Design, modelling and simulation of the water detritiation system (WDS) of the ITER project with EcosimPro.

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The purpose of this project is to model a water detritiation system (WDS) using a process known as CECE (Combined Electrolysis-Catalytic Exchange). The goal is two-fold: reach a current with a high tritium concentration for its subsequent recovery and another current that is detritiated enough so that it can be discharged to the atmosphere.

A library has been developed with this tool. It includes all the required components that are modelled to simulate the process for the elimination of tritium from water. The process needs to meet a series of requirements: including a simple and user-friendly model that also has the complexity of the system that is simulated and incorporates a database of the compounds intervening in the process. Finally, the results obtained need to be analysed to check that the model works correctly.

Key words: EcosimPro, model, simulation, detritiation.

1.- Introduction.

This article focuses on the modelling and simulation of a part of the ITER tritium plant known as WDS (Water Detritiation System). Its purpose is to remove as much tritium as possible from the waste water flow from the fusion reactor. This simulation shall be done by means of the EcosimPro tool. This tool allows the user to analyse the most relevant aspects of the simulation, such as the system inlet flows and their compositions.

The model has been developed by creating the TRITIUM_CECE library.

As regards the validation of the results obtained, they shall be compared with data obtained from laboratory plants and with the output requirements for the process output currents.

Different components, functions and a database of system compounds have been developed to model the detritiation process.

Below are the various steps to be followed to develop the model of the facility.

- Generation of a database of the species existing in the detritiation process. It shall provide the information required for the simulation of the process.
- Modelling of the system components. The modelling of the equipment intervening in the process shall be developed.
- Joints of the components within one schematic diagram of the whole plant.

- Simulation of the detritiation process and validation of the results obtained.

2.- Methodology.

This section shall focus on the procedure followed for the development of the library in which the model of the water detritiation plant is included.

2.2.- System data.

The process information required has been obtained from the official ITER project web page, as well as from articles on similar simulations and from reviews of the tritium plant. In some cases, lack of information has made it necessary to estimate some relevant information for the equipment modelling.

2.3.- Database.

The information obtained from the above sources shall be used to establish the species that occur within the detritiation process. These species are all the isotopes of both gas hydrogen and liquid water, which are as follows: H_2, HT, HD, D_2, DT and T_2 for hydrogen gas and H_2O, HTO, HDO, D_2O, DTO and T_2O for tritiated water.

2.4.- Modelling of the equipment.

Below is an explanation of the procedure applied for the modelling of the equipment that make up the tritiated water detritiation process.

2.4.1.- Electrolyser.

This unit transforms the tritiated water into tritiated hydrogen and oxygen by means of an electric current.

In the system it is better to have tritium in its gaseous phase (as HT) to allow its recovery, so an electrolyser is necessary.

A unit efficiency has been assumed for its modelling. The following equations have been used to calculate the output flows and compositions.

H2O (l) → H2 (g)+ ½ O2 (g)

HDO (l) → HD (g) + ½ O2 (g)

HTO (l) → HT (g) + ½ O2 (g)

D2O (l) → D2 (g)+ ½ O2 (g)

DTO (l) → DT (g) + ½O2 (g)

T2O (l) → T2 (g)+ ½ O2 (g)

2.4.2.- Permeator.

This unit has a dual function: it uses a Pd-Ag membrane system to separate and concentrate a current of steam-free hydrogen (and its isotopes), which shall be channelled to the isotopic separation system (ISS).

It is essential to ensure there are no remains of steam isotopes in the permeate, since they would have a negative impact on the operation of the following process. Forms HT and T_2 of tritium also need to be concentrated.

The model used simplifies these stages so that the flow of permeate Q (mol/s) of each isotope can be related to:

- The surface area of the membrane (m2).
- The thickness of the membrane (m).
- The isotope permeation coefficient.
- The pressure differential between the supply and the permeate.
- The following equation shall be applied:

$$Qi = P_i \times \frac{A}{t} \times \left(\sqrt{P_{Alim.}} - \sqrt{P_{Perm.}}\right)$$

2.4.3.- Exchange column.

The isotopic exchange column is divided into two areas that alternate along its whole length. The two areas are divided into: fill distillation area and bed catalytic reaction area.

A. Catalytic area.

Two gas phase chemical reactions occur in this area:

$HT (g) + H_2O (v) \leftrightarrow HTO (v) + H_2 (g)$ (1)

$T_2 (g) + H_2O (v) \leftrightarrow T_2O (v) + H_2 (g)$ (2)

The compositions are calculated using the balance reactions as a basis, considering that the kinetics are fast enough to ensure the balance of all the species at the outlet of the reaction area, within a system of equations that is solved simultaneously. There are six species in the reaction area, so there are six unknowns that need to be solved.

B. Distillation area.

In the same way as dish distillation, fill distillation is based on the liquid-vapour balance between the species to be distilled. In this case, the reaction occurs between the vapour HTO and the liquid H_2O:

$H_2O(l) + HTO(v) \leftrightarrow H_2O(v) + HTO(l)$

The fill is balanced when the rising steam HTO comes into contact with the liquid H2O, which flows down the column. Thus the lightest component (H2O) evaporates and the heaviest one (HTO) condenses. The tritium contained in the HTO slowly concentrates in the liquid current that will feed the electrolyser at the outlet of the column.

Certain assumptions that need to be taken into account throughout the fill area are considered.

- Constant molar flow rate along the whole column.
- Negligible heat effects within the column.
- Negligible gaseous phase accumulation in comparison with the liquid phase.
- Negligible mass transfer resistance in the liquid.

The model of the EcosimPro component has been based on models of fill column models found in reference documentation and applying the assumptions and species of this system.

2.5.- Joints of components.

Once all the system components have been modelled, the following step involves joining them within a schematic diagram for the joint simulation of the whole process. Figure 1.1 shows the schematic diagram used for the simulation of the in EcosimPro.

3.- Validation of results.

This section shall be used to analyse the results of the process simulation with EcosimPro and to check by means of graphs that the system evolves correctly as the process conditions (such as the head and side supplies, for water and tritiated water respectively, and the efficiency of the electrolyser) are changed.

The validation shall be divided into:

- Simulation of the process at the operating point.
  Figure 2.2 shows the radioactivity of the permeate current under normal operating conditions of the process. The water supply through the catalytic exchange column head will be altered in order to validate that the simulation progresses adequately and correctly.

- Simulation of the process reducing and increasing the head water flow.

  Figures 1.3 and 1.4 show that the process has been simulated by introducing the changes that were commented above in the head current.

- Simulation of the process varying the efficiency of the electrolyser.

  As in the previous simulations, the evolution will be checked by modifying the efficiency of the equipment upstream from the permeator: the electrolyser.

4.- Conclusions.

Once the process has been modelled and simulated it is possible to reach certain conclusions about certain aspects of this project.

The creation of a process model presents a way to efficiently simulate the detritiation facility. The conditions under which the system has been placed are as required by ITER, but they could be altered as necessary.

The results of the simulation are satisfactory. The system evolves correctly under the changes performed in the process input flows.

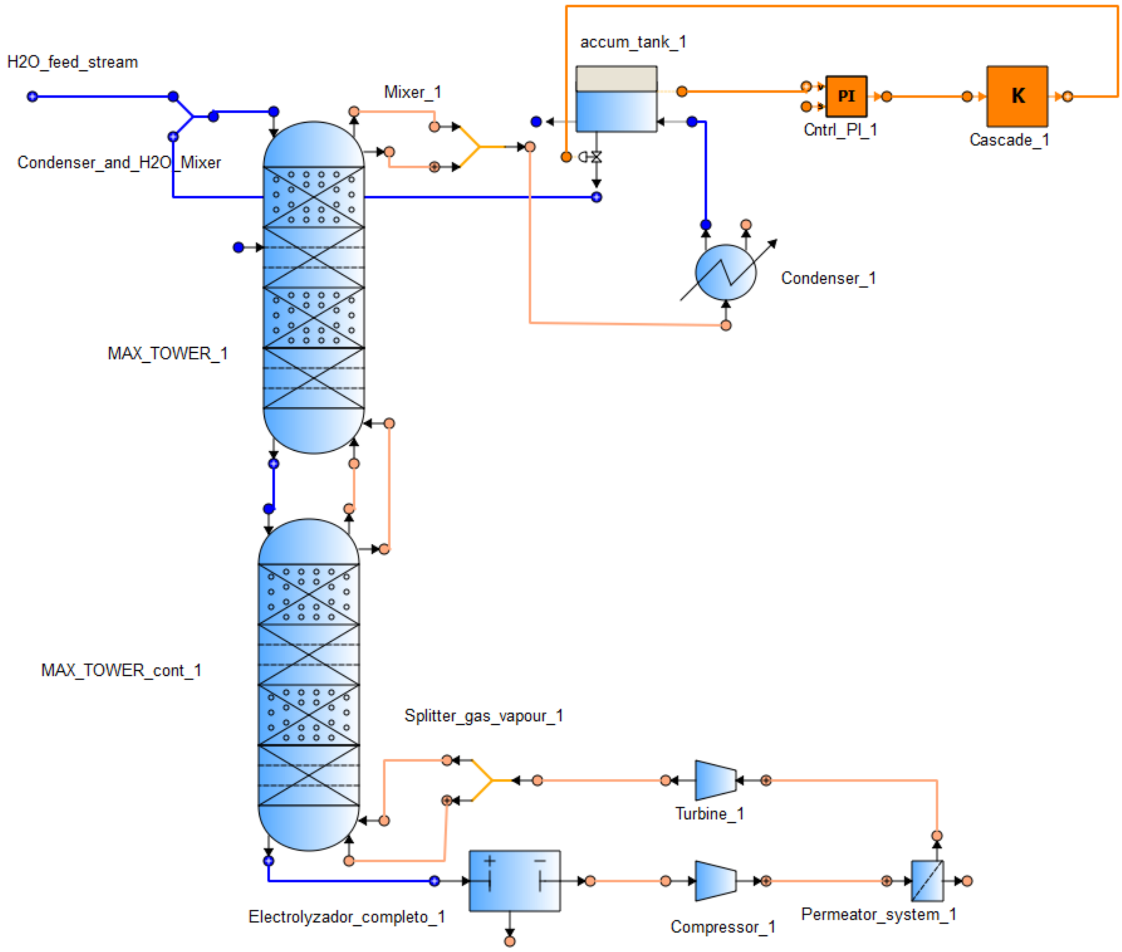

Figure 1. 1.- Final schematic diagram of the process simulated with EcosimPro.

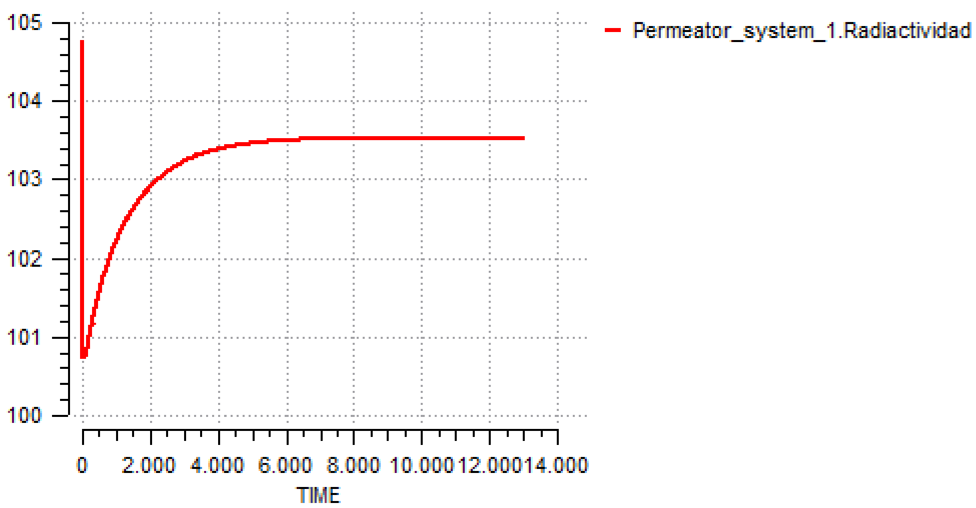

Figure 1. 2.- Radioactivity of the permeate current at the operating point.

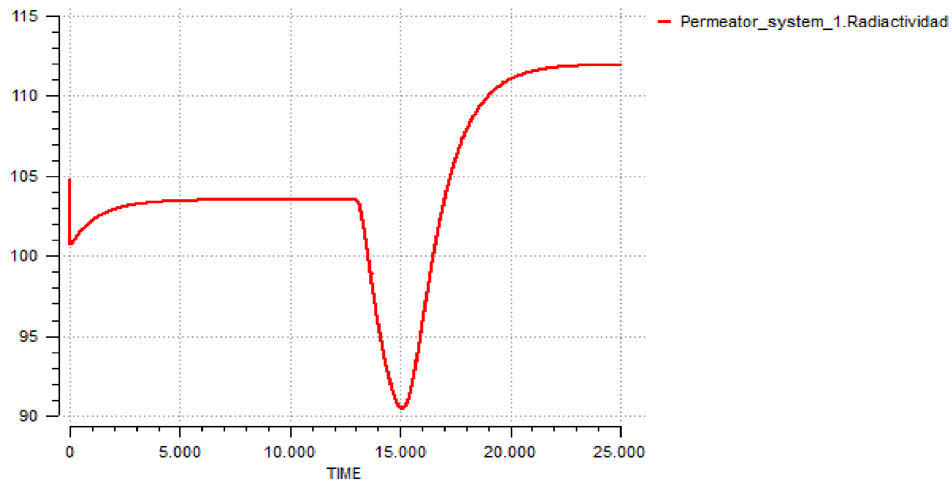

Figure 1. 3.- Radioactivity of the permeate halving the top water flow.

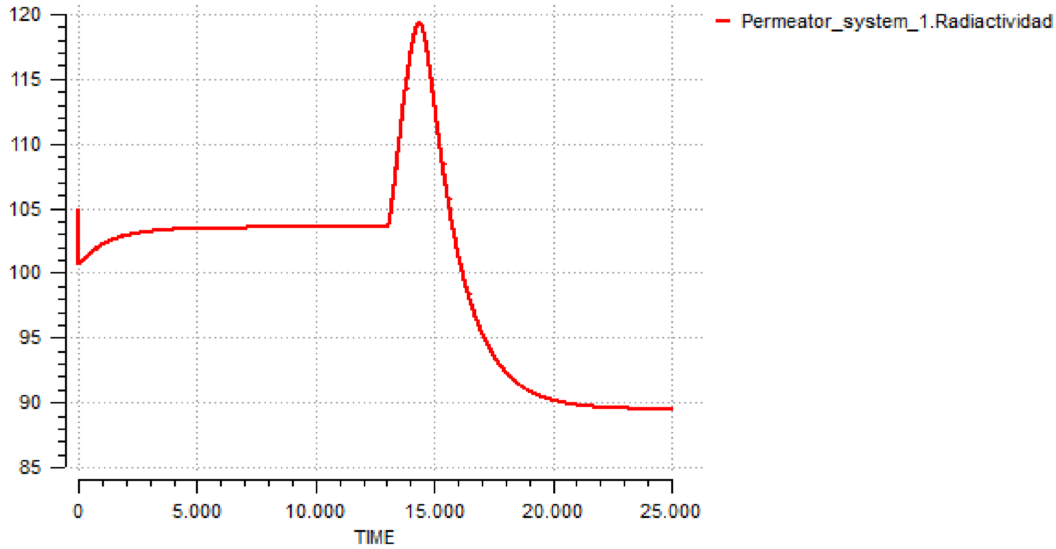

Figure 1. 4.- Radioactivity of the permeate doubling the top water flow.

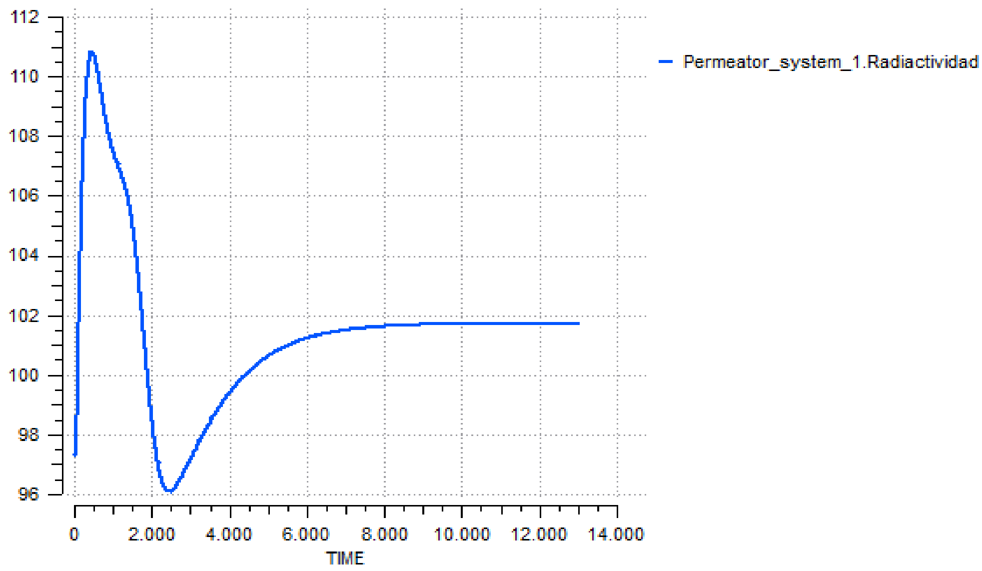

Figure 1. 5.- Radioactivity of the permeate when the electrolyser efficiency is changed.