT = 25.0)

3.4.3 Soil parameters

The following parameters describe the soil characteristics as well as some special re-emission conditions (re-emission rate of the soil during the nighttime and during rain events; overall change of re-emission rate).

The most important parameter which is listed in the following is BODEIN, the initial water content of the soil (of both areas). Test calculations demonstrated that the collective and individual dose from the ingestion pathways reacts very sensitive to changes of BODEIN. Therefore it is planned that in a further code version the initial water content of the soil is precalculated by a hydrological model for each hour of the meteorological dataset.

There exists a possibility to select an extended soil transport model (IBODEX = 1), which includes water transfer between the soil layers due to matrix forces.

- SOILMX** = Fraction of the maximum free pore volume of soil
(DEFAULT = 0.5)
- BODEIN** = Initial value of the fraction of the soil water content
0.2 means 20% water content in the free soil pore volume which is
SOILMX*100% of the soil matrix
(DEFAULT = 0.2)
- WILTP** = Wilting point, stomata closure occurs
(DEFAULT = 0.1)
- IBODEX** = Choice of the model for calculation of the water transport in soil
= **1** extended model will be used with the calculation of the suction
tension and soil conductivity:
formula for suction tension:
$$SS = 1.5E5 * PSI1^{**}(AP + BP*PSI1 + CP*PSI1^{**}NP)$$

formula for conductivity:
$$COND = AKP / (SS^{**}MKP + BKP)$$

= **0** simple model will be used
(DEFAULT = 1)
- IARTBO** = Only valid if IBODEX = 1; selects the soil characteristics
= **1** humus sandy loam; (special default values used)
= **2** loamy sand; (special default values used)
= **3** sand; (special default values used)
= **4** the user may define his own soil type with the following 7 param-
eters
(DEFAULT = 1)

- SOILAP** = Parameter for calculating the suction tension: AP
(DEFAULT = 1.65)
- SOILBP** = Parameter for calculating the suction tension: BP
(DEFAULT = 7.3)
- SOILCP** = Parameter for calculating the suction tension: CP
(DEFAULT = -3.1)
- SOILNP** = Parameter for calculating the suction tension: NP
(DEFAULT = 7.5)
- SOIAKP** = Parameter for calculating the conductivity: AKP
(DEFAULT = 1000.)
- SOIBKP** = Parameter for calculating the conductivity: BKP
(DEFAULT = 60.0)
- SOIMKP** = Parameter for calculating the conductivity: MKP
(DEFAULT = 1.41)
- REMRE** = Re-emission rate during rain events in % per hour
(DEFAULT = 0.3)
- REMNI** = Re-emission rate during the night in % per hour
(DEFAULT = 1.0)
- REDREM** = Factor varying the re-emission rate
(DEFAULT = 1.0)

3.4.4 Parameters for the short term ingestion pathways

The parameters listed below determine the fractions of the agricultural used land areas and the pasture land areas (FAKC1, FAKC2). The remaining five parameters control the water balance of the atmosphere, the number of cows which are grazing on one square kilometre and the organic and anorganic matter content of the cows.

- FAKC1** = Fraction of the area reserved for grazing animals
(DEFAULT = 0.2)
- FAKC2** = Fraction of the area reserved for agricultural production and vegetation
Note had to be selected as **1 - FAKC1**
(DEFAULT = 0.8)
- NCOW** = Number of cows, grazing on one square kilometer
(DEFAULT = 250)
- WWCOW** = Mass content of the anorganic part (water) of a cow in kg per cow
(DEFAULT = 350.0)
- WOCOW** = Mass content of the organic fraction of a cow in kg per cow
(DEFAULT = 150.0)
- WATM** = Mass of water in the atmosphere in kg / km³
(DEFAULT = 8.0E + 6)
- NASS** = Mass of rain reaching the ground per day in kg / km³ d
(DEFAULT = 1.93E + 6)

3.4.5 Long term ingestion pathways

The parameter presented here are necessary for the calculation of the longer term behaviour of tritium in the environment. They control the compartment module which runs after the dispersion and re-emission model. The most important point is that NBOX, NINI, NINT and NOUT have to be set to the same values. Allowed are the value 6, for agricultural land use only, and the number 10, which announces that both areas have to be taken into account.

- NBOX** = Number of compartments (10 for both areas and 6 for agricultural area only)
(DEFAULT = 10)
- NINI** = Number of compartments with an initial inventory = **NBOX** (10 for both areas and 6 for agricultural area only)
(DEFAULT = 10)
- NINT** = Number of integrals with an initial inventory = **NBOX** (10 for both areas and 6 for agricultural area only)
(DEFAULT = 10)
- NOUT** = Number of inventories = **NBOX** (10 for both areas and 6 for agricultural area only)
(DEFAULT = 10)
- NTFX** = Number of transfer coefficients (27 for both areas and 15 for agricultural area only)
(DEFAULT = 27)
- NTIM** = Number of integration times for dose calculation (**max values = 10**)
(DEFAULT = 3)
- TIMC(NTIM)** = values of the integration times for dose calculation in days
NOTE: the results are calculated for integration times TIMC + duration of re-emission process
(DEFAULT = 0., 30., 365., 7*0.) **NOTE:** first value has to be 0

3.4.6 Parameters for dose calculations

The parameters in the equations for the dose calculations consist of two groups. Three parameters contain values for the dose conversion factor, dependent on the age of the individual and the integration time, whereas other parameters determine the breathing rate, the rate of uptake through the skin and the ingestion habits of the population group of interest. However, for a standard run an adult and the 50 year committed dose are recommended.

BRRATE	=	Breathing rate of an individual in m^3 / s (DEFAULT = 3.3E-4)
SKRATE	=	Rate of skin uptake of an individual in m^3 / s (DEFAULT = 1.4E-4)
IMEAT	=	Consumption rate of meat for an individual in gram per day (DEFAULT = 300)
IVEGE	=	Consumption rate of vegetables for an individual in gram per day (DEFAULT = 500)
IMILK	=	Consumption rate of milk products for an individual in gram per day (DEFAULT = 300)
ITIMD	=	Index of the TIMC array for defining the integration time for the dose calculation (DEFAULT = 3)
DOSF	=	Dose conversion factor in Sv/Bq (HTO) for an individual and an integration time selected with ITIMD for dose calculation (DEFAULT = 1.7E-11)
DOSHT	=	Dose conversion factor in Sv/Bq (HT) for an individual and an integration time selected with ITIMD for dose calculation (DEFAULT = 1.7E-15)
DOSFOB	=	Dose conversion factor in Sv/Bq (OBT) for an individual and an integration time selected with ITIMD for dose calculation (DEFAULT = 4.5E-11)

3.4.7 Parameters controlling a fixed stationary run

If the user selects a run with fixed meteorology (METIN = 1 in the input group METEOROL) the both remaining input parameters temperature and solar insolation have to be set to fixed values, too. Additionally a fixed re-emission rate of HTO from the soil and the plants may be chosen. Because of the strong implications and the dynamic interactions of all processes concerning the vegetation, a fixed exchange rate plant-atmosphere can hardly be defined. However there exists a second possibility to have nearly stationary run conditions. If the environmental parameters remain constant, the model calculates implicitly a nearly constant exchange rate plant-atmosphere. Only the exchange soil to atmosphere will vary due to loss of water from the soil.

- IRFIX** = Flag to specify the re-emission rate
= 1 fixed re-emission rate
Note should be used carefully. It is a relict of the first stages of the development of the program. The fixed values of re-emission and plant deposition rate have to be changed in the program , if desired
= 0 re-emission rate will be calculated by the program (normal mode)
(DEFAULT = 0)
- REFEST** = Value of a fixed re-emission rate in % per hour
(DEFAULT = 5.0)
- ITEMPE** = Fixed value for the air temperature during the whole run in °C × 100;
Note will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
(DEFAULT = 1000)
- ISTRBE** = Fixed value for the radiation balance during the whole run in Watt **Note** will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
(DEFAULT = 100)
- RELFA** = Fixed value for relative humidity in air in percent **Note** will be considered if **METIN** is set to 1 (METIN belongs to another namelist called METPAR, input group METEOROL)
(DEFAULT = 0.5)

3.4.8 Parameters controlling input and output listings

The parameters listed above control the storage of results on permanent files as well as the output listing on line printer.

- IFACHS** = Index of the sector position in the polar grid system for printer control output
(DEFAULT = 28)
- IEINR#** = 4 values: IEINR1 - IEINR4
Index of the radius position in the polar grid system for printer control output
(DEFAULT = 6, 8, 12, 16)
- IZUAUS** = Flag steering additional control output during each time step on line printer (very lines consuming)
= 1 very much control output
= 0 no special control output
(DEFAULT = 0)
- KAUSDR(12)** = Array of 12 flags steering additional control output which will be printed on line printer (very lines consuming)
= 1 control output
= 0 no control output
KAUSDR(1) - KAUSDR(6) controls output of the main dispersion program
KAUSDR(7) controls output of subroutine which calculates the transfer factors
KAUSDR(8) controls output of subroutine which calculates the re-emission area and source strength
KAUSDR(9) controls output of subroutine which calculates the processes in the soil and in plants
KAUSDR(10) controls output of subroutine which calculates the dispersion process and environmental conditions of the re-emission process
KAUSDR(11) controls output of subroutine which calculates the dispersion process and environmental conditions of the re-emission process
KAUSDR(12) controls output of subroutine which calculates the long term ingestion doses
(DEFAULT = 12*0)

- IPRPLT** = Controls whether a printerplot is created for the chemical form of tritium and for each phase
= 0 no printerplot
= 1 printerplot for all weather sequences
= 2 printerplot only for the weather sequences defined by LKZ (see i. g. PRINTOUT, namelist OUTPAR)
(DEFAULT = 0)
- INUKL** = Index of the chemical form of tritium for which the concentrations are plotted by printerplot
(DEFAULT = 2)
- IWRITE** = Controls whether doses from inhalation + skin absorption and doses from the ingestion pathways are stored on the logical UNIT 9 for each weather sequence and each phase
= 0 no storage
= 1 storage on the logical UNIT 9
(DEFAULT = 0)
- LWETE** = For each weather sequence LW with $(\text{MOD}(\text{LW}, \text{LWETE}) = 0)$ a control printout will be created; should be-used only for testing
(DEFAULT = 1000)

4. Run the model

4.1 Introduction

At first it has to be pointed out, that UFOTRI needs some special subroutines from a mathematical library called **IMSL**. The long term ingestion model calculates with the help of these subroutines the eigenvectors and eigenvalues of the matrix of transfer rates (see Table 1). If the computer system of the user does not include the IMSL library, another library with these special subroutines in **double precision** mode has to be selected. Most of the rest of the program code is written in standard FORTRAN 77 except the NAMELIST (see chapter 5) and the INCLUDE statement.

The easiest way to gain experience is to start the example calculation proposed in chapter 4.4. With the variation of the input parameters and the corresponding changes in the results, the user may find out the main influencing parameters which should be defined very carefully.

An additional way to get a better understanding is to read the main report of UFOTRI, which describes the physical behaviour of tritium in the environment, as it is included in the model /12/. A list of all subroutines called within UFOTRI (Fig. 3 - Fig. 5) as well as 3 flow charts (Fig. 6 - Fig. 8) are intended to give the user a first understanding of UFOTRI.

4.2 Special input data-set for UFOTRI (meteorological file)

The meteorological data file contains information on the stability (Pasquill Turner categories), the wind direction, the wind speed, the precipitation intensity, the air temperature the relative humidity and solar radiation balance. These data should be available for one meteorological observation station representative for the site with a temporal observation interval of one hour. The data have to be available on a Direct ACCESS File. One record of the file contains the following 7 data in the described order:

WR(J), IDIFF(J), IRAIN(J), WG(J), ITEMP(J), ISTRB(J), RELF(J), J = 1,24

No. of variable	Variable	Type	length in byte b_i	meaning
1	WR	INT*4	4	Wind direction in °C
2	IDIFF	INT*4	4	Pasquill-Turner Stability class; conversion in (1=A, 2=B, 3=C, 4=D, 5=E, 6=F)
3	IRAIN	INT*4	4	Rain intensity in mm/h*100
4	WG	INT*4	4	Wind speed in meter * 100
5	ITEMP	INT*4	4	Air temperature in °C x 100
6	ISTRB	INT*4	4	Solar radiation in Watt / m**2
7	RELF	REAL*4	4	Relative humidity in % / 100.

In the current version the length of one record equals 672 byte (= $\sum_{i=1}^7 b_i \times 24$).

Generally the meteorological input data file has the following characteristics :

```
ACCESS      : DIRECT
RECL        :  $\sum_{i=1}^7 b_i \times 24$ 
BLKSIZE     : = RECL
RECFM      : F = FIXED
```

The **whole** dataset contains **NDAYS** records, where

NDAYS = NYEARS * MAXDAY = max. number of days with met. data

The meteorological data have to be prepared unformatted and binary. They have to be available on logical input **unit 11**.

4.3 Output of UFOTRI

Up to now there exists no evaluation program for the results calculated in UFOTRI. For testing, some selected values will be stored on the logical **units 91 and 92**. A description of these values can be found in the program. The final results of one run concern 3 different dose values. Doses will be calculated for inhalation + skin absorption from plume passage only and secondly with re-emission. The third value is the chronic dose from ingestion. These doses can be printed on paper for each selected weather sequence as well as stored on the logical **unit 21**. Additionally, collective doses will be calculated and printed on paper but they will not be stored on a permanent file. All dose values are potential doses.

In the future, the evaluation programs COCDOS, CORPER and CORARE of the COSYMA package, might be modified for the output of UFOTRI.

4.4 Example of a Job Control data set

Table 3 shows an example of a Job Control file with all the parameters of the general input groups of UFOTRI which are necessary to run the program. The parameters which belong to the input group TRIDAT are only a selection of those parameters which can be chosen by the user. But for each run the user should take care which parameters have to be modified and which can remain unchanged.

For running the program the user needs 5 FORTRAN members namely **TEILO, TEIL1, TEIL4, SCOMMON and PARAM**. TEILO includes the data statements for the general and most of the optional namelists as well as the read statements and control output of the frame of UFOTRI. TEIL1 contains the main program. As mentioned at the beginning, the COMMON blocks used in the UFOTRI-frame are implemented in the SCOMMON part which will be imbedded by an INCLUDE statement in the single program parts. Due to some historical reasons the COMMON blocks in the dispersion part of UFOTRI are separated from those of the SCOMMON part. Nevertheless most of the COMMON blocks which are in SCOMMON occur in the dispersion part too. So be careful if you change one of the COMMON blocks. Some general dimension parameters are defined in PARAM which is imbedded in SCOMMON. TEIL4 contains the main subroutine calculating the dispersion-, ingestion- and dose part of UFOTRI.

All necessary and optional input/output units are listed in Table 2.

5. Examples of NAMELIST input

The programs of UFOTRI are written in standard FORTRAN-77 with the use of two additional features, the INCLUDE and NAMELIST statements.

The INCLUDE statement causes the FORTRAN compiler to insert lines taken from another file into the file being compiled. It is used to insert COMMON blocks into most of the subroutines of the UFOTRI programs. The statement takes the form

```
INCLUDE(filename)
```

in the source code provided. This may need to be modified for some computers. For example, the equivalent statement on a VAX computer is

```
INCLUDE 'file.FOR'/LIST
```

where file.FOR is the name which has been given to the file to be included as it was copied from the UFOTRI tape to the user's computer.

If the INCLUDE statement is not available on the user's computer, then the required lines must be inserted using an editor.

Within UFOTRI FORTRAN NAMELISTs are used to provide a free format input together with default values for all the parameters considered. The user-supplied input only needs to specify values for those parameters for which the default is not considered applicable. Full details of the way this is done will be given in the Fortran language manual for the computer system in use. This section gives a brief summary of the main features of NAMELIST input. The input routines will have to be extensively re-written if the package is to be used on computer systems without this feature.

The Fortran program contains statements like the following:

```
DIMENSION REALS(5),INTEG(5)
DATA REALS/1.0,2.0,3.0,4.0,5.0/
DATA INTEG/5,5,3,0,0/
DATA PARAM/10.0/
DATA INTPAR/0/

NAMELIST /EXAMPL/ REALS, INTEG, PARAM, INTPAR

READ(5,EXAMPL)
```

These statements define floating point (ie for storing decimal numbers) variables REALS and PARAM. REALS is an array of 5 members which have default values REALS(1) = 1.0, REALS(2) = 2.0, REALS(3) = 3.0, REALS(4) = 4.0, and REALS(5) = 5.0 PARAM is a single variable and has the default value of 10.0. The statements also define integer variables INTEG and INTPAR. INTEG is also an array of 5 members which have default values INTEG(1) = 5, INTEG(2) = 5, INTEG(3) = 3, INTEG(4) = 0, and INTEG(5) = 0. INTPAR is a single variable with default value of 0.

All or any of these default values can be changed from the input file. The section of the file referring to these parameters is introduced by

```
&EXAMPL
```

Note that the & must be in the second column of the line on which it appears. The rest of the input section is written in free format, and terminated by &END.

Examples of the input file follow.

```
&EXAMPL  
  INTEG(1) = 1,  INTEG(5) = 1  
&END
```

This sets the values of INTEG(1) and INTEG(5) to be 1, and leaves all the other parameters, including the other members of the array INTEG, at their default values. Note that the variable names used in the input must be identical to those used in the program.

```
&EXAMPL  
  REALS = 5*2.3  
&END
```

This sets all five members of the array REALS to the value 2.3, and leaves all other parameters at their default values.

```
&EXAMPL  
  PARAM=5.0,  INTPAR=3  
&END
```

This sets only the variables PARAM and INTPAR, leaving the other variables at their default values.

```
&EXAMPL      &END
```

This leaves all variables at their default values. Note that this must be used to leave the variables at default values unless the NAMELIST is optional or keywords are used to input certain NAMELISTs only.

subroutine	description
EBALAF	balances a matrix
EHESSF	reduces the matrix to the upper Heisenberg form
EHBCKF	formes the matrix of accumulated transformations
EQRH3F	calculates the Eigenvalues and Eigenvektores
EBBCKF	transformes the Eigenvektores to a balanced matrix to those of the original unsymmetric matrix
VSRTRD	orders the Eigenvalues in descending order

Table 1. 6 IMSL-subroutines called in the long term ingestion part (COMA)

unit	output	input	definition
NEIN	----	INDAT	user NAMELIST input (default: 5)
NAUS	INDAT	----	printout of input data and results (default: 6)
11	----	UFOTRI	meteorological data in UFOTRI form; direct access file
13	(METSAM)	METEO	starting times and probability of the weather sequences (only if LWOPT = 2 and LPOPT = 2)
21	UFOTRI	----	results of UFOTRI
31	(GRIDS)	METEO	input file for the population data (if NSTOPT = 3)
91	UFOTRI	----	plot information for testing some parameters for special grid points
92	UFOTRI	----	plot information for testing some parameters (areas)

Table 2. Sorted list of I/O-Units for the tritium model UFOTRI

```
//INR303X1 JOB (0303,102,POD5S),RASKOB,REGION=6000K,NOTIFY=INR303,
// MSGCLASS=H,TIME=(0,30)
//*****
//*                                     *
//* ---> TEST JCL                       *
//*                                     *
//*****
//**MAIN LINES=50
// EXEC F7CLG,PARM.C='INCLUDE',
//          IMSL=DP
//C.SYSPRINT DD DUMMY
//C.SYSINC DD DISP=SHR,DSN=INR303.UFOTRI.FORT
//C.SYSIN DD DSN=INR303.UFOTRI.FORT(TEILO),DISP=SHR
//          DD DSN=INR303.UFOTRI.FORT(TEIL1),DISP=SHR
//          DD DSN=INR303.UFOTRI.FORT(TEIL4),DISP=SHR
//G.SYSIN DD *
@
@
@          FK2
@
POLGRID
&GRDPAR
  IMAX=20,JMAX=72,
  R= 65., 100., 145., 210., 320., 460., 680., 1000.,
  1500.,2100., 3200., 4600., 6800., 10000., 15000., 21000., 32000.,
  46000., 68000., 100000.,
  RA= 80., 120., 170., 260., 390., 570., 840.,
  1250., 1750., 2600., 3900., 5700., 8400., 12500., 17500., 26000.,
  39000., 57000., 84000., 125000.
&END
ISOTOPE
&ISOPAR
  NABL=2,
  VA=5.E-4,0.005
&END
SOURCE
FKxy          1          0          0
              1          20  0.000E0  0.000E0  0.000E0
METEOZON
  KARLSRHE    1          1  0  1  2  10
              4020
OOHOMOGEN    0  1.00E- 0          1
              5.00E+01  0
PRINTOUT
&OUTPAR
  NOOTKZ=2,NOOTMT=2
&END
METEOROL
&METPAR
  METIN=0,IWNR=315,IWNG=300,IREGN=100,IDIKAT=4,
  MIXLH=1600,1200,800,560,320,200
&END
END
```

Table 3: Example of an UFOTRI Job Control file (cont. on next page)

```
&TRIDAT
NJAHRE=1,LWETE=1,INUKL=2,IPRPLT=1,IWRITE=0,Q(2,1)=1.,Q(1,1)=0.0,
Q1(1)=3.7e16,IDMP=8,IDMPMX=20,NSTOP=70,
IZFREI=36000,IFACHS=28,IEINR1=6,IEINR2=8,IEINR3=12,IEINR4=16,
BODFAK=1.,REMRE=0.3,BODEIN=0.2,ISTRGR=200,
BEWG=1440.,BEWGZ=160.,RCMIN=4.,LEAF=3.,
LEAF2=3.,BEWG2=680.,BEWGZ2=170.,RCMIN2=4.,
FAKC1=0.2,FAKC2=0.8,
NBOX=10,NINI=10,NINT=10,NOUT=10,
BRRATE=3.3E-4,IMILK=300,IVEGE=521,IMEAT=300,
NTIM=3,ITIMD=3,TIMC=0,10,365,7*0,NCOW=250,
IMODEL=1,IARTBO=4,
WILTP=0.10,IBODEX=1,SOILMX=0.5,
KAUSDR=0,0,0,0,1,1,1,1,1,1,1,0
&END
//G.FT11F001 DD DISP=SHR,DSN=INR303.TRYKLIMR.DATA,LABEL=(,,IN)
//G.FT13F001 DD DISP=SHR,DSN=INR303.STRTTIME.DATA,LABEL=(,,IN)
//G.FT21F001 DD UNIT=SYSDA,DCB=DCB.VBS,SPACE=(TRK,500)
//G.FT31F001 DD DISP=SHR,DSN=INR482.HEADER.DATA,LABEL=(,,IN)
/*
//G.FT91F001 DD DISP=SHR,DSN=INR303.BEISPIEL.TRITDA8,LABEL=(,,OUT)
//G.FT92F001 DD DISP=SHR,DSN=INR303.BEISPIEL.TRITDA9,LABEL=(,,OUT)
```

Table 3: Example of an UFOTRI Job Control file (cont.)

Figure 1. Key processes of tritium behaviour in the environment

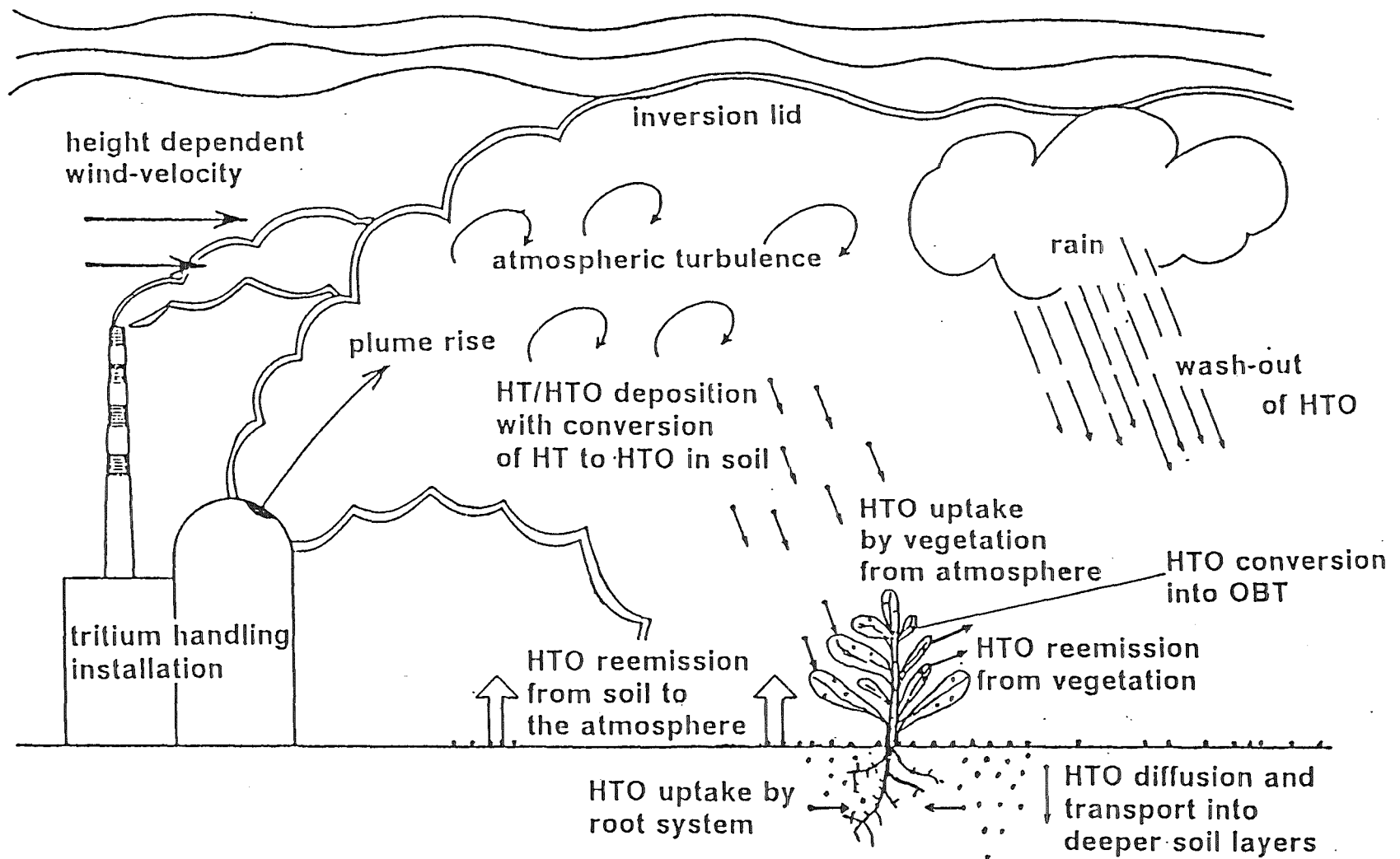
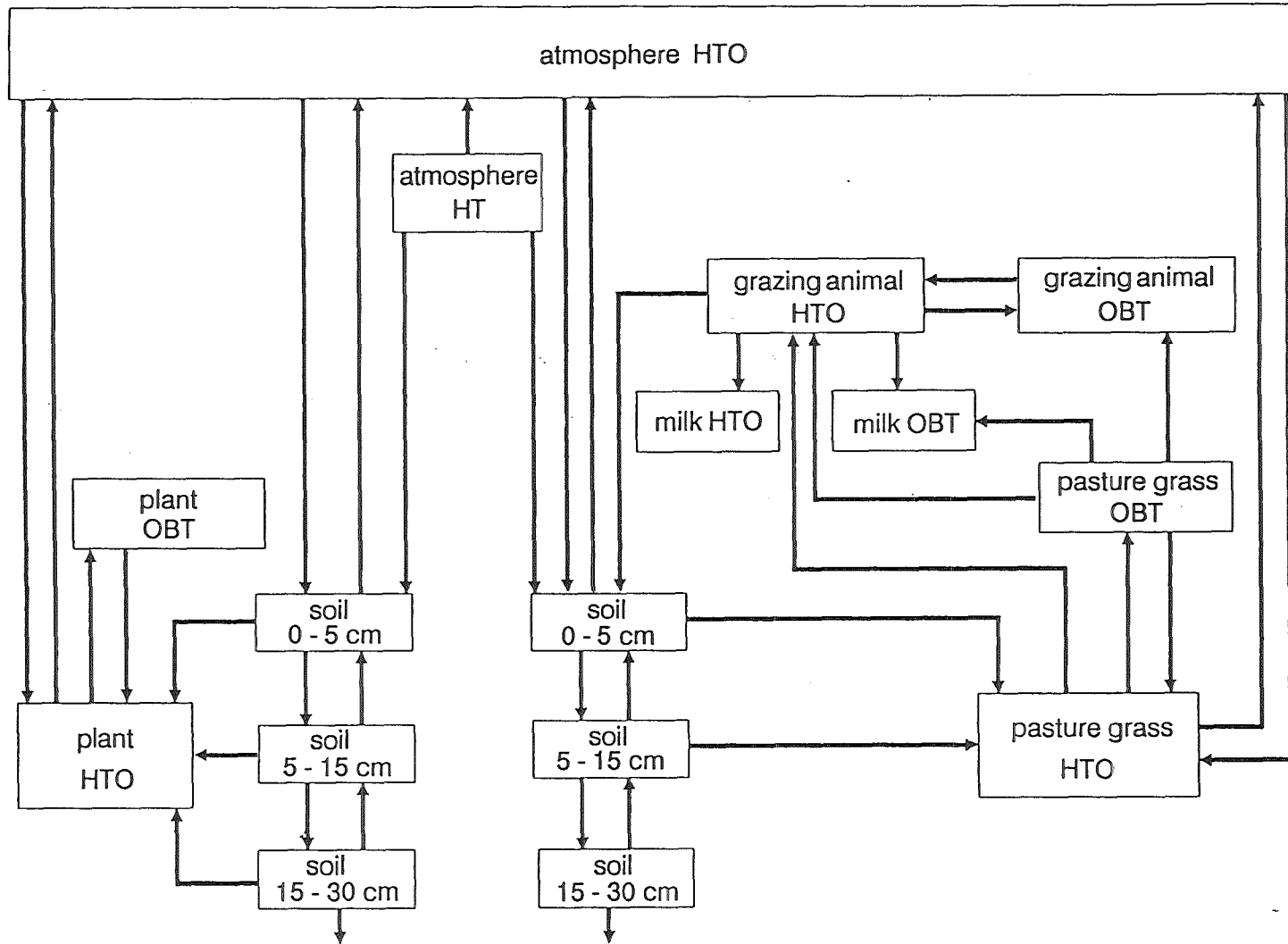


Figure 2. Diagram of transfer pathways in UFOTRI



	- INPUT	input namelist UFODAT
	- PUNKTE	specifies grid points
	- AUSBPF	area source dispersion + ingestion
	- PLRISE - HOEHE	final rise
	- PQYZFO	vert. interpolation of diff. coefficients
	- PQYZF2	vert. interpolation of diff. coefficients
	- DRYDEP - INTEG	dry deposition to soil
	- DRYPF	deposition to plants
UFOTRI	- RISEFX	rising phase of the plume
	- OUTPA	control output
	- METOUT	controls output of met. data
	- TRANSF	calculates transfer rates
	- COMA	long term ingestion pathway
	- RAUSDR	printout of concentrations
	- RAUSD2	printout of concentrations
	- RAUSDD	printout of ingestion dose
	- DOSIS	collective dose calculation

Figure 3. Subroutines called in UFOTRI

	- BODENR	soil parameter + re-em. from soil
	- MASSCH	mass balance check for plants
	- WATER	extended soil transport module
	- DRYPF	deposition to plants
AUSBPF	- FLAE3	area source module (narrow)
	- RESUS	re-emission rate from plants
	- FLAE	area source module (normal)
	- PQYZFO	vert. interpolation of diff. coefficients
	- DRYDE2 - INTEG	dry deposition to soil
	- TRANSF	calculates transfer rates

Figure 4. Subroutines called in the area source module AUSBPF

COMA	- COMAS- ERRSET	long term ingestion pathway
	- COMA1	calculation of the transfer matrix (in the subroutine EIGENS the vector operations will be performed)
	- COMA2	calculation of the actual and integral concentrations in all boxes

Figure 5. Subroutines called in the long term ingestion module COMA

Figure 6. Flow-chart of UFOTRI

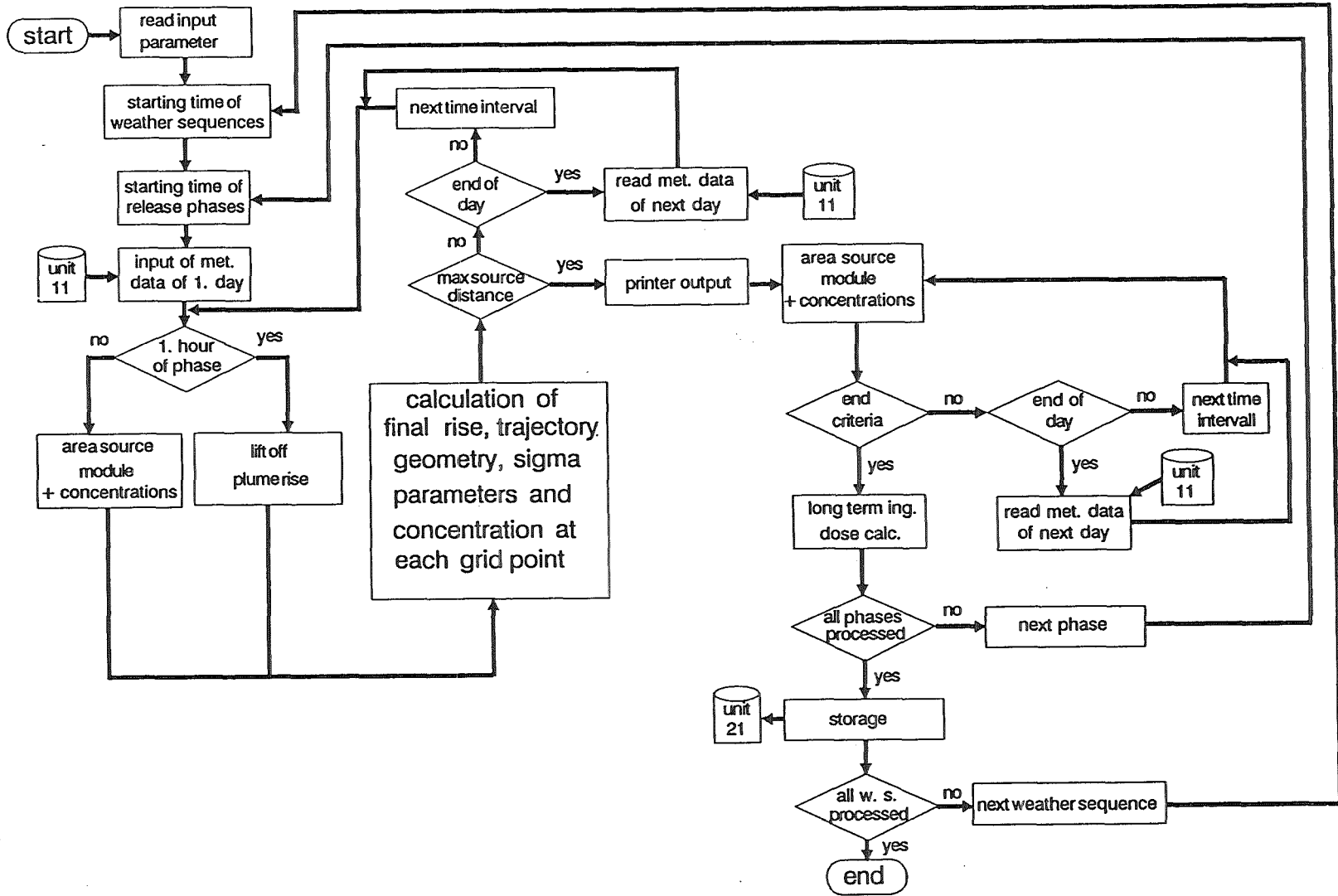


Figure 7. Flow-chart of area source dispersion module AUSBPF

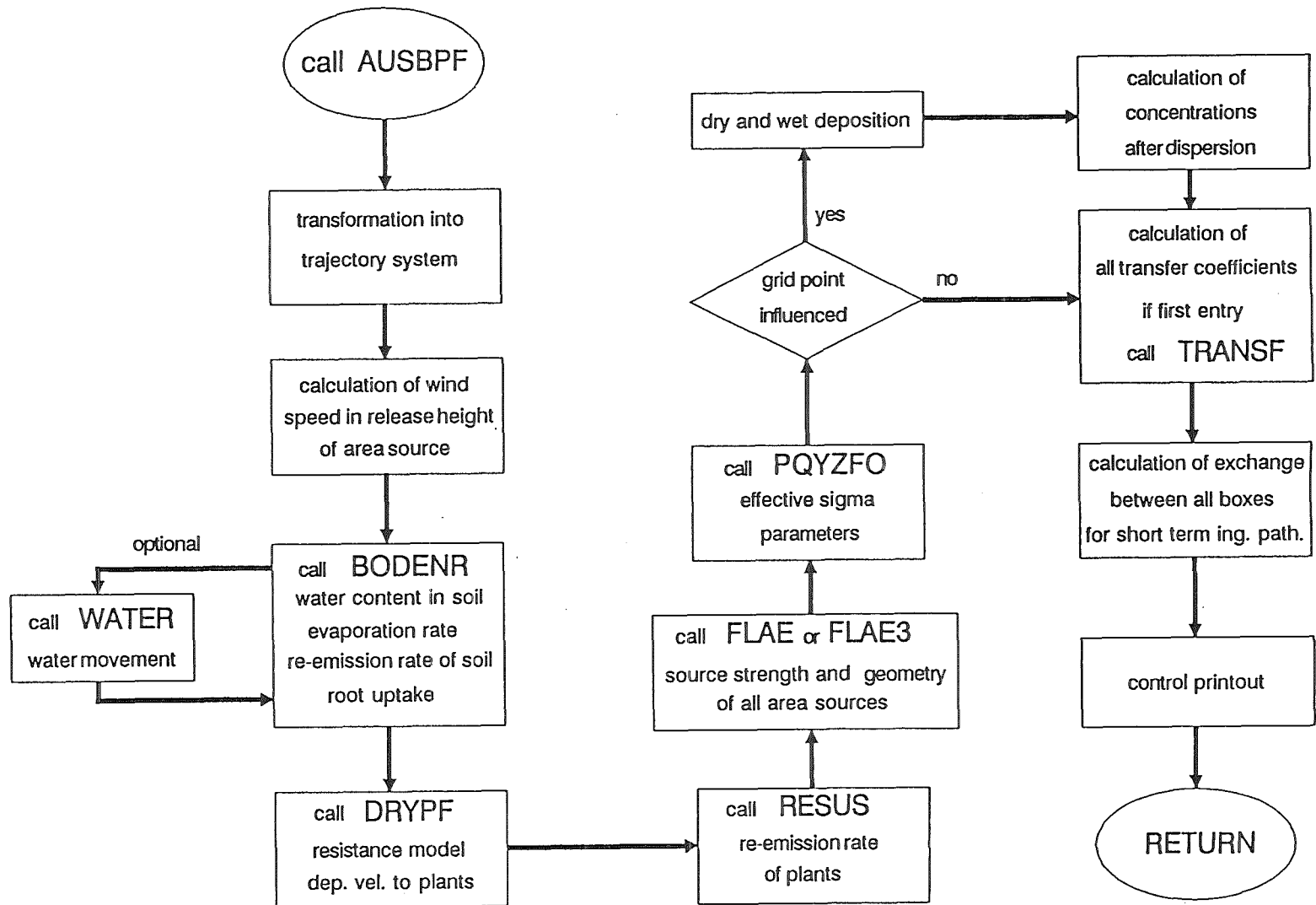
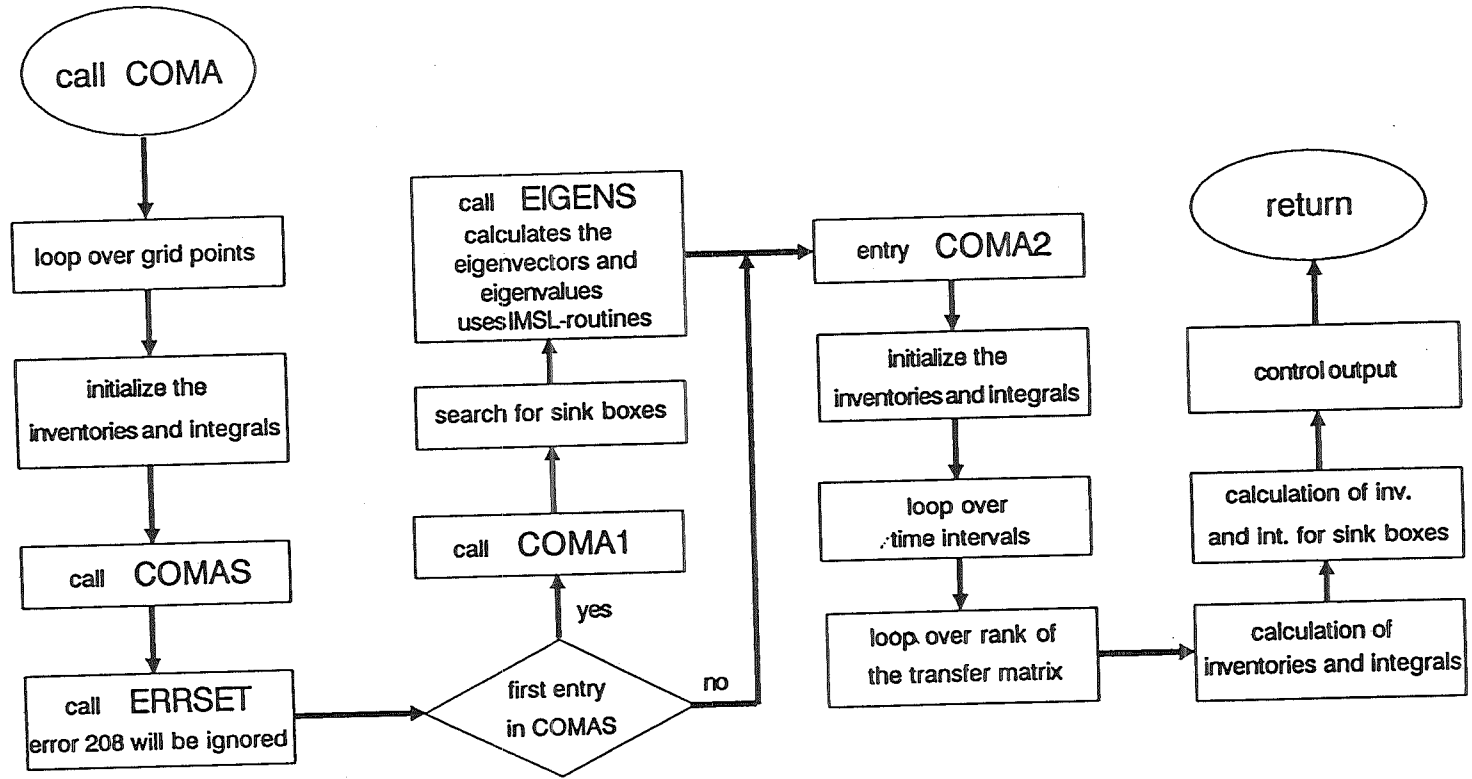


Figure 8. Flow-chart of long-term ingestion module COMA



Acknowledgement

This work has been performed in the framework of Nuclear Fusion Project of the Kernforschungszentrum Karlsruhe and is supported by the European Communities within the European Technology Program.

References

- /1/ Baldocchi, D.D., Hicks, B.B. and Camara, P.
A Canopy Stomatal Resistance Model for Gaseous Deposition to Vegetated Surfaces
Atmospheric Environment, Vol. 21, No. 1, pp. 91-101 (1987)
- /2/ Belot, Y., Gauthiers, D., Camus, H. and Caput, C.
Prediction of the Flux of Tritiated Water from Air to Plant Leaves.
Health Physics, Vol 38, pp. 575-583 (1979)
- /3/ Fisher, M.J. et. al.
An Analysis of the Effects of Repeated Short-term Soil Water Deficits on Stomatal Conductance to Carbon Dioxide and Leaf Photosynthesis by the Legume *Macroptilium atropurpureum* cv. Siratro
Australian Journal of Plant Physiology, Vol. 8, pp. 347-357 (1981)
- /4/ Garland, J.A.
The Absorption and Evaporation of Tritiated Water Vapor by Soil and Grassland
Water, Air and Soil Pollution, Vol. 13, pp. 317-333 (1980)
- /5/ A. Groh und C. Steinhauer
COMA: Programmbeschreibung
Interner Bericht, Kernforschungszentrum Karlsruhe (1987)
- /6/ Guenot, J. and Y. Belot
Assimilation of ^3H in Photosynthesizing Leaves Exposed to HTO
Health Physics Vol 47, No.6, pp. 849-855 (1984)
- /7/ Hasemann, I. and Jones, J.A.
COSYMA: User Guide
CEC Brussels EUR-report 13045 (1991)
KfK-report 4331 B, Kernforschungszentrum Karlsruhe (1991)
- /8/ Jarvis, P.G.
The Interpretation of the Variation in Leaf Water Potential and Stomatal Conductance Found in Canopies in the Field
Phil. Trans. R. Soc. London, Vol. B 273, pp. 593-610 (1976)
- /9/ COSYMA: A New Program Package for Accident Consequence Assessment
A Joint Report of KfK and NRPB
Commission of the European Communities, Report EUR-13028 EN (1991)

- /10/ McIntosh, D.H., and Thom, A.S.
Essentials of Meteorology.
Wykeham Science Series 3, London (1969)
- /11/ Penman, H.L.
Evaporation: An Introductory Survey
Netherl. J. Agric. Sci., Vol. 4, pp. 9-29 (1956)
- /12/ Raskob, W.
UFOTRI: Program for Assessing the Off-Site Consequences from Accidental Tritium Releases
KfK-report 4605, Kernforschungszentrum Karlsruhe, June 1990
- /13/ Rutter, A.J.
The Hydrological Cycle in Vegetation.
in: Monteith, J.L. (Ed.): Vegetation and the Atmosphere, Vol. 1, Academic Press
London (1975), pp. 111-154
- /14/ Shaw, P.V., Haywood, S.M.
A Dynamic Model for Predicting the Movement of Tritium in the Environment
Radiation Protection Dosimetry, Vol. 16, No.1-2, pp. 59-62 (1986)
- /15/ Spencer, F.S., and Dunstall, T.G.
Molecular Tritium Conversion in Vegetation, Litter and Soil.
Radiation Protection Dosimetry, Vol. 16, No. 1-2, pp. 89-93 (1986)
- /16/ Straka, J., Geiß, H. and Vogt, K.J.
Diffusion of Waste Air Puffs and Plumes under Changing Weather Conditions
Contr. Atm. Phys., Vol. 54, pp. 207 - 221 (1981)
- /17/ Turner, D.B.
Workbook of Atmospheric Dispersion Estimates. Public Health Service Publication
No. 999-AP-26 (1970)