

AN INVESTIGATION OF PLASMA-FACING COMPONENT MATERIAL EFFECTS ON TRITIUM REPROCESSING SYSTEMS

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ABSTRACT

Plasma-facing component (PFC) materials directly affect tritium inventories by the creation of a characteristic set of volatile impurities inside the torus. Impurity creation processes were modeled and incorporated into the Tritium Fusion Fuel cycle dynamic Simulation, TRUFFLES, which simulates dynamic inventories in the tritium reprocessing systems.¹ These surface processes include net erosion and "outgassing". The estimated impurity outflow is coupled with the tritium reprocessing models in TRUFFLES to calculate inventories. Be and C were evaluated as examples of plasma-facing materials. It is found that for C a constraint limiting its net erosion rate is necessary in order to keep the tritium inventory in the cryopumps below a specified value. In contrast, Be may present no problem because of its non-production of volatile species when eroded during reactor power operation. "Outgassing" of H₂O and the DT reflection coefficient were also investigated.

I. INTRODUCTION

Previous fuel cycle models did not take into account the role of impurities on the calculation of dynamic tritium inventories in the fuel cycle.^{2,3} This impurity effect along with impurity control characteristics links PFC materials with tritium reprocessing systems, such as cryopumps, the fuel cleanup unit, impurity processing, and the isotope separations system.

The approach for this initial investigation starts with the identification of torus impurity sources. Simple models are then used to investigate the fuel cycle dependence upon various averaged parameters

characterizing these impurity sources. The simulation of dynamic inventories in the tritium fuel cycle can increase in accuracy with the inclusion of these PFC material processes. A foundation is thus laid for more detailed studies of vacuum vessel effects coupled with plasma dynamics on the fuel cycle.

II. TRUFFLES PLASMA AND IMPURITY CONTROL MODEL

In terms of the fuel outflow rate, the primary plasma parameters that influence its value are the fractional fuel burnup, β , and the fusion power level, P_f . If β is given, then the torus fueling rate (i.e. the DT inflow rate for DT burning fusion reactors) is:

$$F_{\text{torus, in, DT}} = \frac{F_{\text{burn}}}{\beta} \quad (1)$$

$F_{\text{torus, in, DT}}$ is the DT fueling rate and F_{burn} is the fuel burnup rate. F_{burn} , which is equivalent to the He production rate, J_α , is directly related to the power level of the fusion reactor by:

$$F_{\text{burn}} = J_\alpha = \frac{P_f}{Q_f} \quad (2)$$

P_f is the fusion power and Q_f is the energy released per fusion event. For the DT fusion reaction, Q_f is 17.6 [MeV/fusion]. β can be further decomposed into more general plasma and impurity control structure parameters. In particular, it is now possible to determine a β -plasma-impurity control performance parameter relationship with the following equation:

$$\beta = \frac{J_{\alpha}}{\left(\frac{N_{DT} V_p}{2\tau_p}\right) (1 - R_{DT}) + J_{\alpha}} \quad (3)$$

N_{DT} is the DT plasma density, V_p is the plasma volume, τ_p is the confinement time of DT, and R_{DT} is the DT reflection coefficient of the PFC impurity control structure (i.e. divertor/limiter) material. TRUFFLES is thus able to account for variations in these parameters rather than β .⁴

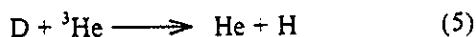
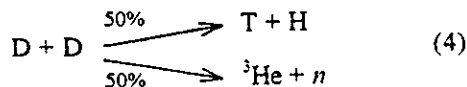
III. IMPURITY SOURCES

To accurately estimate the true values of the torus exhaust rates for both DT and He, the impurities from a variety of sources must be included in the model. These impurities include H_2 , He, and volatile compounds.

A. H_2 and He IMPURITY SOURCES

H_2 protium impurities are expected to originate from the following sources:

- Isotopic exchange of protiated impurities (e.g. H_2O) inside the vacuum vessel.
- Nuclear reactions inside the plasma.⁵ For these impurity sources, the only significant reactions are the D-D and D- 3He reactions. This reaction yields the following products:



The reactivity of the D-D and D- 3He reaction are approximately several hundred times less than the D-T reaction in the 20 keV range.

- Vacuum vessel material (n-p) reactions.
- Non-purity of fuel. The expected purity of the fuel due to ISS isotope separation is ~99.99 %-99.999 %.
- H_2 propellant contamination from the pellet injection system (PIS).

The last 3 sources are expected to be negligible. He will originate from the same sources as H_2 but with different rates of formation. For example, if He is used as a coolant rather than water, this will increase He impurities while lowering H_2O 's. These He sources are also expected to contribute negligible amounts to the torus exhaust.

B. VOLATILE IMPURITY SOURCES⁶

Volatile impurities other than H_2 and He will significantly affect fuel cycle operation and design, especially the impurity separation and processing subsystems. Although outgassing will be performed prior to reactor operation, a sizable quantity of desorbed and dissolved gases will still reside inside the vacuum vessel. This quantity will of course depend upon the state of cleanliness of the materials. During normal operation, expected sources for these impurities include the following:

- Sputtered surface material. Surface material will sputter and redeposit throughout the torus. If volatile compounds are created when the sputtered elemental species react with the plasma, these volatile impurities must be pumped away. The quantity of bulk impurities as well as bulk alloy elements will play a major role in the volatile compounds being created during sputtering.
- Ion- and electron-stimulated desorption and chemical reactions. The vacuum vessel will contain a large quantity of adsorbed and dissolved gases from previous atmospheric exposure and manufacture. Ion and electron bombardment can desorb these impurities.
- Surface desorption and diffusion. Chemical desorption is the most likely process by which chemisorbed impurities and dissolved diffusing gases inside the bulk are released. Both first order and second order desorption will occur. Gross surface contamination will determine the importance of this process.
- Permeation of atmospheric gas and coolant gas. Atmospheric and coolant gases will permeate through the vacuum vessel, especially during high temperature operation.
- Internal leaks. Internal leaks may be produced which will increase the release of dissolved gases inside the bulk material. Real surfaces are characterized by a large number of imperfections which greatly increase the impurity flow rate into the torus.

C. TORUS EXHAUST RATE CALCULATIONS

To estimate the torus exhaust rate and composition with the inclusion of impurity sources, all the above impurity sources can be simply simulated using averaged aggregate parameters. Sputtering as well as stimulated and chemical desorption and reactions due

to ion bombardment can be approximated with an average net erosion rate during power operation. Nuclear reactions can be modeled using the average reactivity ratio between D-D / D-³He and D-T in the ion temperature range of operation and using this value as the fraction of H, and He being produced. Finally, all other remaining sources (e.g. previously adsorbed and dissolved gases in addition to atmospheric and coolant permeating gases) can be approximated with an average "outgassing" term.

Eroded material species will produce protiated, deuteriated, and tritiated impurity compounds if volatile species are formed from their interaction with the hydrogen isotope, Q, ions. This will result in a corresponding reduction of the Q₂ torus exhaust rate. Additionally, if "outgassing" impurities containing protium are included, mainly water, a large fraction of this protium will be lost to the plasma through isotope exchange. To account for the above processes, the resulting exhausted impurities are assumed to contain an equivalent composition of Q isotopes as the total mixture of Q isotopes inside the torus. Thus,

$$\left(\frac{H}{Q}\right)_{imp} = \left(\frac{H}{Q}\right)_{plasma} = \frac{\sum F_{torus, in, H, j}}{2(F_{torus, in, DT} - F_{burn})} \quad (6)$$

(H/Q)_{imp} is the protium to hydrogen isotope ratio inside impurity compounds, (H/Q)_{plasma} is the equivalent ratio in the plasma, and F_{torus, in, H, j} is the protium inflow rate from impurity source j.

When taking into account this impurity uptake of plasma Q ions and assuming that all the D and T ions in the plasma are exhausted as DT molecules and H ions as H₂ molecules, the torus exhaust flow rates for each hydrogen isotope compound, F_{torus, out, DT} and F_{torus, out, H₂}, are:

$$F_{torus, out, DT} = F_{torus, in, DT} - F_{burn} - \left[1 - \left(\frac{H}{Q}\right)_{plasma}\right] \sum_{imp\ source\ j} \sum_{k=1}^{#\ of\ imp} q_k F_{j, k} \quad (7)$$

$$F_{torus, out, H_2} = \sum_{all\ sources} F_{torus, in, H, j} - \left[\frac{1}{2} \left(\frac{H}{Q}\right)_{plasma}\right] \sum_{imp\ source\ j} \sum_{k=1}^{#\ of\ imp} q_k F_{j, k} \quad (8)$$

F_{j,k} is the kth impurity flow rate being released into the torus chamber from source j and q_k is the number of Q atoms contained in the kth impurity compound.

Finally, the He and kth impurity torus exhaust flow rates, F_{torus, out, He} and F_{torus, out, k}, can be approximated by:

$$F_{torus, out, He} = J_{\alpha} + F_{nuc1, He} + F_{outgas, He} \quad (9)$$

$$F_{torus, out, k} = \gamma_k F_{j, k} \quad (10)$$

F_{nuc1, He} is the D-D and D-³He reaction production of He, F_{outgas, He} is the "outgassing" rate (particularly from the coolant if He is used), and γ_k is the volatility factor of the kth impurity species which is defined as follows:

$$\gamma_k = \begin{cases} 0 & \Rightarrow \text{non-volatile} \\ > 0 \text{ and } < 1 & \Rightarrow \text{partly volatile} \\ 1 & \Rightarrow \text{completely volatile} \end{cases} \quad (11)$$

It is assumed that non-volatile species are not pumped out of the torus but are redeposited back to the surfaces. The above flow rate equations are for the steady state case. However, these equations are equally valid for pulsing operation where the burn and dwell times are much greater than the rampup and pumpdown times.

IV. SIMPLIFIED MODEL OF IMPURITY SOURCES

A. NET EROSION

For use with TRUFFLES, the average net erosion rate with appropriate deviation values can be given as input parameters for each surface material or it can be obtained from corresponding sputtering yields. The various molecular species which are subsequently created are generalized as average mole fractions from the total eroded amount. Typical compositions of the resulting sputtered molecular species can be gathered from experimental data to be used in this model. Table 1 defines 2 plasma-facing-material designs and their net erosion characteristics for use in the analysis. The volatility factor is assumed to be 1 for all given volatile species. No bulk impurity was assumed for both C and Be in this initial study. An erosion estimate from characteristic sputtering yields of the material has also been included in the model and can be used if necessary.

Plasma Facing Component Material #1	Be
Area [m ²]	1000
Net Erosion Rate [mm/year]	0.3
<u>Volatile Impurities Created</u>	<u>Erosion Mole Fraction</u>
none	n/a
Plasma Facing Component Material #2	C
Area [m ²]	1000
Net Erosion Rate [mm/year]	0.3
<u>Volatile Impurities Created</u>	<u>Erosion Mole Fraction</u>
CQ ₄	0.8
C ₂ Q ₆	0.2

Table 1: Vacuum Vessel Material Physical Characteristics for 2 Different Surface Materials

B. TORUS "OUTGASSING" DURING NORMAL REACTOR OPERATION

The "outgassing" of various molecular gaseous species from various sources will contribute a large percentage of exhausted impurities and will thus significantly affect the torus exhaust impurity composition. For simplicity, the value of the "outgassing" rate for several expected volatile impurities are provided as input in Table 2 along with the estimated outgassing area of the torus surface. These values are calculated from the expected production of about a 1% H₂O exhaust with the assumptions from Section III.

"Outgassing" Species	"Outgassing" Value [torr lit / cm ² sec]			
	Ave	Dev	Min	Max
H ₂ O	10 ⁻⁸	50 %	10 ⁻⁸	10 ⁻⁷
O ₂	10 ⁻⁸	50 %	10 ⁻⁹	10 ⁻⁶
N ₂	10 ⁻⁸	50 %	10 ⁻⁹	10 ⁻⁶
NH ₃	10 ⁻⁸	50 %	10 ⁻⁹	10 ⁻⁶
CO ₂	10 ⁻⁸	50 %	10 ⁻⁹	10 ⁻⁷
CO	10 ⁻⁸	50 %	10 ⁻⁹	10 ⁻⁶
Total Outgassing Area	10000 [m²]			

Table 2: Reference "Outgassing" Species

C. PLASMA DISRUPTIONS

For our modeling needs, the impurity contribution from plasma disruptions can be assumed to be negligible because of 2 reasons. The disruption frequency is very low and if a disruption occurs, then

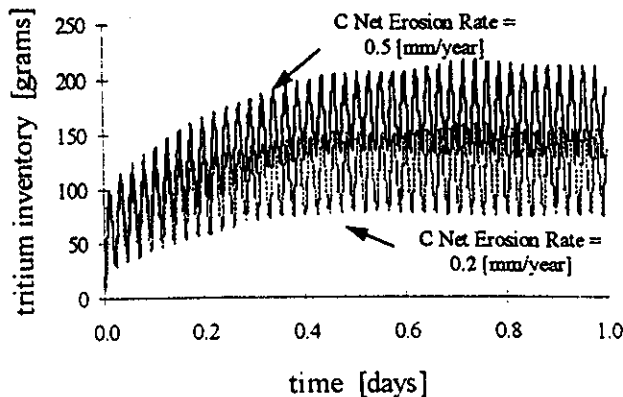


Figure 1: Dynamic Cryopumps Tritium Inventories for 2 Different Graphite (Carbon) Net Erosion Rates

maintenance and shutdown of the reactor is likely to follow.

V. SIMULATION AND ANALYSIS

The various tritium reprocessing components must be able to handle the impurity load originating from the torus and any changes in its composition. However, the only fuel cycle components affected by these changes are limited to the tritium components upstream of the impurity processing unit.

A. EFFECTS FROM NET EROSION RATE

Changes in the average net erosion rate of C and their effect on the cryopumps tritium inventory is examined on Figure 2 where a pulsing scenario was simulated. An increase in the net erosion rate from 0.2 [mm/year] to 0.5 [mm/year] results in an increase in

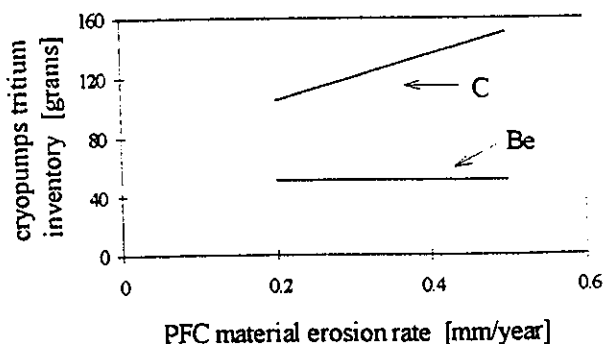


Figure 2: Average Cryopumps Tritium Inventory vs. Net Erosion Rate

the inventory of about 50%. The dynamics however remain similar in behavior. Figure 2 plots the averaged cryopumps tritium inventory against the net erosion rate of C and Be, the 2 leading plasma facing components. Gaseous "outgassing" as given in Table 2 is included in the calculation. Because Be is eroded as a non-volatile component, it will not be exhausted and thus will not have an effect on tritium reprocessing systems. However, Be sputtering and redeposition may hold a large quantity of tritium trapped on the first wall. Nevertheless, during power operation, Be is a more appropriate material to use because of its non-effect on the tritium reprocessing systems. On the other hand, if C is used and the maximum allowable tritium inventory requirement inside the cryopumps is limited to 100 [grams], then the design of the plasma facing components must be able to limit the net erosion to less than about 0.17 [mm/year] if the average "outgassing" rates are as given in Table 2.

Figure 3 illustrates the dynamics of the impurity processing waste stream to the TWT (Tritium Waste Treatment) when the permeator and PMR (Palladium Membrane Reactor) efficiencies are 99.9 %.⁸ The dynamics of this effluent flow rate are characterized by pulses which range up to ~400 [Ci/day]. These pulses are caused by a variety of factors, mainly pulsing, the cryopumps stagger operation, and the batch operation of buffer tanks. The average tritium flow rate to the TWT for this case is about 51 [Ci/day].

It is found that this tritium outflow rate does not significantly change with corresponding changes in the C net erosion rate, though it is expected that the change in CQ₄ impurity production will effect a

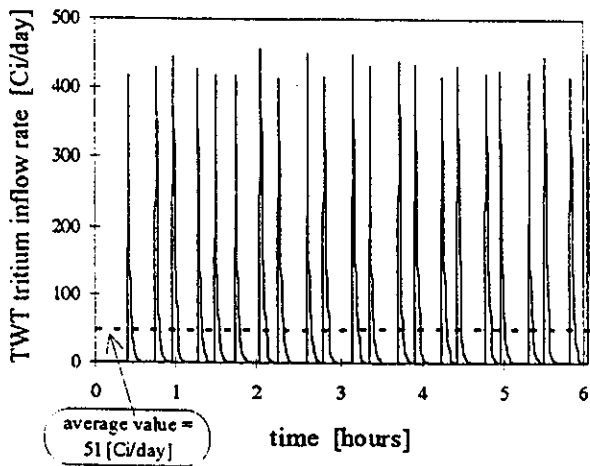


Figure 3: Dynamic TWT Tritium Inflow Rate from Impurity Processing

change in the impurity processing tritium effluent value. The reason for this near-constant behavior is due to the fact that the tritium outflow rate in the form of Q₂ species changes in an opposite direction to the increase or decrease of CQ₄ impurity, thus balancing it.

B. TORUS "OUTGASSING" EFFECTS

The "outgassing" rate as defined previously in Section III.D is also a contributing factor on the impurity composition of the torus exhaust. However, this "outgassing" rate will actually have a greater impact on the ISS design rather than the other tritium reprocessing units mentioned so far (i.e. the cryopumps and fuel cleanup unit). Figure 4 illustrates the effects of varying the average "outgassing" rate for H₂O.

As can be seen from the figure, values of this "outgassing" rate higher than ~7x10⁻⁸ [torr lit/cm² sec] will produce H₂ impurities higher than 1 % of the torus exhaust flow. Since H₂ impurities are very difficult to separate from other Q₂ species, this H₂O "outgassing" (i.e. from a physical perspective, the cleanliness of the vacuum vessel material, moisture content, and seal inleakage tightness) is expected to impact fuel cycle design more strongly than net erosion rates of surface materials.

C. EFFECTS FROM IMPURITY CONTROL STRUCTURE MATERIAL

Finally, the impurity control structure (i.e. divertor/limiter) is expected to affect the fuel cycle reprocessing systems through impurity control structure performance parameters rather than through erosion or "outgassing" through its material. Although

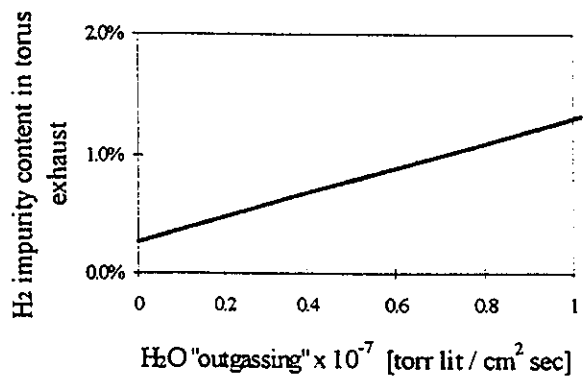


Figure 4: Torus Exhaust H₂ Impurity vs. H₂O "Outgassing" Rate

size considerations are part of the reason, plasma and fusion burnup considerations will control its impact.

The DT reflection coefficient is considered the primary material surface parameter affecting plasma-divertor/limiter interactions and is thus investigated and analyzed using TRUFFLES. From Figure 5, it can be observed that both the ISS and cryopump inventories will vary in a wide range of inventory values when R_{DT} is varied from 0.4 to 0.9. Furthermore, the ISS tritium inventory will be impacted more strongly by changes in R_{DT} due to its greater effect on the Q_2 exhaust rate than impurity exhaust rates.

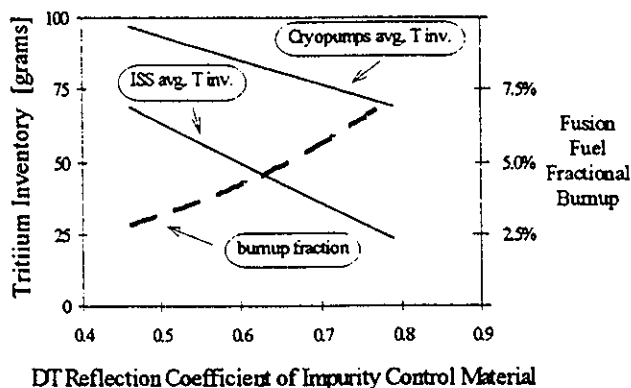


Figure 5: Effect of DT Reflection Coefficient on Various Tritium Reprocessing Tritium Inventories

SUMMARY

Dynamic fuel cycle tritium inventories and tritium losses as a result of torus impurity production parameters were investigated. It was found that for C, a design constraint limiting its allowable net erosion may be required if the cryopumps allowable tritium inventory is set at a low value (e.g. a 0.17 [mm/year] constraint for an allowable cryopumps tritium inventory of 100 [g]). On the other hand, although Be produces no volatile species when eroded, the quantity of tritium trapped during redeposition of Be may impact tritium reprocessing systems during torus conditioning. Also, no bulk impurity effects were included. Further investigation is needed in these 2 areas.

For the "outgassing" problem, which will be affected by all material inside the vacuum vessel, it was found that this presents a potentially more

complex and difficult problem because of its H_2 impurity source affecting ISS design. If the torus exhaust H_2 impurity concentration needs to be lower than 1 %, then the H_2O "outgassing" needs to be mitigated, since H_2O is expected to be a primary H_2 source. Finally, impurity control performance parameters, especially the DT reflection coefficient, are expected to dominate the divertor/limiter material effects on tritium reprocessing systems. Therefore, tritium fuel cycle considerations should play a role in the selection of plasma-facing component materials.

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