

# Comparison of two modelling tools for the evaluation of tritium and hydrogen transfers in nuclear reactors or complex systems

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## ABSTRACT

In the framework of the TRANSAT project, started in 2017 (TRANSversal Actions for Tritium supported within the H2020 Euratom program), the ability to measure and to assess the tritium inventory and migration within different kinds of reactors or processes is one major challenge to control the potential releases and personal dosimetry in nominal operating conditions.

A benchmarking activity between two calculation tools developed either for the fusion machines (EcosimPro developed between CIEMAT and EAI) or for the fission reactors (KUTIM developed at CEA), was initiated to improve the level of confidence in the tritium and hydrogen balances estimated by such codes in complex systems.

An application to a conceptual fission reactor based on the technology of Sodium Fast Reactors was carried out on the base of a shared data set used for the design characteristics of circuits and components as well as for physico-chemical properties of liquid sodium, of wall materials and of operating conditions. The modeling of specific components or physical equilibriums involved in sodium cooled reactors was adapted and implemented in EcosimPro libraries. In particular the major recovery of tritium and hydrogen impurities in purification systems (cold traps) is evaluated as well as the dissolution equilibrium of both hydrogen isotopes at the primary sodium surface between the liquid metal and the gas plenum.

Calculations results with both codes are presented and compared in terms of tritium activities and hydrogen concentrations in each circuit of the reactor, but also in terms of transfer fluxes and releases. In addition, the distribution of the various transfer contributions (between primary, secondary and tertiary circuits) is analyzed. Comparisons between both codes results associated with sensitivity studies on the influence of main parameters (such as tritium and hydrogen source terms, temperature profiles) are also used to propose perspectives of modeling improvements.

## 1. Introduction

The ability to measure and to assess the tritium inventory and migration in different kinds of nuclear reactors or processes is one key challenge to control the potential releases and personal dosimetry in nominal operating conditions. This purpose is of major interest for the security control of nuclear reactors at the design stage as well as the operating stage. Indeed, tritium is produced in the core of all fission nuclear reactors and is able to diffuse through the fuel claddings and through structural materials. Tritium mobility is particularly enhanced in case of higher temperatures such as in the walls of heat exchangers

between reactor circuits. On the other hand in fusion reactors, the management of tritium produced in breeding blankets and collected in the tritium extraction system is also a critical issue with the aim to reduce tritium permeation and losses while ensuring fuel self-sufficiency.

Consequently the development of reliable and validated modeling tools for the assessment of tritium transfers and inventories is crucial for the future of fission and fusion energy. Due to the presence of different circuits and specific process components (in particular for the coolant purification and the tritium management) and due to the thermal coupling between sections separated by heat exchangers, a large variety

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of chemical transfers or transformations involving tritium (and other hydrogen isotopes) have to be described by the modeling.

In the framework of the European TRANSAT project (TRANSversal Actions for Tritium supported within the H2020 Euratom program [1]), a benchmarking activity between two calculation tools developed either for fusion (EcosimPro developed between CIEMAT and EAI) or for fission reactors (KUTIM developed at CEA), was started to improve the evaluation of tritium and hydrogen balances in complex systems such as nuclear reactors.

A first application to a conceptual Sodium Fast Reactors was carried out on the base of a shared data set used for operating conditions, for physico-chemical properties of liquid sodium and for design characteristics of circuits and components. Numerical values of design characteristics are not communicated due to confidentiality limitations for the project of this future reactor. The study is focused on the modeling description and evaluation of the different transfers of tritium and hydrogen in a complex system like a nuclear reactor. Thanks to the large variety of transfer phenomena or physico-chemical mechanisms that are covered in the present study applied to the complex system of a nuclear reactor, perspectives of adaptation to the description of different processes involved in the field of fusion system can be foreseen. For example, the modularity and the flexibility of these calculation tools could be used for the simulation of tritium behavior in helium purification system (and tritium reprocessing) or in breeding blankets systems. In this paper, calculations results with both codes were compared in terms of tritium activities and hydrogen concentrations in each circuit of the reactor, but also in terms of transfer fluxes and releases. A sensitivity study was also carried out on the influence of permeation level through IHX (between primary and secondary circuits), since the effective value of metallic wall permeability is subject to potential uncertainty.

## 2. Theory and calculation description

### 2.1. Tritium and hydrogen transfers in SFR

Like in other fission reactors (PWR), tritium is produced in the core of SFR by ternary fissions in the fuel pins and by neutron activation of  $^{10}\text{B}$  boron isotope present in control rods made of boron carbide. The fission of fissile radioisotopes ( $^{239}\text{Pu}$ ;  $^{235}\text{U}$ ) may generate a ternary fragment which is a light nucleus such as an alpha particle or a tritium nucleus, in addition to the formation of other fragments. The probability of a tritium nucleus formation is estimated by the rate of ternary fission  $y_T$  for a given fissile nucleus  $i$ . The tritium production rate by ternary fissions for a SFR operated at a thermal power  $P_{th}$ , is theoretically given by the following expression ( $\alpha$  is the number of fissions per unit of thermal energy of the reactor) :

$$S_T^{fuel}(\text{atoms/s}) = \alpha \cdot P_{th} \cdot y_T \quad (1)$$

In control rods made of boron carbide ( $\text{B}_4\text{C}$ ), tritium is mainly produced from neutronic reactions with boron isotope  $^{10}\text{B}$ . The corresponding tritium production rate is defined by different parameters such as “N” number of  $^{10}\text{B}$  atoms present in control rods,  $\sigma$  the absorption cross section of the reaction  $^{10}\text{B}(n,2\alpha)^3\text{H}$ ,  $\phi$  the neutronic flux density,  $\tau_r^{B4C}$  the retention factor of tritium within the material and a simplified estimation is given by the following expression :

$$S_T^{B4C}(\text{atoms/s}) = (1 - \tau_r^{B4C}) \cdot N \cdot \sigma \cdot \phi \quad (2)$$

While it is generally assumed that the stainless steel cladding allows the diffusion of the total tritium production from the fuel, the partial retention of tritium within control rod material is not so easy to evaluate. Indeed a part of this production may be chemically trapped (probably with lithium in the form of  $\text{LiT}$ ) or physically trapped in  $\text{B}_4\text{C}$  material characterized by reduced diffusivity. Due to the strong dependence to temperature profiles and neutronic beam profiles, the

effective release of tritium production from control rods is difficult to evaluate. Though a large proportion of the global tritium source term is transferred and dissolved in primary sodium, this key parameter for the assessment of tritium balance is subjected to uncertainty. This is why a benchmarking of available calculation tools will provide a preliminary verification for further validation studies with experimental results.

The tritium source transferred from the reactor core into primary sodium migrates towards all other circuits because of different phenomena:

- by permeation through metallic walls due to gradients of concentrations in different circuits and enhanced by higher temperatures: major transfer contributions are through heat exchanger tubes (Intermediate Heat Exchanger “IHX”), but also through auxiliary circuit piping such as “EPuR” circuits dedicated to residual heat removal in case of pumps dysfunction,
- in cover gas (argon) above primary sodium, a concentration equilibrium at interface between liquid sodium phase and argon gas phase controls the tritium transfer into the cover gas and is used for the calculation of the tritium release due to gas leaks in purification circuits of cover gas,
- a major part of the tritium amount transferred into primary sodium is trapped in purification systems (cold traps) integrated in primary (and also in secondary circuits),
- radioactive decay is also impacting tritium inventory.

In order to evaluate a global balance of tritium inventory in circuits and the potential releases in environment (in atmosphere and in tertiary water effluents), the transfers into other circuits (secondary, tertiary and ancillary cooling circuits) has to be evaluated as well as the quantities trapped in sodium purification systems.

A source term of hydrogen (protium) has to be considered also in primary and in secondary circuits. In primary sodium hydrogen atoms are dissolved due to the production of protons in the core by fission reactions and neutron activation of materials. In secondary sodium a more important source of hydrogen has to be considered due to permeation through steam generators and from tertiary circuits where steel surfaces in contact with water or steam are subjected to potential corrosion. In this study hydrogen source term in secondary sodium was considered as a constant input data estimated from dedicated measurements in french Superphenix reactor, carried out by monitoring the concentration in sodium of hydrogen impurity after a temporary interruption of purification with cold traps. The presence of stable hydrogen (in larger quantities than tritium inventory) has an impact on the tritium behavior in gas phase (such as in the cover gas used for inert sodium circuits and capacities) and in the sodium purification units (cold traps). In particular, due to its higher (more than 1000 times) source term (expressed in atoms / time unit independently from the atomic weight of each isotope) and its higher concentration in secondary sodium, hydrogen crystallization in cold traps (as sodium hydride) enhance the recovery and trapping of tritium in these components, thanks to co-crystallization mechanism involving both hydrogen isotopes.

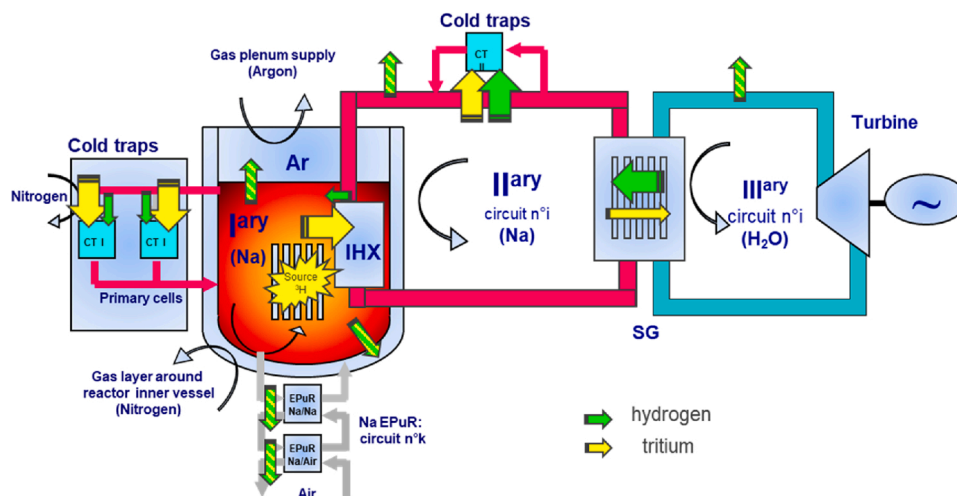
The main transfer fluxes of both isotopes (hydrogen and tritium) to be considered in a SFR (Sodium Fast Reactor) are represented by different arrows (green for hydrogen, yellow for tritium) on Fig. 1.

### 2.2. Mathematical approach for both modeling tools

The two modeling tools are based on different mathematical and computational implementations of the physical models to be used for the simulation of all transfers in the reactor.

#### 2.2.1. EcosimPro

The multi-domain simulation platform EcosimPro was used to develop (by CIEMAT and EAI) a modeling tool with a dedicated tritium transport toolkit devoted to fusion system [2] and implementing



**Fig. 1.** Main transfer fluxes in a Sodium Fast Reactor.

different phenomena such as: tritium generation, 1D diffusion model through materials and coolants, different surface phenomena like recombination-dissociation reactions or Sieverts equilibrium at gas - material interface, 1D simulation of tritium/hydrogen transfer along piping for coolant circuits (possible discretization of materials and piping), different system modules (TBM, piping, tritium recovery components such as oxidizers, adsorption column, getter beds...). Calculations are possible either in static or dynamic modes and for modeling 0D or 1D multidisciplinary continuous-discrete systems and any kind of system based on differential-algebraic equations and discrete events.

### 2.2.2. Kutim

A 0D and steady state modeling tool was developed at CEA for the evaluation of tritium/hydrogen balance in the main circuits and components of a Sodium Fast Reactor and was also adapted to the configuration of fusion reactor like DEMO [3]. Equilibrium concentrations are calculated by solving the two equation systems of both isotopes, built with the material balance calculated in each circuit with the different transfer contributions such as permeation through metallic walls (piping, heat exchangers between circuits, main reactor vessel), concentration partition by liquid-gas equilibrium and co-crystallization in purification system (cold traps). Potential tritium releases (in gas phase or in the form of liquid tritiated water) are also evaluated.

For the purpose of the present benchmarking, the models of material transfers associated with the design characteristics and the operating conditions of a conceptual SFR were implemented in both calculations tools. In particular, specific models related to sodium chemistry and SFR technology (such as the description of co-crystallization in cold traps) were integrated in EcosimPro. Equations and permeation regimes were configured in EcosimPro to operate under the same conditions as Kutim. The main characteristics of physical models are given hereunder.

### 2.3. Permeation through metallic walls

Depending on the metallic walls considered and the fluid phase on each side, different permeation configurations are encountered:

- from a liquid sodium circuit (or capacity) to another liquid sodium circuit (IHX tubes between primary and secondary sodium, heat exchangers used for ancillary cooling circuits),
- from a liquid sodium circuit (or capacity) to a gas phase (piping of all sodium circuits in contact with air environment, inner reactor vessel protected by a nitrogen outer chamber, ancillary cooling circuits cooled by aerothermal coolers),

- from a gas phase to another gas phase (parts of cover gas circuits in contact with air atmosphere).

In stationary mode, the global diffusion through a plate with thickness " $\delta$ " and surface area " $A$ " is expressed from the 1st Fick's law as :

$$\Omega = D \cdot \frac{A}{\delta} \cdot (C_1 - C_2) \quad (3)$$

with  $\Omega$  = diffusion flux of H or T through the metallic wall (atoms/s)

$D$  = diffusivity of H or T in the wall material ( $\text{m}^2/\text{s}$ )

$C_1, C_2$  = concentrations of H or T on both sides surfaces of the metallic wall (atoms/m<sup>3</sup>)

Considering the Sieverts relation defining equilibrium on side « i » between partial pressure of diatomic molecule  $Q_2$  ( $Q = H$  or  $T$ ) in gas phase and concentration of atoms dissolved in liquid sodium ( $C_{Qi}^{Na}$ ) or at metal surface ( $C_{Qi}^{met}$ ), a relation can be established between these concentrations, which involves the partition coefficient based on the ratio of Sieverts constants in liquid sodium and in the wall metal  $K_{SO}^{Na}$  and  $K_{SO}^w$ :

$$C_{Q,1}^{met} = \frac{K_{SQ}^{met}}{K_{SQ}^{Na}} \cdot C_{Q,1}^{Na} \text{ and } C_{Q,2}^{met} = \frac{K_{SQ}^{met}}{K_{SQ}^{Na}} \cdot C_{Q,2}^{Na} \quad (4)$$

This relation is obtained by considering a common value of a fictive “Q<sub>2</sub>” gas pressure in equilibrium simultaneously with both media: liquid sodium and wall metal ( $C_{SO,i}^{media} = K_{SO}^{media} \cdot \sqrt{p(Q_2)}$ ).

Consequently, in the case of liquid sodium circuits on both sides of the metallic wall, the permeation flux is described by a correlation introducing the permeability of metal relatively to hydrogen isotopes. For example, in the case of H isotope we consider the following expression:

$$\Omega_H = D_H \cdot \frac{A}{e} \cdot (C_{H,1}^{met} - C_{H,2}^{met}) = D_H \cdot \frac{K_{SH}^{met}}{K_{SU}^{Na}} \cdot \frac{A}{e} \cdot (C_{H,1}^{Na} - C_{H,2}^{Na}) \quad (5)$$

In this expression is included the permeability  $pe_Q$  of hydrogen isotope (Q = H or T) through the metallic wall which is expressed in (atoms.  $m^{-1}.s^{-1}$ ,  $Pa^{1/2}$ ) and is defined by the product of the diffusivity  $D_Q$  ( $m^2.s^{-1}$ ) and the Sieverts constant in the metal  $K_{SQ}^{met}$  (atoms.  $m^{-3}$ .  $Pa^{-1/2}$ );

$$pe_o = D_o \cdot K_{so}^{met} \quad (6)$$

In the case of a gas phase in contact with the metallic wall, because of the Sieverts relation  $C_{M,i}^{met} = K_{SQ}^{met} \cdot \sqrt{P_i}$  between the concentration (in atoms/m<sup>3</sup>) and the partial pressure in Pa, we express the concentration in metal in function of the concentration at equilibrium in gas phase calculated on the base of the ideal gas law.

For conversion of the results into values reported to the mass of coolant (in ppm for hydrogen concentration and in kBq/g for tritium activity) the concentrations in sodium can be converted in (atoms/kg) using the density of sodium  $\rho^{Na}$  (kg/m<sup>3</sup>):

$$[Q]_i = C_i / \rho^{Na} \quad (7)$$

The metal involved in the model is generally stainless steel 316 L [4] for almost all structures, pipings and components except for steam generators made of Incoloy 800 [5].

#### 2.4. Accumulation transfer in cold traps

The purification of liquid sodium operated in cold traps is based on crystallization of sodium impurities (hydrogen and oxygen principally) in the form of sodium hydride and sodium oxide. A major proportion of tritium is deposited in cold traps thanks to a co-crystallization mechanism with hydrogen impurities. This phenomenon is governed by the solubility of hydrogen in sodium and its dependence with temperature.



The solubility of hydrogen in liquid sodium is given by the Whittingham [6] correlation:

$$\log_{10} \left( C_{H,sat}^{Na} \right) = 6.467 - \frac{3023}{T} \quad (8)$$

With:  $C_{H,sat}^{Na}$  = hydrogen concentration in sodium at saturation (mass ppm)

T = temperature of liquid sodium (K)

The solubility of tritium in liquid sodium is supposed to be the same as hydrogen. In fact, in the usual operating conditions of SFR, the tritium concentrations in sodium circuits are too small to reach the saturation value, and consequently its deposition in cold traps is due to co-crystallization with sodium hydride (as a mixture of crystals NaT + NaH). The flux of tritium deposition in cold traps is based on the crystallization flux of hydrogen depending on different parameters such as the sodium flowrate ( $Q_{Na}^{PF}$ ), the purification efficiency of cold trap ( $\epsilon$ ) and proportional to the hydrogen concentration overtake above saturation value. On the base of hydrogen crystallization flux, a ratio of both isotopes concentrations is applied to calculate the flux of tritium deposition in cold traps defined by the following correlation:

$$\Omega_T^{PF} = \frac{[T]}{[H]} \cdot Q_{Na}^{PF} \cdot \epsilon \cdot ([H] - [H]_{sat}) \quad (9)$$

#### 2.5. Hydrogen – tritium equilibrium in gas phase and transfer into cover gas

In gas phase such as in cover gas above primary sodium, diatomic molecules of hydrogen and tritium are not independent and react together to form HT molecules. Both isotopes are involved in a reaction equilibrium:



The thermodynamical constant of this equilibrium is function of temperature and can be expressed by the following correlation from data in [7].

$$K_{eq}(T) = \frac{p_{HT}^2}{p_{H_2} \cdot p_{T_2}} = e^{\left( -\frac{133}{T} + 1.4966 \right)} \quad (11)$$

Moreover, in the primary vessel, at the sodium surface in contact with the cover gas (argon), the transfer of hydrogen isotopes can be evaluated considering the simplified assumption of a concentration equilibrium (Sieverts law) between both phases. The transfer fluxes ( $\Omega_H$ ,  $\Omega_T$ ) of hydrogen isotopes released from liquid sodium into the gas phase can be expressed in function of different parameters (in particular  $Q_{cgl}$ , the estimated leak flowrate assumed in the cover gas circuits) detailed in

the expression below for protium transfer flux. In this case, a simplification related to concentrations levels ( $[H] \gg [T]$ ) can be made (while complete expression is saved in the case of tritium transfer flux):

$$\begin{aligned} \Omega_H &= \frac{2 \cdot N_A \cdot Q_{cgl} \cdot [H]^{Na}}{R \cdot T \cdot (K_{SH}^{Na})^2} \cdot \left( [H]^{Na} + \frac{\sqrt{K_{eq}}}{2} \cdot \frac{K_{SH}^{Na}}{K_{ST}^{Na}} \cdot [T]^{Na} \right) \\ &\approx \frac{2 \cdot N_A \cdot Q_{cgl} \cdot ([H]^{Na})^2}{R \cdot T \cdot (K_{SH}^{Na})^2} \end{aligned} \quad (12)$$

#### 2.6. Tritium radioactive decay

The rate of radioactive decay considered for the tritium material balance is expressed in (atoms/s) with a radioactive decay constant  $K_D = 1.7857 \cdot 10^{-9} \text{ s}^{-1}$ , by the following expression:

$$\Omega_T^{rad} = K_D \cdot m_{Na} \cdot [T] \quad (13)$$

with:  $m_{Na}$  = mass of the media (liquid sodium, water, gas...) containing tritium (kg)

[T] = tritium concentration in the media (atoms/kg)

### 3. Results and discussion

The calculations were carried out with both codes with the particularity that for EcosimPro, transient behavior is evaluated before reaching equilibrium at steady state. Comparisons are analyzed for results in terms of concentrations in the different circuits, for major contributions of transfer rates in the whole system and for the evaluation of tritium releases. Concentrations (hydrogen and tritium) were calculated in all sodium circuits (primary, secondary, EPUr circuits) but also in the water-steam tertiary circuit and in the nitrogen volume of the primary vessel outer chamber.

#### 3.1. Hydrogen and tritium inventories in circuits

In addition to the tritium balance (Fig. 2), the inventory of hydrogen (protium) migrating from tertiary circuit (produced from water dissociation due to aqueous corrosion of tertiary circuits) is calculated (Fig. 3). Kutim results are presented in blue color and EcosimPro results are presented in orange color. In complement to the reference calculation, a second one was carried out with an enhanced value (factor x 5) of permeation transfer through IHX tubes from primary to secondary sodium, since this key parameter is identified as potentially underestimated in liquid sodium due to its reducing properties (the metal oxide layer potentially present on metal surface formed spontaneously in contact with air is supposed to be eliminated in sodium).

Both codes give similar results in all different circuits, as well for tritium activities and for hydrogen concentrations. The influence of a potential higher permeability of IHX has a major impact on tritium activity in primary sodium which is significantly reduced (factor  $\approx 1/3$ ). The activity in ancillary coolant circuit is also reduced in a similar ratio since it is directly coupled (with heat exchangers) to primary sodium. This is not the case in secondary sodium where tritium activity is very low in both cases (reference or enhanced) of permeation through IHX. This different impact on tritium activities is related to the effect of the important capture of tritium in secondary cold traps due to co-crystallization with higher hydrogen concentrations (a major hydrogen source is coming from tertiary circuit). Consequently even with higher permeation transfer through IHX, a major proportion of tritium activity is still captured in secondary cold traps and residual activity in secondary sodium remains very low.

A comparison of tritium activities between both codes is also presented in Table 1. Though graphical representation presented in Fig. 2 indicate a good coherence between both codes especially for reference calculation and for circuits with largest tritium inventories (primary sodium and EPUr ancillary cooling circuits), the ratio of tritium

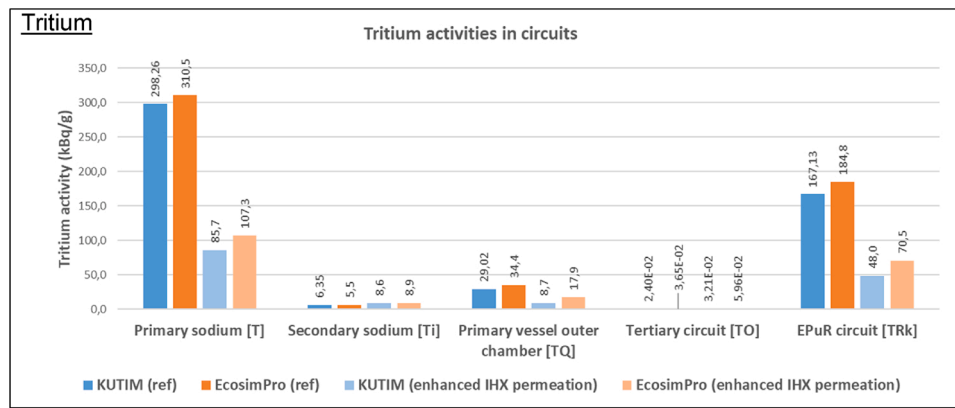


Fig. 2. Tritium activities in main circuits of the reactor.

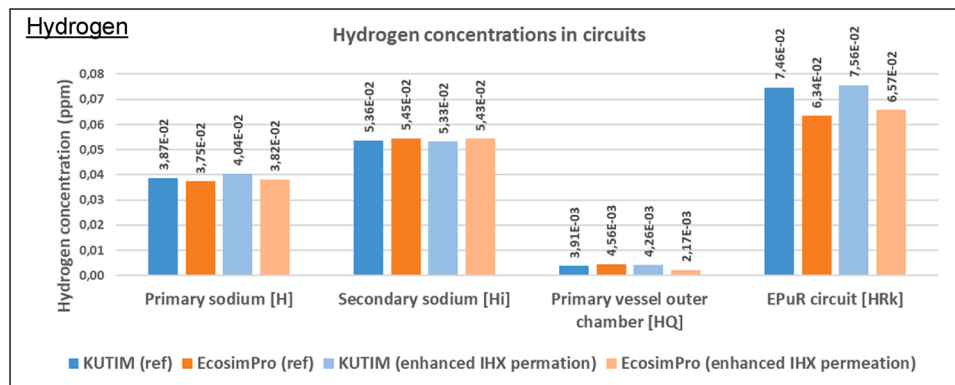


Fig. 3. Hydrogen concentrations in main circuits of the reactor.

Table 1

Ratio of tritium activities calculated by both codes (EcosimPro / Kutim) in each circuit.

Ratio of tritium activities calculated by both codes (EcosimPro / Kutim)	Reference	Enhanced IHX permeation
Primary sodium [T]	1.04	1.25
Secondary sodium [Ti]	0.86	1.03
Primary vessel outer chamber [TQ]	1.18	2.06
Tertiary circuit [TO]	1.52	1.85
EPuR circuit [TRk]	1.11	1.47

activities calculated by both codes reveal higher relative discrepancies in the case of enhanced permeation through IHX and particularly in circuits with small tritium inventories.

Though the overall results of this study are clearly showing a good agreement between both calculations for all important contributions in the material balances, some difference may be induced by the fact that EcosimPro takes into account the temperature profiles of wall materials (circuit pipings, heat exchangers tubes) while Kutim code considers a permeation coefficient calculated with a mean temperature. The fact that EcosimPro calculation is performed in transient mode before reaching steady state equilibrium may also contribute to these differences.

### 3.2. Main transfer fluxes in circuits and components

For a more detailed analysis of the different transfer contributions, the main tritium transfers to be surveyed in the global system are compared between the both calculation tools and for the two conditions of permeation level through IHX. The calculated values of tritium

transfer fluxes presented in Table 2 are expressed in % of the tritium source produced in the reactor core. It can be noticed that a major part of the tritium source (generally more than 90%) transferred into primary sodium is captured globally in the purification systems (primary and secondary cold traps). In particular it is interesting to observe that the tritium transfer flux through IHX is almost completely captured in secondary cold traps, this is due to the effect of higher hydrogen source term in secondary sodium (from permeation through steam generators) in favor of a resulting co-precipitation of tritium in cold traps.

In the case of enhanced permeation through IHX, the values of main tritium transfer contributions are very similar while a small difference is

Table 2

Main tritium transfer contributions in the reactor (in % of tritium source transferred into primary sodium).

Tritium transfer contributions (% tritium source into primary sodium)	Kutim (reference)	EcosimPro (reference)	Kutim (enhanced IHX perm.)	EcosimPro (enhanced IHX perm.)
Accumulation in primary cold traps	40.3%	35.0%	29.5%	27.9%
Permeation fluxes through all IHX	51.6%	45.4%	68.0%	70.1%
Accumulation in secondary cold traps	51.4%	45.0%	67.8%	69.5%
Permeation fluxes through all SG	0.2%	0.3%	0.2%	0.4%
Global gaseous releases	5.1%	5.0%	1.5%	2.0%
Global tritiated water releases	0.2%	0.3%	0.3%	0.4%



observed between both codes for the reference calculation.

### 3.3. Tritium releases

Though they are very limited (less than 6% of the tritium source transferred into primary sodium), two kinds of tritium releases are evaluated: tritium in gaseous form (HT, T<sub>2</sub>) due to permeation through circuit walls and liquid form (HTO) released from pressurized (water/steam) tertiary circuit. In this case, HTO releases from tertiary circuits corresponds to the leaks of pressurized coolant used in tertiary circuit which are considered as a very low fraction (< 1%) of the nominal tertiary coolant flowrate (on the base of Superphenix feedback).

Results presented in Fig. 4 are relative values (in %) reported to the tritium source term produced in the reactor core. They are also very similar between both codes either for reference calculations or for the sensitivity study to IHX permeation level. Due to lower tritium activity in primary sodium and in ancillary cooling circuits, the concentration gradient within piping walls thickness is also reduced and so is the gaseous release related to the permeation determined by this driving force.

In terms of tritium releases in gaseous form, the distribution of the different contributions is presented in Fig. 5 for both codes and for the two permeation levels through IHX.

The major contributions are identified to be the leaks estimated in the purification circuit of cover gas and also the permeation through the walls of EPuR ancillary cooling circuits. The slight difference on this last contribution between the results of both codes (−14% for EcosimPro : corresponding to the difference between 2,20% of tritium source for Kutim to 1,90% for EcosimPro) may explain the slightly higher tritium activity in primary sodium for EcosimPro. Moreover, because of its direct impact (decrease) on tritium activity in primary sodium, the influence of enhanced IHX permeation reduces the main gaseous tritium releases (contributions of cover gas leaks and ancillary cooling circuits).

### 3.4. Accumulation transfers into cold traps

The accumulation of tritium in primary and secondary cold traps ensures the capture of a major part of the tritium source flux (more than 90%) as it can be verified in Fig. 6. EcosimPro evaluates slightly lower values of accumulation fluxes in cold traps (−13% in the case of reference level for the permeation in IHX) probably because of the different approach of the circuits description (estimation of all circuits volumes and systematic use of temperature profiles along circuits).

### 3.5. Analysis and comparison of results

Though very similar results were globally obtained from both codes different interpretations can be proposed for the slight discrepancies observed for a few particular results such as permeation transfer through IHX and accumulation transfer into cold traps. These interpretations are

presented hereafter :

- a specific calculation of permeation profile along circuit piping is implemented in EcosimPro while Kutim considers a mean temperature (between hot and cold sides) in the whole circuit for the evaluation of metallic walls permeability,
- the equations solving for material balance is carried out with different concentration units in both codes (in at/kg for Kutim and in mol/m<sup>3</sup> for EcosimPro): the fluid density which is needed for the unit conversion is function of temperature and may have an influence since the temperature profiles are not treated in the same way in both codes,
- in addition an estimation of the volume of fluid in each part of the circuit is carried out in EcosimPro, especially in piping where temperature profiles are considered, while Kutim considers an average value of concentrations in the whole volume circuit,
- Kutim calculation is performed by resolution of equation system at steady state while EcosimPro converges to equilibrium state after a transient phase evolution of the solution.

In order to evaluate the impact of the temperature profiles which cannot be directly taken into account in the case of Kutim modeling, a complementary calculation was carried out with this code taking into account a discretization of the tubes of main heat exchangers (IHX and steam generators) in 10 sections with the simple assumption of a linear temperature profile along the heat exchange tubes and with the corresponding profile of permeability coefficients (ideally a 2D or 3D calculation with a CFD code would be necessary to calculate temperature profiles more accurately). The results obtained for the evaluation of tritium gaseous releases and of accumulation transfer in cold traps (Fig. 7) show that the application of this correction has a limited influence and does not explain the discrepancies between both codes. This verification confirms the general coherence of both codes and provides an example of the calculations robustness.

## 4. Conclusions and perspectives

With the aim of the development of reliable and validated modeling tools for the assessment of tritium balance in different systems (reactors or processes) operated in the field of nuclear activity, a first benchmarking activity was carried out in the framework of the European TRANSAT project between two calculation tools developed either for fusion (EcosimPro) or for fission reactors (KUTIM). As a first application, this study focused on the case of conceptual Sodium Fast Reactors and on a common data set used for operating conditions and design characteristics. After a general description of the different terms of tritium transfers to be considered in the different circuits and components integrated in this kind of nuclear reactor, the principal models used for the evaluation of material transfer and physico-chemical transformations were presented for both hydrogen isotopes (protium and tritium) that must be considered similarly due to their partial combination by chemical equilibrium.

Calculations results with both codes were compared in terms of tritium activities and hydrogen concentrations in each circuit of the reactor, but also in terms of transfer fluxes and releases. The influence of permeation level through IHX (between primary and secondary circuits) was also investigated.

Generally, a very good coherence of both codes results (larger discrepancies were lower than 15% and only for particular transfer terms) was observed despite the different calculation approaches. Consequently, in the case of steady state evaluation, the simpler approach of Kutim code seems to be sufficient for a good estimation of tritium balance since it provides equivalent results as EcosimPro taking into account a few complementary description such as the temperature profiles along piping or the transient phase preceding the steady state.

Both codes are similarly sensible to key parameters like the

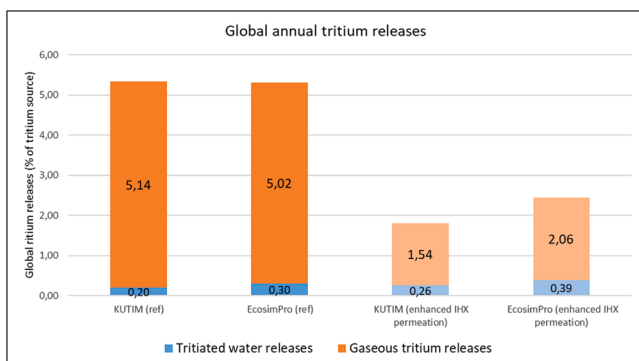


Fig. 4. Global tritium releases (gaseous and liquid form).

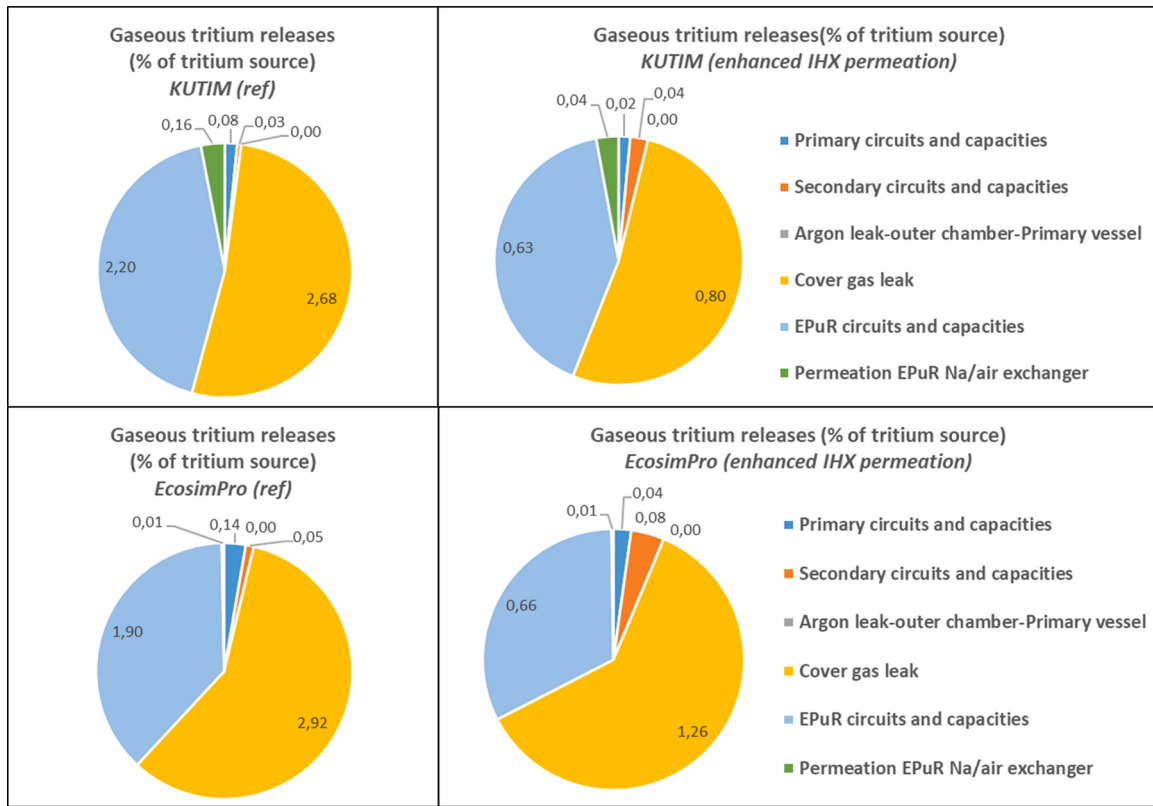


Fig. 5. Contributions of tritium gaseous releases in the overall system.

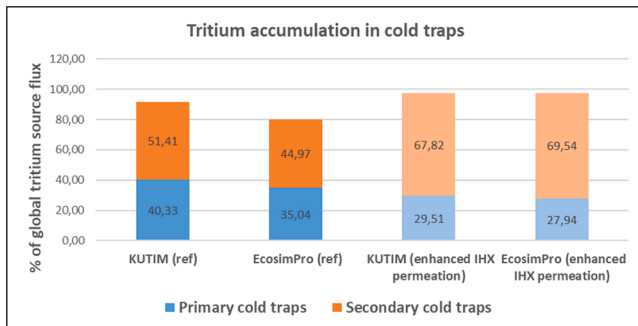


Fig. 6. Global accumulation of tritium in cold traps (primary and secondary sodium).

permeability of wall material used for the assessment of major transfer fluxes such as the permeation contribution through the tubes of main heat exchangers and consequently for all other material balances in the reactor. Due to the modularity and adaptability of these tools, this important result is also an indicator of their robustness for potential application to the simulation of fusion systems.

In perspectives, other comparative studies can be foreseen for further investigations such as a broader analysis of the influence of temperature profiles on overall permeation in the different sections of circuits and components or complementary sensitivity studies of key parameters (hydrogen source terms in secondary sodium, permeation surfaces of circuits and heat exchangers, sodium flowrate in purification systems...). The influence of sodium velocity on permeation rate could be also an interesting study to carry out at the local scale of a single component or a piping section, by comparison with a CFD code calculation. Moreover, the consolidation of this benchmark activity with future applications to other systems involving the management of

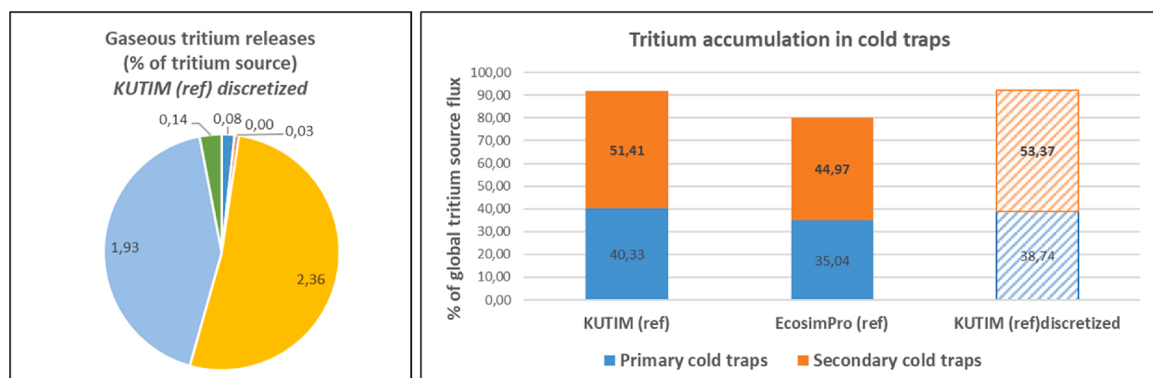


Fig. 7. Tritium gaseous releases and accumulation in cold traps calculated by Kutim with discretization of IHX and SG tubes.

tritium transfers (like an application to purification system for tritium recovery in fusion reactors) would be interesting to confirm the flexibility and the robustness of these calculation tools.

In further steps, this kind of benchmark studies applied to comparisons with experimental measurements in reactor could be also used to help the consolidation of not well known parameters (effective permeation coefficients, tritium source term, hydrogen source term...) thanks to the crosschecking of results from both calculation tools.

### Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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### References

- [1] European Commission – Directorate General Research & Innovation - project TRANSAT number 754586 (identification: NFRP-14) – Annex 1 – Part A.
- [2] F.R. Ugorri, C. Moreno, E. Carella, D. Rapisarda, I. Fernández-Berceruelo, I. Palermo, A. Ibarra, Tritium transport modeling at system level for the EUROfusion dual coolant lithium-lead breeding blanket, *Nucl. Fusion* 57 (11) (2017).
- [3] F. Masse, C. Latge, Kutim : an efficient approach for tritium balances in fast breeder and fusion reactors », *Fusion Technol.* 28 (1995) 1039–1044.
- [4] K.S. Forcey, et al., Hydrogen transport and solubility in 316L and 1.4914 steels for fusion reactor applications, *J. Nucl. Mater.* 160 (1998) 117–124.
- [5] G. Esteban, et al., Diffusive transport parameters and surface rate constants of deuterium in Incoloy 800, *J. Nucl. Mater.* 300 (2002) 1–6.
- [6] A. Wittingham, An equilibrium and kinetic study of the liquid sodium hydrogen reaction, *J. Nucl. Mater.* 60 (1976) 119.
- [7] W.M. Jones, *Chemphyschem* 16 (11) (1948) 1077–1081.

### Glossary

- IHX*: Intermediate Heat Exchanger (/)
- PWR*: Pressurized Water Reactor (/)
- SFR*: Sodium Fast Reactor (/)
- TBM*: Test Blanket Module (/)
- $\Omega$ : diffusion flux of H or T through the metallic wall (atoms/s)
- $D$ : diffusivity of H or T in the wall material ( $\text{m}^2/\text{s}$ )
- $C_1, C_2$ : concentrations of H or T on both sides surfaces of the metallic wall (atoms/ $\text{m}^3$ )
- $A$ : Surface area of the permeation wall ( $\text{m}^2$ )
- $\delta$ : Thickness of the permeation wall (m)
- $C_{Q,i}^{\text{Na}}$ : Concentration of atoms “Q” (Q = H or T) dissolved in liquid sodium on side “i” (atoms/ $\text{m}^3$ )
- $C_{Q,i}^{\text{met}}$ : Concentration of atoms “Q” (Q = H or T) dissolved in metal on side “i” (atoms/ $\text{m}^3$ )
- $K_{SQ}^{\text{met}}$ : Sieverts constant of diatomic molecule “Q<sub>2</sub>” in equilibrium with liquid sodium interface (atoms.  $\text{m}^{-3}$ .  $\text{Pa}^{-1/2}$ )
- $K_{SQ}^{\text{Na}}$ : Sieverts constant of diatomic molecule “Q<sub>2</sub>” in equilibrium with the wall metal interface (atoms.  $\text{m}^{-3}$ .  $\text{Pa}^{-1/2}$ )
- $D_Q$ : Diffusivity of hydrogen isotope (Q = H or T) through metallic wall ( $\text{m}^2.\text{s}^{-1}$ )
- $p_{eQ}$ : Permeability of hydrogen isotope (Q = H or T) through metallic wall (atoms.  $\text{m}^{-1}.\text{s}^{-1}$ .  $\text{Pa}^{-1/2}$ )
- $[Q]_i$ : Concentration of atoms “Q” (Q = H or T) dissolved in liquid sodium on side “i” (atoms/kg)
- $\rho^{\text{Na}}$ : Sodium density ( $\text{kg}/\text{m}^3$ )
- $C_{H,\text{sat}}^{\text{Na}}$ : Saturation concentration of H impurity in sodium (atoms/ $\text{m}^3$ )
- $Q_{\text{Na}}^{\text{PF}}$ : Sodium flowrate purified in cold traps (kg/s)
- $\varepsilon$ : Purification efficiency in cold trap (/)
- $[H]_{\text{sat}}$ : Saturation concentration of H impurity in sodium (atoms/kg)
- $K_{\text{eq}}(T)$ : Constant of chemical equilibrium between H<sub>2</sub>, T<sub>2</sub> and HT (/)
- $K_D$ : Tritium radioactive decay constant ( $\text{s}^{-1}$ )
- $m_{\text{Na}}$ : Mass of the media (liquid sodium...) containing Q species (kg)