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Tritium control in fusion reactor materials: A model for Tritium Extracting System



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HIGHLIGHTS

- A modeling work has been performed to address these issues in view of its utilization for the TES (Tritium Extraction System), in the case of the HCPB TBM and for a Molecular sieve as adsorbent material.
- A computational model has been setup and tested in this paper.
- The results of experimental measurement of fundamental parameters such as mass transfer coefficients have been implemented in the model.
- It turns out the capability to model the extraction process of gaseous tritium compounds and to estimate the breakthrough curves of the two main tritium gaseous species (H2 and HT).

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ABSTRACT

In fusion reactors, tritium is bred by lithium isotopes inside the blanket and then extracted. However, tritium can contaminate the reactor structures, and can be eventually released into the environment. Tritium in reactor components should therefore be kept under close control throughout the fusion reactor lifetime, bearing in mind the risk of accidents, the need for maintenance and the detritiation of dismantled reactor components before their re-use or disposal. A modeling work has been performed to address these issues in view of its utilization for the TES (Tritium Extraction System), in the case of the HCPB TBM and for a molecular sieve as adsorbent material. A computational model has been setup and tested. The results of experimental measurement of fundamental parameters such as mass transfer coefficients have been implemented in the model. It turns out the capability of the model to describe the extraction process of gaseous tritium compounds and to estimate the breakthrough curves of the two main tritium gaseous species (H2 and HT).

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1. Introduction

One of the main objectives of the experimental campaign on the Test Blanket Systems (TBS) in ITER is the demonstration of the efficient processing of the tritium generated in the Test Blanket Module (TBM) [1]. On the other hand, efficient tritium processing in a TBS has deep implications on safe operation of TBS itself and of the entire ITER system.

The successful development and validation of tritium transport modeling codes is essential for this purpose. Tritium Transport

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http://dx.doi.org/10.1016/j.fusengdes.2015.06.052 0920-3796/© 2015 Elsevier B.V. All rights reserved. modeling tools must be such accurate as to be potentially able to predict the tritium concentration in any point of the system and at any time.

A tritium permeation analyses code (FUS-TPC) was previously developed by some of the authors [2,3], in order to perform the tritium transport analysis in fusion reactors, based on the mass balance equation for various chemical forms of tritium, coupled with a variety of tritium sources, sinks, and permeation models. Concerning tritium transport and release during operation, the analysis showed that tritium losses and inventories in the reactor components are strongly dependent on the presence of tritium permeation barriers, on the performances of the Coolant Purification System and of the Tritium Extraction System.

The experience gained in the development of FUS-TPC has been useful in order to setup a new model, specific for the Tritium Extraction System (TES) of one of the four test blanket models proposed and developed for ITER, the HCPB (Helium Cooled Pebbles Bed) TBM. In this blanket [4], tritium is produced in solid breeder, it has to be extracted using Helium purge gas flowing through pebbles bed. At the outlet of TBM, He stream must be cooled down and processed. All these steps are carried out in the TES (Tritium Extraction System) allowing separation of both gaseous and liguids tritium compounds. Many techniques have been proposed over the years, based on different adsorbent materials and operating conditions. Typically, liquid compounds are extracted in cold traps operating at low temperature, while a cryogenic adsorption inside special columns is used for gaseous tritium. Main issues related to the latter process concern adsorbent column saturation and behavior of helium-flow through a porous medium. Because of column saturation, regeneration process is needed after a certain time, that must be estimated. Also, because of material porosity, velocity profile associated to He-flow could influence the adsorption process itself. A modeling activity has been performed to address these issues for the TES (Tritium Extraction System), in the case of the HCPB TBM and for molecular sieve Zeolite 5A as adsorbent material. A computational model of the system has been setup in order to identify potential solutions. The results of experimental measurement of fundamental parameters such as mass transfer coefficients have been implemented in the model too

The paper describes the model and reports its verification versus experimental results. Its main scopes are to be able to model the extraction process of gaseous tritium compounds and to estimate the breakthrough curves of the two main tritium gaseous species.

In fact, a useful technique to characterize adsorption is the breakthrough curve. It represents evolution of adsorbate concentration in the gas flow at the outlet of absorber bed, over time. The typical "S" shape of this curve is displayed in a figure shown later in the paper (see Figs. 5 and 8 in Section 3). Three regions can be identified: since during initial phases, all adsorbate is adsorbed near the column inlet, relative concentration value is initially null. After a certain time, this value starts to increase because saturation has already taken place in regions of the column near the inlet boundary. Relative concentration keeps increasing up to when its value is about 1. This means that concentration of absorbate at the column outlet is almost equal to that at the inlet, and solid adsorbent material is almost all saturated. Afterwards, value stays constant at 1 and gas stream is not purified anymore, thus, at this point regeneration process is needed. Area under breakthrough curve during purification is called Mass Transfer Zone (MTZ) and it can be computed through an integration. Shape of breakthrough curve, and MTZ, are influenced by different parameters. The most important are: gas flow-rate, adsorbent column height, and void fraction inside the bed. As introduced above, adsorption of tritium and other hydrogen isotopes can be performed using many materials, but molecular sieve is the most important one. This material, which is also known as Zeolite, will be used in the simulation work described hereafter. Zeolite has pores in the range 4–14 Å.

2. Model description

Modeling work is has been performed by setting up a new code by means of the COMSOL Platform [5]. Here, the verification of the model by testing it against experimental results published in Ref. [6] is described.

The computations were performed considering a uniform velocity for helium stream. Afterwards, a velocity profile has been considered. All breakthrough curve calculations have been achieved using a simulation program. This is COMSOL Multiphysics 4.3: it has been used to solve equations and modeling the hydrogen isotopes extraction, through molecular sieve, from helium purge gas. For our purposes, species transport in porous media has been used since molecular sieve can be represented as a porous medium. Also, Brinkman equations interface has been used in order to perform a more realistic calculation. As demonstrated by partial pressure of hydrogen isotopes, we can assume that these species are quite diluted: this means that their concentration in the helium purge flow is low. Thus properties necessary for calculations, like density and viscosity, can be assumed equal to those of helium.

Species transport in porous media is solved by usual timedependent mass balance equations; by solving them, effective diffusion coefficient for hydrogen mass species can be obtained. Equations are valid in a general case, thus coefficients have to be set in order to consider the real phenomena occurring inside cryogenic adsorption column. Also, geometry and dimensions of CMSB column [6] and properties of materials have to be specified. Since the real component is a cylinder, it can be studied in 2D geometry like a rectangle. Thus, this simplified configuration is pretty easy to be represented. Concerning materials, Zeolite 5A is the porous medium and He gas which flows through solid matrix. Additionally, properties like partial pressure, molecular diffusivity and Langmuir constant, were defined for hydrogen isotopes (H2 and HT). This is a 2D symmetric model: the experiment does not need, as a first approach, a 2D axisymmetric model. Further details on the numerical model are available in Ref. [6].

3. Results

Despite its simplicity, experimental facility configuration [7] is similar to that of a real plant. Fig. 1 shows the experiment configuration.

In this scheme, flow rate seems uniformly distributed over the whole cross section. However, because of smaller dimensions, experimental results obtained in Ref. [7] are not directly applicable to the TES cryosorption column. Observing column dimensions, we can notice that they are very small with respect to pebbles diameter. In fact, only 11 pebbles can be contained on the cross section. This means that the packing factor of the bed is small. This is not true for real TES CMSB because diameter of the column is about 10 times larger: since pebbles diameter is the same, packing factor will be much higher. Dimensions of the test facility and other physical properties of adsorbent and used in the code are listed in Table 1.

Concerning adsorption process in the bed, we assumed that two independent active adsorption sites coexist on the pore surface of adsorbent and that Langmuir-type adsorption occurs at each site [7,8]. This assumption leads to have two values of surface diffusivity for both chemical species. Also, there are two values of Langmuir constant for each species, however some simplifying assumptions can be done: in fact, it has been considered that Langmuir constants that are related to the second adsorption site, are about one order of



Fig. 1. Configuration of experimental facility.

Time=500 s H₂ Concentration (mol/m³)

Table 1

Data on the experimental facility.

Parameter	Symbol	Value
Inner diameter of tube (m)	rD	$2.2 imes 10^{-2}$
Bed height (m)	ZB	$4.0 imes10^{-2}$
Packed bed/bulk density (kg/m ³)	ρb	660
Particle diameter (m)	dP	$2.0 imes10^{-3}$
Porosity	\in	0.51
Pore radius (m)	rP	2.5×10^{-10}
Tortuosity	τF	3.0

Table 2

Langmuir constants of molecular sieve 5A.

	1/Pa	mol/kg Pa
H2	$2.7 imes 10^{-3}$	4.1×10^{-3}
HT	$5.6 imes 10^{-3}$	7.8×10^{-3}

magnitude smaller than those ones for the first site. This means that their contribution is almost negligible and can be neglected. Values of Langmuir constants in molecular sieve 5A for both species are shown in Table 2.

Due to previous assumption, total number of constants is 4. Other parameters necessary for calculation, which describe operating conditions in the experiment, are listed in Ref. [4]. Superficial velocity and helium properties are calculated at 77.4 K and 0.1013 MPa since the column operates at atmospheric pressure. Inlet concentrations of hydrogen isotopes have been obtained from their partial pressure (Fig. 2).

Results of computation can be plotted on a 2D surface plot (Figs. 3 and 4) and on a 1D line graph (Fig. 5). First one allows checking the evolution of the adsorption process inside the bed, while the second one is important to observe the breakthrough curve. Fig. 3 shows the concentration of H2 in the helium stream.

Figures display concentrations at the same times: this allows better comparison between the two cases. A longer time is required to reach bed saturation for HT. Concentration of HT is plotted in Fig. 4.

As mentioned before, 1D line graph is very useful to observe the breakthrough curve which describes phenomenon just analyzed. Fig. 4 displays curves for both chemical species.

Saturation in case of H2 is reached after about 5200 s, while for HT after about 9500 s. These values are comparable to experimental results [7].





▲ 0.0889

Fig. 3. H2 concentration in the adsorption column (dimensions in meters).



Fig. 4. HT concentration in the adsorption column (dimensions in meters).



Fig. 5. H2 and HT breakthrough curves.

A 0.0889

Time=2200 s H₂ Concentration (mol/m³)



Fig. 6. Velocity profile in experimental column.



Fig. 7. HT concentration (velocity profile, dimensions in meters).

Even if it is not directly applicable to the experiment in Ref. [7], better modeled with a constant velocity profile, we have implemented in our model a velocity profile, which will be necessary to analyze the TES cryosorption column. In fact, since porosity and permeability are not constant on the column cross section, velocity varies as well. For this reason, Brinkman equations module in Ref. [5] was used to compute a velocity and pressure profile.

Since molecular sieve 5A is in form of pebbles, adsorption column is represented as a bed of packed spheres. In this case, porosity sharply varies near the wall because the geometry of packing is interrupted. Also, this behavior is valid in case of packed irregular granular particles as well. For this study, since flow velocity is low, an exponential porosity profile was considered. Velocity profile and constant velocity for experiment in Ref. [7] are shown in Fig. 6.

The velocity peak is in the near-wall region. Flow channeling region is very wide with respect to the tube diameter because of low value of aspect ratio. In fact, for a cluster of few spherical particles like this one, wall region effects are dominant over the entire column. Peak velocity is higher than in case of constant superficial velocity, but in the central region the value is smaller.



Fig. 8. HT breakthrough curves (velocity profile).

Concerning breakthrough curves, due to breakthrough curve definition, all points are located on the outlet boundary. Point #1 is placed on the column centerline, where velocity is lower. Point #2 is located on the wall and #3 in the middle [7]. In Figs. 7 and 8, predicted HT concentrations and breakthrough curves are displayed. Concentration has the same shape as velocity profile. In fact, considering a certain height in the bed, concentration is higher near the wall. This means that porous medium in this area reaches saturation earlier. Fig. 8 shows that saturation occurs faster in point #2 because of velocity profile. Time necessary is 9100 s in #2 and 10,200–10,500 s in #1 and #3.

4. Conclusion

If we compare breakthrough curves obtained in Figs. 4 and 5 and relative times with the experimental results in [6], it turns out the full capability of our model to deal with the extraction process of gaseous tritium compounds and to estimate the breakthrough curves of the two main tritium gaseous species (H2 and HT).

It will be possible then to perform in the future a modeling work to address tritium processing issues for the TES (Tritium Extraction System), in the case of the HCPB TBM and for Molecular sieve 5A as adsorbent material, assuming velocity profile as done in Figs. 7 and 8. As a future development, the model presented here, a simplified 2D one, will be improved into a 3D model.

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