Forschungszentrum Karlsruhe
in der Helmholtz-Gemeinschaft

Wissenschaftliche Berichte
FZKA 7281

Test and Validation Studies Performed with UFOTRI and NORMTRI

TW5-TSS/SEP2 – deliverable 4

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Institut für Kern- und Energietechnik
Programm Kernfusion

März 2007

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2007

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Mitglied der Hermann von Helmholtz-Gemeinschaft
Deutscher Forschungszentren (HGF)

ISSN 0947-8620

urn:nbn:de:0005-072819

Abstract

Several test and validation studies have been performed for the two tritium codes UFOTRI and NORMTRI in the frame of international exercises in particular in the BIOMOVS and the BIOMASS programs, supported by the IAEA. Validation of NORMTRI confirmed that the specific equilibrium approach is appropriate for routine releases as long as yearly averages are of interest. It also strongly depends on the quality of the primary dispersion model except an HT release is of interest. In case of UFOTRI applied for accidental releases, the situation is much more complex and dynamic approaches are mandatory. Testing and validation focused here mainly on the ingestion pathways as it was identified as the most critical pathway in many studies. In particular for crops it could be demonstrated that the generic and physically based approach used in UFOTRI is able to treat the various foodstuffs with sufficient accuracy.

Test- und Validierungsuntersuchungen für die beiden Tritiummodelle UFOTRI und NORMTRI

Zusammenfassung

Ziel dieser Arbeiten war der Test und die Validierung der beiden Tritiummodelle UFOTRI und NORMTRI im Rahmen von internationalen Projekten wie BIOMOVS und BIOMASS. Beide Studien, die von der IAEA unterstützt wurden, zeigten, dass die Modelle für die Abschätzung von Freisetzungen bei Unfällen oder im Normalbetrieb angewendet werden können. Tests mit dem Normalbetriebsmodell NORMTRI bestätigten die Anwendbarkeit des sogenannten „Gleichgewichtsansatzes“ solange Jahresmittelwerte von Interesse sind. Hier liegt der Schwerpunkt auf der Qualität des Ausbreitungsmodells. Nur wenn Tritium in Form von HT-Gas freigesetzt wird, sind auch weitere Prozesse wie die der Reemission zu berücksichtigen, welche auch in NORMTRI realisiert ist. Bei unfallbedingten Freisetzungen ist die dynamische Modellierung der Umwelteinflüsse notwendig. Die Tests in diesem Rahmen fokussierten sich auf die Nahrungskettenmodellierung und hier insbesondere auf die Modellierung der Pflanzenparameter. Der pflanzenphysiologische Ansatz, der in UFOTRI gewählt wurde, zeigte sehr gute Ergebnisse in allen Tests und kann alle notwendigen pflanzlichen Nahrungsmittel mit ausreichender Genauigkeit beschrieben.

"This work, supported by the European Communities under the contract of Association between EURATOM and Forschungszentrum Karlsruhe, was carried out within the framework of the European Fusion Development Agreement. The views and opinions expressed herein do not necessarily reflect those of the European Commission."

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1 Introduction

The test of a computer program is an essential part of the development stage before it can be delivered to a customer. This is valid for commercial products as well as for research tools. In case of a scientific assessment model, however, not only tests but also validation studies are necessary. One objective of the validation studies for example is to clarify in which situation the model can be applied.

2 Quality Assurance

Quality Assurance procedures in the industry and in research and development are often treated differently. Industrial products often follow ISO standards and are certificated at the end of their development. Research and development projects (RTD) on the contrary are often characterised by the fact that new information becomes available during the time of the contract and therefore a project is often prolonged to incorporate this information into the software package. Furthermore, the scientific content of the software has a higher importance than the way how to code the program. Therefore, ISO standards are often not followed within RTD projects.

To overcome this problem in case of a software which is used by external partners, the Accident Consequence Assessment Group of FZK, which was mainly responsible for the development of the COSYMA package and the tritium models UFOTRI and NORMTRI, followed a slightly different approach. The software was quality assured by the feedback from its users. Both software packages were well documented with user guides and test procedures. In particular the test procedures assured that the installation produced exactly those results which were documented for this test case. With the wide distribution of the software, COSYMA has more than 100 users, UFOTRI more than 20 and NORMTRI about 10. The use of the software in many different applications provided feedback to the developers to remove bugs or limitations of the software as soon as they were detected. This approach of the users feedback seems to be more appropriate for RTD software than a formal approval of software code which was never tested in real applications.

3 Test and validation exercises for UFOTRI (version 93/4.4)

3.1 Introduction

During a workshop in Aiken, South Carolina, in 1990, the most important processes which have to be considered in an assessment model for accidental tritium releases were defined /MUR90/. From Table 1 it can be clearly stated, that besides the processes relevant for atmospheric dispersion and deposition, the consideration of tritium in the foodchains and in particular the conversion of HTO (tritiated water) to OBT (organically bound tritium) is of importance. In further studies with UFOTRI, the contribution of the individual exposure pathways to the total dose were investigated /RAS97/.

Process	Importance	Status of modelling	Experimental data need
Atmospheric dispersion	H	H	
Atmospheric conversion HT to HTO	L	-	
Wet deposition	M / H	L*	
Condensation / dew	L / M	L	
Dry deposition HTO			
Plants	H	M / H	x
Soil	H	M*	x
Free water surface	L	-	
Dry deposition HT			
Plants	L	-	
Soil	H	M	
Free water surface	L	-	
Re-emission			
Soil surface	M / H	M / H	x
Root / plant uptake	H	M / H	
Synthesis of T into organics			
Plant	H	L / M*	x
Soil	L	-	
Transport through food chain	H	M*	x
Absorption of tritium from			
air in humans HT	L	M	
HTO	H	H	
Translation of exposure to dose	H	M / H*	

Table 1: Tritium transport processes ranked by importance as contributors to the dose and by confidence in ability to model them following short term releases (H = high, M = medium, L = low, - = not needed for modelling, x = important, * = ranking still unclear)

Even if this study was limited by the use of only one assessment code, it highlighted the high importance of the contribution of the foodchain part to the total exposure of the population in the longer term. Initiated by the review studies and the workshop, a model intercomparison exercise was scheduled which was hosted in the frame of the BIOMOVS-II study.

3.2 BIOMOVS II

Within the BIOMOVS II (BIOsheric MOdel Validation Study - phase II) study tritium models including UFOTRI were tested and compared with each other and with experimental data. In a first step, a model intercomparison exercise was carried out /BIO96a/. The key findings from the model intercomparison exercise can be summarised as follows:

- In most cases, predicted concentrations obtained with the different models agreed within an order of magnitude
- A number of processes were identified which require further study to improve the overall model performance. This includes processes such as:
  - deposition and reemission of HTO to soil below canopies,
  - deposition and reemission to plant canopies at night,
  - root uptake,
  - rates of OBT formation at night,
  - translocation of TWT (tissue free water tritium) and OBT to plant storage organs and
  - rate of loss to OBT from milk and meat.

Besides artificial model-model comparisons, scenarios have been outlined covering the reemission process from the soil and the vegetation as well as the OBT formation during daytime and night-time conditions /BIO96b/.

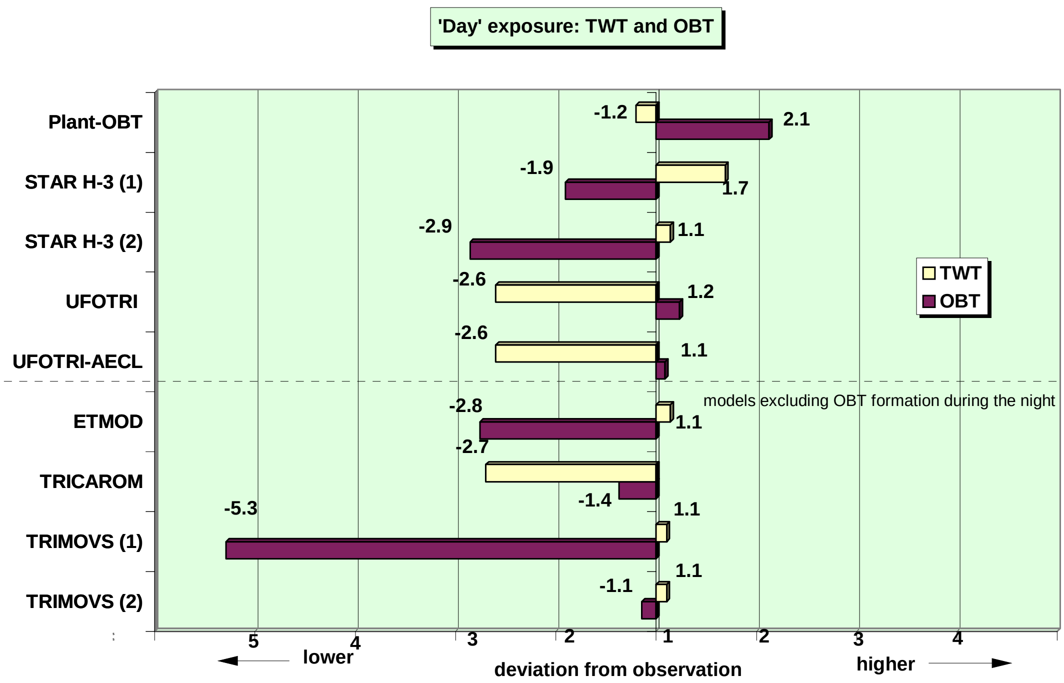

Figure 1 OBT formation following a daytime exposure

The model results of UFOTRI for the reemission scenario showed in principle a rather good agreement with the calculations. However, the flux out of the soil and plants in the morning and evening was always slightly overestimated. The approach used within UFOTRI for modelling the build-up of organically bound tritium performed well in the exercise, in particular when compared with the tritium concentration at time of harvest. However, in the initial stage after exposure, the OBT formation was always underpredicted. This problem is interesting from a scientific point of view as it demonstrates that some processes might still be not fully understood, but as long as the performance for the end product, the edible part at harvest time is sufficiently correct, no refinement of the OBT model in an assessment code seems to be necessary (see Figure 1). Only the OBT formation during night-time was slightly modified to account for an higher build-up of OBT during night (see Figure 2).

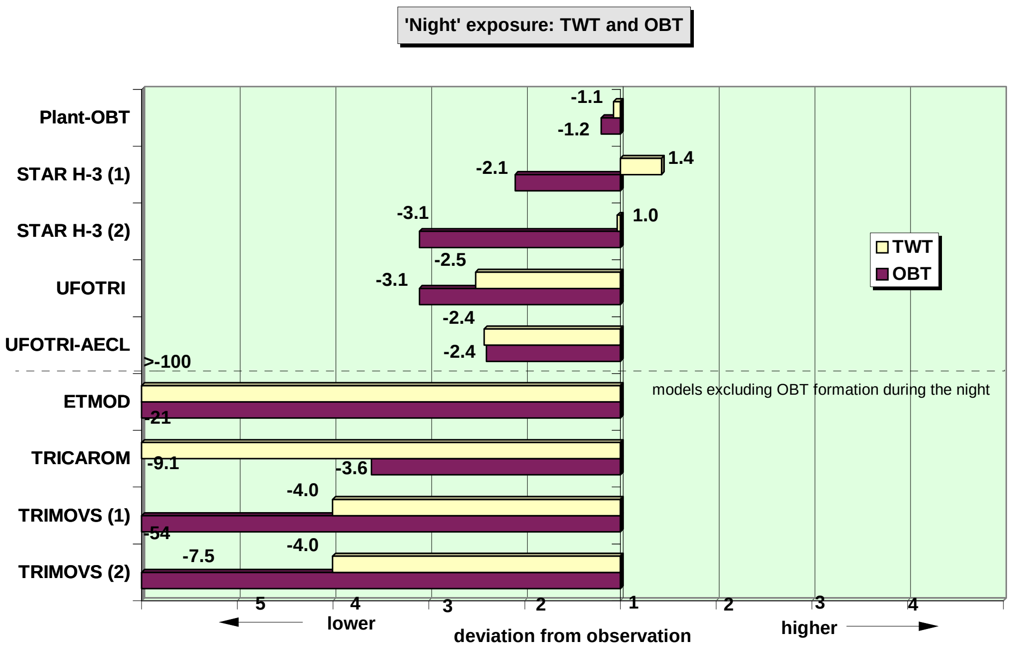

Figure 2 OBT formation following a night-time exposure

One limitation of the exercise is the number of crops for which data is available. Scenarios were selected for wheat crops, but other products could not be tested due to missing data at this time. Furthermore, animal data for validation studies are missing in general.

3.3 Experiments performed at FZK

At FZK, experiments were performed to investigate the uptake and loss of tritium from winter wheat, the build-up of OBT and finally its translocation into the edible part of the crop. To follow the results of the experiments in more details, the so called ‘Plant-OBT’ for describing the OBT formation and translocation in wheat plants was developed. This model uses the OBT formation engine developed for UFOTRI, however the number of compartments was increased. Comparative calculations performed with experimental data from 1995 and 1996 showed, however, that our present understanding of the processes seems not to be deep enough to describe the OBT formation in the seedlings of winter wheat by using only a limited number of environmental parameters /STR98/. In particular, the dynamics of the OBT formation could not be reproduced in detail. The final OBT content at the time of harvest could be predicted within a bandwidth of a factor of two (see Figure 3).

It has to be mentioned that a better performance is often accompanied by an increased complexity. For example the number of compartments in the Plant-OBT model was three times higher than that inside UFOTRI. This causes the problem to derive parameters describing the transfer between these compartments. As this is difficult to measure, assumptions have to be made which might be site and crop specific. As the assessment models have to be operational, such an adaptation of model parameters have to be avoided as much as possible. This together with the small difference in performance between UFOTRI and Plant-OBT supported the decision not to modify the OBT formation engine of UFOTRI.

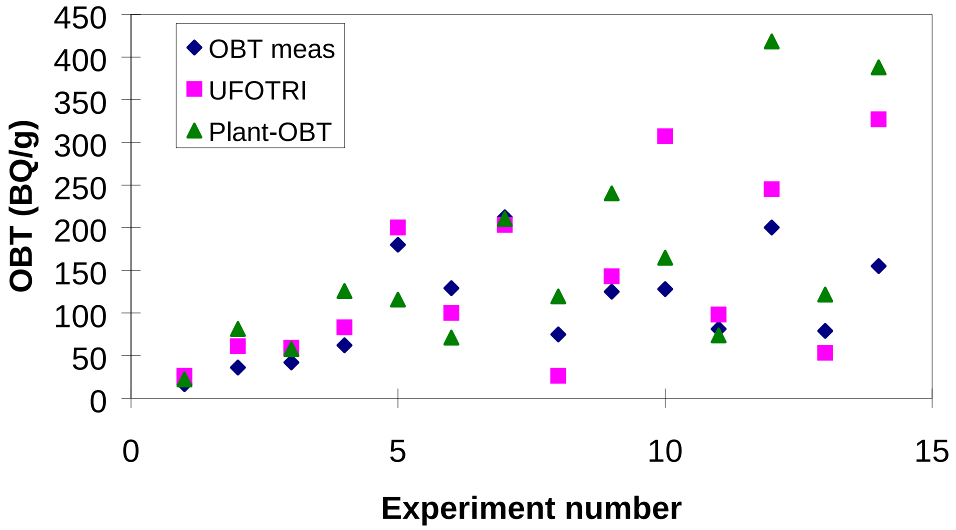

Figure 3 OBT formation following exposure of winter wheat at different development stages and times of the day

3.4 Rice

Model testing was performed for two sets of experimental data (for details see /RAS02/). Within one experiment, potted rice was exposed for one hour to tritiated water /CHO02/ whereas in the other experiment deuterium was applied /ICH00/.

In the tritium experiment, potted rice plants were exposed at different stages of development, ranging from times before anthesis, during the linear growing phase and up to early maturity of the crop. Nine experiments were carried out during daytime (10 AM – 11 AM) with the pots exposed in a small box which was removed afterwards to allow for natural growing conditions until the time of harvest. HTO was measured in air moisture during and shortly after the exposure, whereas TWT and OBT in leaf, stem, ear and seed was collected from the end of exposure to the time of harvest. Only a few parameters were adopted according to /CHO02/.

Measured and calculated ratios were in close agreement for most of the experimental conditions (see Figure 4). The linear growing phase (experiment 5 – 7) can be easily detected in both the measurements and the calculations. There is only one experiment in the beginning of the linear growing phase which is over-estimated by more than a factor of two. There is no apparent explanation, but an indication that the plants exposed in this experiment might not be in optimal conditions. The uptake of HTO into the leaves is lower than for any other experiment and on the other hand, linear growing might be delayed here.

Potted rice plants were exposed over 8 hours with deuterium under daytime and night-time conditions /ICH00/. The exposure was conducted in a greenhouse under controlled conditions. It took place about 23 to 25 days before harvest. In two of the experiments the pot was flooded with water. Deuterium concentration was measured in air moisture during exposure and in various organs of the rice plants until the time of harvest. Recorded meteorological data from the nearest meteorological station was used for the model calculations with UFOTRI.

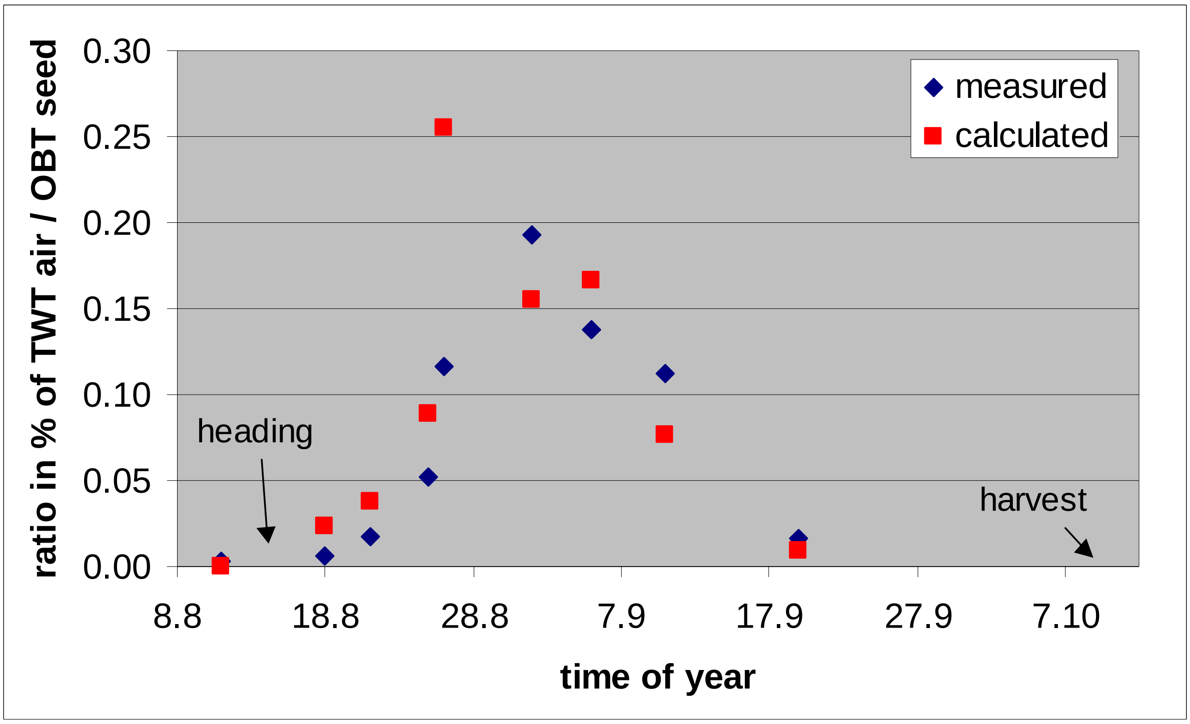

Figure 4 Comparison of measured and predicted ratios of TWT air to OBT in rice seed

Table 2 shows the ratio of the mean air concentration and the organically bound deuterium (OBD) in rice seeds at the time of harvest. Assuming the exposure took place in the linear growing phase would lead to a clear overprediction for the daytime release, whereas the night-time values fit very well. However as the comparison with the tritium exposure of rice and wheat plants suggest ratios of about 0.2% for the exposure of only one hour during daytime and in the linear growing phase, an exposure over 8 hours should lead to much higher ratios. Therefore, by applying the rice characteristics from the tritium experiment, early maturity conditions were assumed which result in a close agreement for daytime but a not so good agreement during night-time. The latter results fit more to the theory, but need further experimental confirmation.

	Measured ratio	Predicted (linear growing)	Predicted (early maturity)
Daytime	0.25	0.89	0.29
Day-flooded	0.21	0.79	0.28
Night-time	0.20	0.23	0.11
Night-flooded	0.23	0.22	0.11

Table 2 Comparison of measured and predicted ratios of deuterium in air moisture to organically bound deuterium (OBD) in rice seed under various growing conditions

In general, the rice experiments demonstrated that the plant engine developed for winter wheat can be easily applied for other crops without significant modifications. The overall performance seems to be good and the difference between the model and the measurements is limited in most cases to a factor of two.

3.5 EMRAS

3.5.1 Soybean scenario

The soybean scenario addresses tritium absorption by soybean foliage and subsequent tritium behaviour in the plant. To provide data for model testing, soybean plants were exposed to elevated levels of airborne tritium in a glove box. The exposure was carried out for one hour at various stages in the growth of the soybeans. A total of six experiments (SB1 to SB6) were carried out. Two of the experiments (SB1 and SB4) were designed to study the time-dependent HTO concentration in various parts of the soybeans. After the exposure, the soybean parts were sampled with time to quantify the rate of transfer from leaves to other plant parts or to the air as time elapsed. In all experiments, the OBT concentrations were measured in the plants parts at harvest.

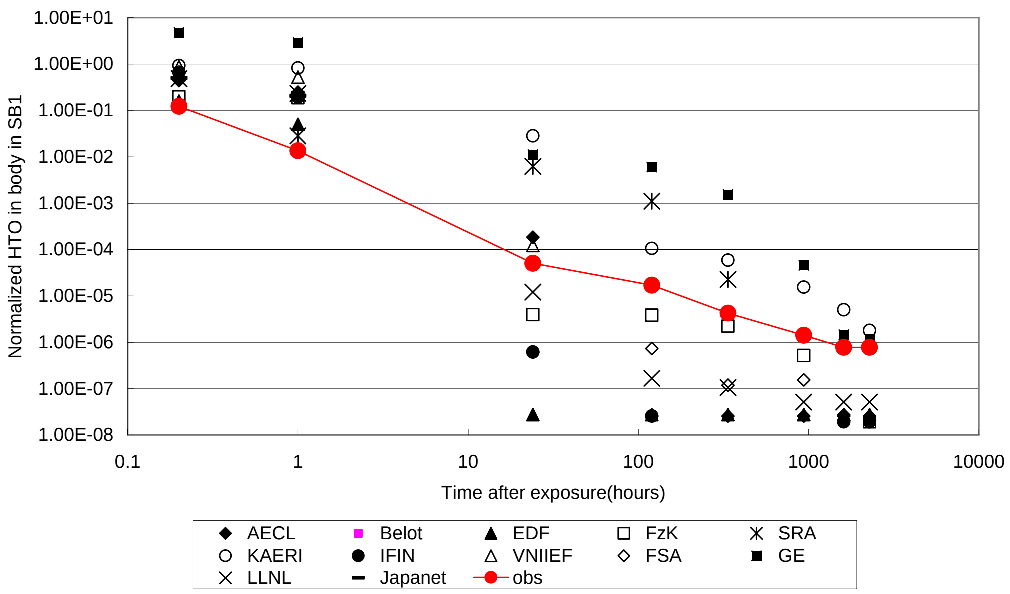

Figure 5 Predicted and observed normalised HTO concentration in plant body in SB1 (from /EMR06a/)

Figure 5 shows the result of the time dependent HTO concentration in the plant body. UFOTRI calculates the initial concentration with an extremely low deviation and follows the time function within a factor of 10 up to harvest time. This deviation at later stages is not important for dose calculations as the HTO concentrations are low and OBT formation is completed within one to two days following the exposure.

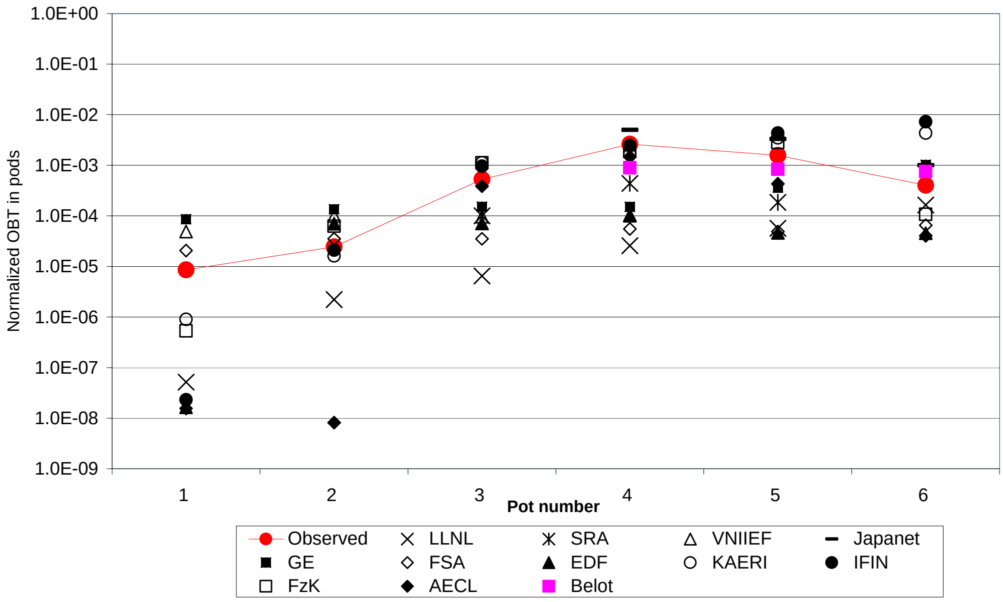

Figure 6 Predicted and observed OBT concentrations in the pods at harvest (from /EMR06a/)

The performance of UFOTRI in relation to the final OBT concentration at the time of harvest can be seen in Figure 6. Except for the first and the last scenario, an exposure before flowering and an exposure close to harvest, UFOTRI is within a factor of two to the experimental results. For the first experiment, the build-up of OBT is extremely high and the scatter of the models demonstrate that the experimental result is not fully understood. The last experiment with an exposure close to harvest showed a discrepancy of a factor of about four between UFOTRI and the experiment. As the UFOTRI model is designed as a general engine for all types of crops, such an underprediction might be only typical for soybean. In the rice scenario, exposure close to harvest was reproduced quite well.

3.5.2 Hypothetical scenario

The hypothetical scenario aims to analyse the consequences of an acute atmospheric release of tritium evaluating the importance of the individual exposure pathways and the contribution of the various forms of tritium (HT, HTO, and subsequent OBT) to the total exposure. In this way, some practical guidance to decision-makers in the case of a severe release is expected. It does not compare models but demonstrate how models may differ and if this might be considered in case that several neighbouring countries are affected by a tritium release.

Three different release conditions, ranging from release under stable atmospheric conditions (night-time) via neutral stratification (daytime with high solar radiation) to a release with heavy rain, were investigated. A release of 10g of tritium, either HT or HTO, were assumed. Endpoints were concentrations in various compartments of the environment and also doses from inhalation and ingestion.

The huge variety of results is demonstrated in the Figure 7 and Figure 8. Even if all the input parameters were defined, some countries might have used nation specific parameters and thus over-written the definition. However, it also shows the difference in the model approaches and capabilities. Important to note, that the French model, an improved version of the GAZAXI code /MON03/, and the German model UFOTRI model performed similar.

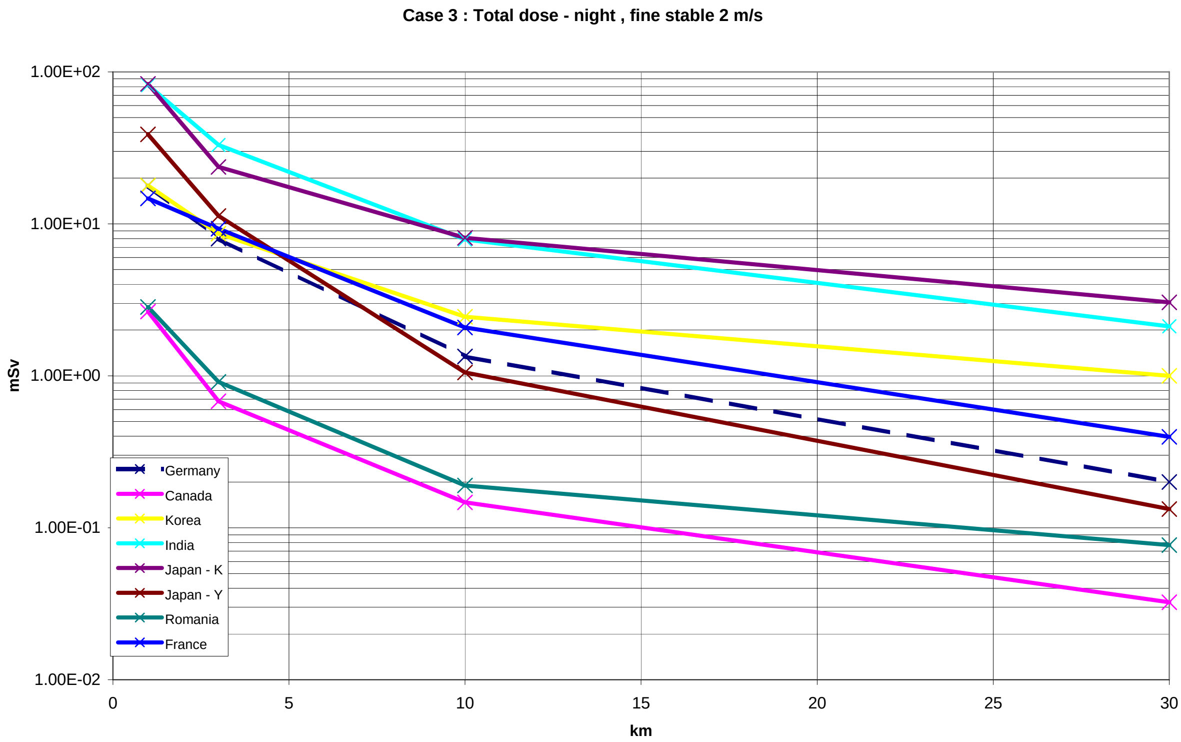

Figure 7 Total dose for the night release (from /EMR06b/)

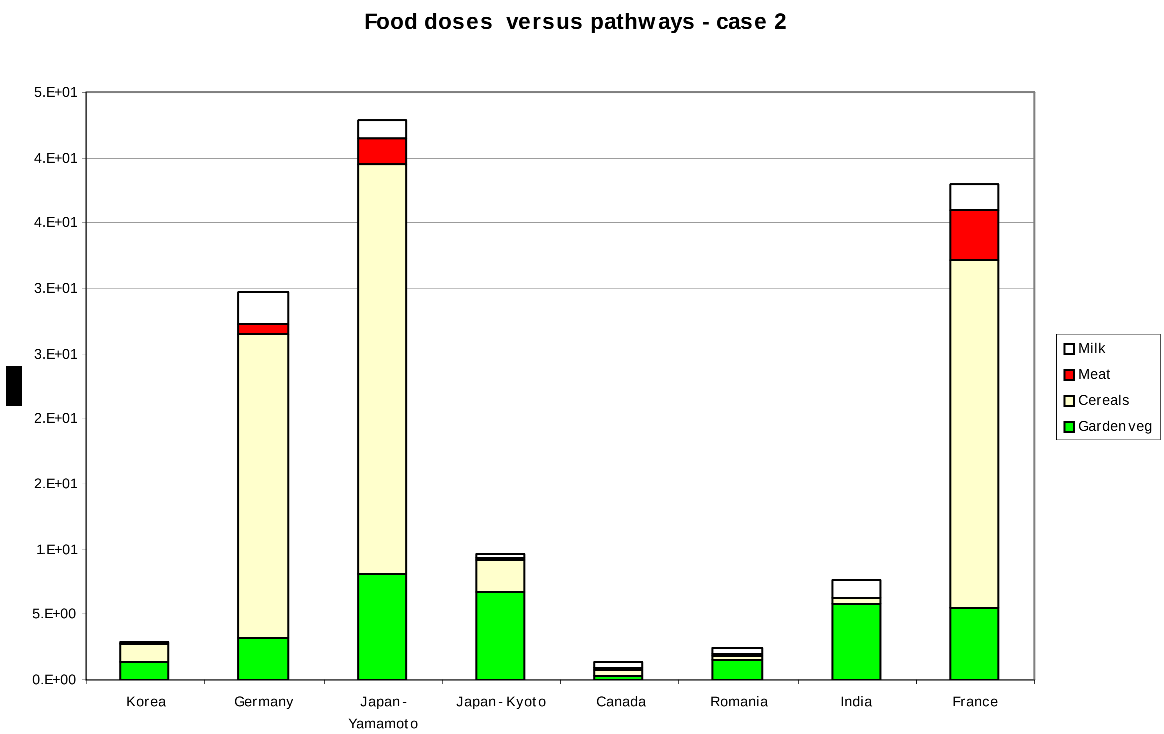

Figure 8 Ingestion dose for the release with rain (from /EMR06b/)

The hypothetical exercise identified that the target ingestion dose is the most important one for decision-making following an accidental release of tritium. It became obvious that the activity concentrations in food products, which is a criterion to stop the trade of a contaminated product might be not appropriate for emergency management. There, the ingestion dose might be more important. This topic was controversially discussed during the various meetings and further clarification seems to be necessary.

Nevertheless, this huge variety is to some extend alarming as decisions will be different from country to country and thus difficult to explain to the public living close to a border. There seems to be some need for harmonisation.

4 Test and validation exercises for NORMTRI (1.1)

4.1 Introduction

In case of routine releases, complex models seem to be not necessary. Extensive measurements at Savannah River site (USA) and also data from Chalk River (Canada) applied within the BIOMASS exercise showed that the equilibrium approach between air concentration and concentration in crops gives a sufficient good estimate of the average contamination (/MUR93/ and /BIO03/). In particular when using the equilibrium factor one between air and crop, concentration and thus dose estimations are conservative. Only in case of HT releases, reemission of converted HTO from soil and vegetation is important and has to be considered. Reemission, however, might be also introduced as a simple conversion factor from atmospheric HT, not depending on the actual site conditions /DAV95/. The computer model NORMTRI /RAS94/ includes both, the equilibrium approach and reemission.

4.2 BIOMASS

Within the BIOMASS (BIOspheric Modelling and ASSessment) project testing of tritium models for routine releases into the atmosphere and hydrosphere has been performed. Five different scenarios have been set up covering both fixed environmental conditions to test individual model features and using measured data from sites in Canada, Russia and France to test the overall performance of existing assessment codes for routine releases. NORMTRI has participated in most of the scenarios. Other computer codes participating in the BIOMASS intercomparison exercise are either still under development (Japan, Russia) or research codes are not available in operational versions.

The first task of the Tritium Working Group (TWG) focused on a model-model intercomparison exercise on the transport of tritium in the vicinity of permanent atmospheric sources /BIO03/. The tritium concentration in air humidity can be derived by using classical models of atmospheric dispersion and also by specially developed models that consider both primary emission from the main sources and secondary emission from the contaminated soil surface. The results obtained in assessing the impact of HTO releases are not very dependent on the way in which the secondary emission has been treated, since the contribution of the latter process is generally relatively small. In contrast, for HT releases, the results are highly dependent on the method used to estimate the secondary emission, because this process is the only one that brings tritiated water into the atmosphere. NORMTRI considers the re-emission of HTO from soil and thus fits to the recommendation of the working group.

A further test exercise has been devoted to a model-data test concerning the transport of tritium in the vicinity of long-term atmospheric sources at the Chalk River Laboratories site of AECL in Canada /BIO03/. Participants were given hourly meteorological data and the observed HTO concentrations in air at three sampling sites. From this information they were asked to predict long-term average tritium concentrations in rainfall, soil water, plant water and plant organic material. Differences between predictions and observations were commonly about a factor of 2 to 3. The observations suggested that, the long-term average soil concentration is typically one-fifth to one-third the average air moisture concentration. This ratio will depend on soil properties and on the joint frequency of wind direction and rainfall occurrence and may be quite different at other sites. The long-term plant water/air moisture concentration ratio lay between 0.50 and 0.85. Results obtained with NORMTRI were closest to the measured values. There was no evidence encountered to modify the present equilibrium approach implemented in NORMTRI.

5 Conclusion

Several test and validation studies have been performed for the two tritium codes UFOTRI and NORMTRI: Validation of NORMTRI confirmed that the specific equilibrium approach is appropriate for routine releases as long as yearly averages are of interest. The results strongly depend on the quality of the primary dispersion model in general. In case of an HT release, the re-emission process and the subsequent dispersion and transport of the re-emitted HTO has to be modelled which is the case for NORMTRI. Re-emission however is not of interest in case of a pure HTO release under normal operating conditions.

In case of accidental releases, the situation is much more complex and dynamic approaches are mandatory. Testing and validation focused here mainly on the ingestion pathways as it was identified as the most critical pathway in many studies. However, the number of test data is limited and for some of the endpoints such as milk and beef, the available data was used to develop the model itself. Therefore, independent tests are not possible in these areas. This was identified within the EMRAS study and the collection of new experimental data was initiated. However, this could not be completed by the end of the project. For crops, more data are available and UFOTRI demonstrated in many tests that the current generalised approach to model the transport through the foodchain including the build-up of OBT, which is based on plant physiology, is capable to reproduce at least the dose relevant endpoints within a factor of 2-3 under most test conditions.

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