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Modeling of Tritium Transport in a Pin-Type Solid Breeder Blanket

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I. INTRODUCTION

This study supplements a larger study of a solid breeder blanket design featuring lithium ceramic pins. This aspect of the study looks at tritium transport, release, and inventory within this blanket design. Li_2O and $\gamma\text{-LiAlO}_2$ are the two primary candidates for ceramic solid breeders. $\gamma\text{-LiAlO}_2$ was chosen for this blanket design due to its higher structural stability. Analysis of tritium behavior in solid breeder blankets is of great importance due to its impact on several critical issues: the generation of an adequate amount of fusion fuel, the safety-related issue of keeping radioactive blanket inventories as low as possible, and the release, purge, and economical processing of the bred tritium without undue contamination of the coolant and other reactor structures.

Tritium inventory is related to both transport (diffusive) and solubility (thermodynamic) properties (1). Tritium recovery is achieved by passing helium through the purge channels and porosity of the ceramic to sweep out the tritium. Tritium diffusion plays a major role in determining tritium inventory: the slower the diffusion, the longer the residence time within the blanket, and the greater the diffusive inventory. This phenomenon is very temperature sensitive, with the diffusion coefficient generally varying as:

$$D = D_0 \exp (-Q/RT) \quad (1)$$

where Q is the activation energy for diffusion in kcal/mol, R is the ideal gas constant equal to 1.987×10^{-3} kcal/mol/°K, D_0 is a pre-exponential factor, and T is in units of degrees Kelvin. Both D and D_0 are in units of cm^2/sec . Experimental determination of diffusion coefficients is very important in estimating blanket inventories. Experiments on both Li_2O and LiAlO_2 show wide variations in the experimental coefficients, likely due to both variations in experimental conditions and in the grain sizes used in each experiment. Figure 1 shows this situation for Li_2O .

For Li_2O , the recent BCSS and FINESSE studies (2,3) have used the diffusion coefficient obtained by Guggi *et al.* (4) because of the well characterized grain sizes used and the controlled experimental conditions:

$$\ln (D/\text{cm}^2\text{s}^{-1}) = -(5.93 \pm 0.48) - (19.52 \pm 1.01 \text{ kcal/mol}/RT) \quad (2)$$

measured between 850 and 1200°K.

LiAlO_2 shows even greater variation in experimental coefficients. Brünig, Guggi, and Ihle (5) determined a value of:

$$\ln (D/\text{cm}^2\text{s}^{-1}) = -5.78 - (19.3 \text{ kcal/mol}/RT) \quad (3)$$

between 878 and 1178°K. However, the TRIO-01 experiment (6) determined a value of:

$$\ln (D/\text{cm}^2\text{s}^{-1}) = (-13.7 \pm 1.8) - (35.8 \pm 3.9 \text{ kcal/mol}/RT) \quad (4)$$

Figure 1 : Temperature dependence of diffusion coefficients of tritium, oxygen, lithium, hydrogen, and deuterium in Li_2O .

which has been taken as the reference value in the BCSS and FINESSE reports. Choice of D can change the calculated tritium inventory by several orders of magnitude; this mandates an accurate characterization of the coefficient for the relevant blanket conditions.

The solubility effect is most significant for Li_2O , with increased tritium inventory from $\text{HTO}/\text{T}_2\text{O}$ dissolution and LiOT formation:

One experiment was reported (1) which measured the solubility of H_2O in Li_2O as a function of temperature from 973 to 1273°K to give an analytical expression for the concentration of dissolved LiOH :

$$\log (X_{\text{LiOH}}) = (0.427 + 1.700 \times 10^{-4} T) \log (P_{\text{H}_2\text{O}}) + (-17.667 + 2.502 \times 10^{-2} T - 9.62 \times 10^{-6} T^2) \quad (6)$$

where X_{LiOH} is the mole fraction of LiOH , $P_{\text{H}_2\text{O}}$ is the gas phase partial pressure of H_2O in atmospheres, and the temperature is in degrees Kelvin. The chemical properties of hydrogen and tritium are virtually identical.

Above a threshold pressure of H_2O a separate LiOH/T phase will form, tying up tritium in a stable form difficult to remove from the bulk of the Li_2O ceramic. Experimental values for this critical pressure were determined in the range of 573 to 894°K (7):

$$\begin{aligned} \log P_{\text{H}_2\text{O}} &= -6718/T + 6.45, & T < 723^\circ\text{K} \\ \log P_{\text{H}_2\text{O}} &= -4406/T + 3.27, & T > 723^\circ\text{K} \end{aligned} \quad (7)$$

with 723°K the melting point of LiOH . These results are given in Figure 2. Higher temperature allows a higher critical partial pressure of H_2O before onset of LiOH/T phase formation, but it also increases the LiOH/T solubility (equation 6).

Experimental values of activity coefficient data indicate thermodynamic non-ideality for Li_2O (9). A positive deviation from ideality was determined indicating a lower LiOH solubility than for an ideal solution, a favorable result for decreased tritium inventory. The thermodynamic data used for ideal solution calculations was taken from the JANAF tables (10).

The greater LiOH solubility at higher temperatures and partial pressures of H_2O has another unfavorable result: greater LiOH vapor pressure outside the Li_2O ceramic causing lithium transport from the ceramic and the structural corrosion problems associated with LiOH .

2. PREVIOUS EFFORTS IN TRITIUM TRANSPORT MODELING

One of the earliest attempts to model tritium blanket inventory was the STARFIRE (11) reactor study. The model was relatively crude, using macroscopic variables in a percolation model to approximate T_2O partial pressures within the large pores, and using an assumed average partial

Fig. 2: Partial pressure of H_2O above the diphasic Li_2O (solid)- $LiOH$ (solid, liquid) system as a function of temperature

pressure of one torr in the $\text{LiAlO}_2/\text{Al}_2\text{O}_3$ equilibrium to obtain a very approximate value of 13 wppm tritium or 8.1 kg of blanket inventory at 1000°K and 1% lithium burn-up.

Far more refined models were devised for the BCSS and FINESSE studies to approximate blanket inventories. All models begin with the simple analytical solution of tritium diffusion in a spherical ceramic grain. By assuming zero tritium concentration at the grain boundary, a simple equation can be established for the inventory within the grain:

$$I_g = \tau \dot{g} V_g \quad (8)$$

with the mean residence time within the grain given by:

$$\tau = r_g^2 / 15D \quad (9)$$

D is the previously defined diffusion coefficient, r_g the grain radius, $\dot{g}$ the tritium generation rate in grams/sec/cm³, and V_g the grain volume. After applying various summations and correction factors for the temperature and/or generation profiles over unit cells and the blanket as a whole (described below), a value is obtained for the tritium diffusive inventory (I_d) throughout the blanket. Additional inventory can be associated with tritium solubility within the ceramic (I_s), adsorption of tritium on the surfaces of the grains and the larger pellets (I_a), tritium diffusing through the grain boundaries (I_g), and tritium passing out through the purge gas within the porosity/percolation/purge stream convection (I_p). The entire inventory within the breeder can then be represented by:

$$I_b = I_d + I_s + I_a + I_g + I_p \quad (10)$$

These interrelated physical phenomena can be visualized using the schematic in Figure 3. If the entire inventory throughout the blanket is considered, then contributions due to contamination of the coolant (I_c) and the metal structure from permeation (I_m) can be added:

$$I_{\text{total}} = I_b + I_c + I_m \quad (11)$$

Models have been devised to approximate all inventory contributions within the breeder except for grain boundary diffusion. Each model has assumed that, analogous to diffusion within metals, the transport of tritium within the grain boundaries is so rapid relative to the bulk diffusion rates that it could be neglected as a significant contribution to total blanket inventory.

From the basic equation for diffusive inventories within a sphere, an equation can be established to represent the diffusive inventory within a characteristic unit cell of the blanket:

$$I_{\text{cell}} = \int_{V_{\text{cell}}} \tau \dot{g} (1 - \epsilon) dV \quad (12)$$

with ϵ the fraction of porosity within the breeder. The diffusive inventory is calculated by summing over all unit cells.

For plate-type solid breeders, with the length of the plate and the

Figure 3: Schematic of Tritium Inventory Phenomena

coolant path positioned radially from the plasma, the above equation is converted to:

$$(I_d)_{\text{plate}} = \dot{G}_p \int_{-1/2}^{1/2} h(\xi) \left[\int_0^1 \tau(\eta, \xi) d\eta \right] d\xi \quad (13)$$

with $\dot{G}_p$ the total generation rate for the plate in grams/sec, ξ the normalized position along the coolant path, $h(\xi) = \dot{g}(\xi)/\bar{g}$ the normalized tritium production rate along the ξ direction, η the normalized position along the thickness of the plate, and τ defined by equations 1 and 9 but with $T = T(\xi, \eta)$. The only published results from this model (12) used the simplifying assumption of both blanket heating rate and tritium generation rate varying with the same exponential dependence along the coolant path, i.e.:

$$\dot{g}(\xi) = \dot{g}_{\text{max}} \exp [-\alpha(\xi + 1/2)] \quad (14)$$

Different values of α were then used for purposes of comparison. For detailed calculations, this study found equation 14 to be not applicable over the entire blanket. The results of a preliminary neutronics calculation were plotted in Figures 4 through 7 to test this approximation. Although the exponential dependence with radial position is true on average, the greater neutron populations just beyond the beryllium zone and reflected by the shield cause significant deviation from the exponential approximation.

Models of cylindrical unit cells employ the simpler equation:

$$(I_d)_{\text{cyl}} = f \dot{G}_{\text{cyl}} r_g^2 / 15D(\bar{T}) \quad (15)$$

where

$$f = (\beta - 1)^{-1} \int_1^\beta \exp [(Q/RT)(\bar{T}/T - 1)] d\eta \quad (16)$$

with $\beta = r_o^2/r_i^2$ and $\eta = r^2/r_i^2$ for r_i the unit cell inner radius, r_o the unit cell outer radius, and r and T the local position and temperature at any point between r_i and r_o . This equation requires evaluation of the diffusion coefficient at only one value, the volume-averaged temperature $\bar{T}$, for each unit cell. Equations can be used for T and $\bar{T}$, given T_{max} and T_{min} , or actual values can be used for a known or given temperature profile.

For the solubility inventory, BCSS (13) first makes a calculation for an assumed situation for Li_2O to make a qualitative comparison with I_d ; the result was a solubility inventory of about ten times the diffusive. A more realistic evaluation was then employed by BCSS (14) using temperature profiles over a blanket-averaged breeder pellet and calculated pressure and concentration distributions of T_2O within the breeder pores to obtain a solubility inventory about 3300 times that of the diffusive inventory for a Li_2O blanket.

Estimates of low to negligible tritium solubility inventories for LiAlO_2 were thermodynamically evaluated or assumed by several studies: STARFIRE, the GA Technologies Inc. model in BCSS (14), and the TRIO experiment.

Inventory based on surface adsorption is a big question due to limited

Figure 4

VOLUMETRIC HEATING, FIRST ZONE

Figure 5

VOLUMETRIC HEATING FOR ZONE 2

Figure 6

TRITIUM GENERATION RATE, FIRST ZONE

Figure 7

TRITIUM GENERATION RATE, SECOND ZONE

experimental data and problems of interpretation of results. The only experiment attempting to interpret surface effects is the TRIO experiment. Thirty-three irradiation runs of γ -LiAlO₂ pellets were made under varying conditions. Those runs with 0.1% hydrogen in the helium purge gas were interpreted to exhibit bulk diffusion as the rate-limiting step; tritium release was assumed to be uninhibited by surface adsorption, and the surface inventory was assumed to be negligible. Any changes in tritium release due to alteration of purge stream composition was attributed to surface effects and a non-negligible surface inventory. The conclusions drawn were $I_a = 3 \pm 2$ wppm for LiAlO₂ blankets with pure helium purge and $I_a = 0$ for 0.1% H₂ within the purge gas. Both BCSS and FINESSE assumed 0.1% H₂ in the purge gas and used the $I_a = 0$ assumption in modeling LiAlO₂ blankets.

The inventory attributed to porosity/percolation/purge stream transport can be approximated by applying mass balance and ideal gas law considerations to an equation from BCSS (15):

$$P_A = (P_A)_i + \frac{(1/\epsilon - 1) R \bar{T} \dot{g}_A r_i^2 f(\beta)}{4 W_A D_e(\bar{T})} \quad (17)$$

where A is the tritium species, $(P_A)_i$ the partial pressure of A in the purge stream, ϵ the interconnected (as opposed to closed) porosity fraction, $\bar{T}$ the average temperature within the porosity, $\dot{g}_A$ the generation rate of A per unit of 100% dense ceramic volume, W_A the molecular weight of A, $f(\beta) = \ln \beta - \beta + 1$ for maximum P_A or $f(\beta) = (1 - \beta^{-1})^{-1} \ln \beta - 1$ for average P_A , and all else defined as before. These equations assume a cylindrical unit cell with the purge tube located next to the central coolant tube. The ratio of the mean free path for molecular collisions to the average pore radius λ/r_p determines what equation to use for the calculation of $D_e(\bar{T})$. Different values of $D_e(\bar{T})$ are obtained if the transport of the tritium species within the porosity is dominated by Knudsen diffusion, ordinary molecular diffusion, or some intermediate regime. FINESSE (16) reports an error of $\pm 20\%$ with this model and its assumption of an isothermal unit cell, and calculates a typical rise in tritium partial pressure across a unit cell of less than one pascal.

The GA Technologies model of tritium inventories for the BCSS helium-cooled blanket design is the only one to approximate porous inventories in a blanket design. For all BCSS blanket designs, a value of 0.04 g tritium within the porosity was calculated. This GA model, based on the TRIT4 computer code, is the most comprehensive to date in attempting to simultaneously model the diffusive, solubility, and porous contributions to tritium inventory. However, it still suffers from the weaknesses of the assumptions it employs, and the limited experimental basis upon which those assumptions were made. The assumptions of both the GA and other models which require greater scrutiny are discussed below.

No model has yet been compared to a numerical analysis of inventory over the blanket based on calculated temperature and tritium generation profiles. The only model using radial temperature and generation profiles assumed idealized exponential spatial dependencies identical for both profiles, and then analyzed the results for three different examples of exponential decrease. All other models simply applied average volumetric heating and generation rates to a blanket-averaged unit cell, and scaled up to an

approximate tritium inventory. The overall accuracy of this approach has not been evaluated.

All models are based on experimental diffusion coefficients which vary significantly from one experiment to another. This uncertainty is especially true for LiAlO_2 . For example, the Brüning *et al.* values (5) would substantially reduce the calculated diffusive inventory and remove perhaps the greatest argument against the use of LiAlO_2 with respect to Li_2O .

Only one transport mode has been considered significant in any of the models, that of bulk diffusion and release. All models assume the surface inventory and grain boundary effects to be negligible, and only limited attempts have been made to investigate their roles. A real question remains over the relevance of surface effects. As mentioned previously, surface effects and inventories were assumed significant for LiAlO_2 in a pure helium purge stream in the TRIO experiment.

The simplest possible boundary condition has been used in all models, i.e. zero concentration of all tritium species on the spherical grain surfaces. Any non-zero boundary value assumptions would alter the analytical solutions for the diffusive inventories.

Solubility effects are poorly modeled at present. The GA model made solubility calculations for Li_2O , but it appears an average T_2O partial pressure within the porosity was calculated using equation 17, and the thermodynamic equilibrium equations for LiOH solubility were employed for an overall solubility inventory. Lack of background for the TRIT4 calculations precludes detailed analysis. A model more detailed than average equilibrium calculations may be in order.

Effects due to chemical reactions, particularly oxidation and reduction effects within the breeder and purge stream, are very poorly understood. The large majority of experiments prior to TRIO found T_2O to be the predominant tritium species released from the breeder. However, TRIO determined 94% of the release to be in the form of HT and T_2 . The mass of the released species may affect the calculations for I_p (although this is insignificant compared to $I_d + I_s$ values), but more important are the problems of tritium permeation through the metal structures and coolant which are far more severe for HT and T_2 than for HTO or T_2O . Any oxidation effects within the breeder itself could have profound effects on tritium inventory and release, as TRIO discovered when 0.2% O_2 was added to the purge stream and release kinetics were disturbed well after the purge was returned to the H_2/He combination. Experimental evidence (17) of globular elemental lithium, a potent reducing agent, has been found after irradiation. Some thermodynamic calculations indicate preferential release of HT or HTO under different oxygen activity regimes (18). None of these effects has been incorporated into a comprehensive model of tritium inventory.

A major weakness of all inventory calculations is the total lack of any radiation effects models. No firm conclusion of radiation effects can be drawn from the experiments (6,19), most of which were based on small lithium burn-ups relative to blanket lifetimes. Significant radiation trapping and detrapping would have profound effects on tritium release calculations.

No significant modeling of the change of ceramic properties over time has been done, e.g. grain growth, pore closure due to sintering, possible formation of release pathways by internal gas generation, restructuring of the solid and pores over time (as with uranium oxide fuels), effects this restructuring will have on thermal conductivity, temperature, and diffusive profiles, and the effects extended lithium burn-up will have on tritium generation and inventory profiles across the blanket. The discussion of the GA model mentions the use of reduced thermal conductivities for Li_2O and LiAlO_2 under high neutron fluence, but no discussion is made of any time-dependent effects.

Additional modeling is also needed for change of inventory and release profiles under start-up, shutdown, and non-continuous operation. Little work has been done in this area: limited modeling of a few TRIO transients and some calculations of tritium release and inventory fractions over time for one of the BCSs LiAlO_2 blankets.

3. MODELING OF TRITIUM TRANSPORT FOR THE CURRENT BLANKET DESIGN

Blanket tritium release and inventory for this pin-type solid breeder design is based on the DIFFUSE code developed by M. Baskes (20,21). This code provides numerical solutions of the diffusion equation for one or two diffusing species in up to five different materials. Although primarily designed to study hydrogen permeation effects in metals, it can also model tritium generation, inventory, and release in solid breeders by a convenient choice of input parameters.

DIFFUSE calculates the one dimensional diffusion of atoms within a material of specified properties for a variety of initial, source, and boundary conditions. The diffusive equations used are given by Fick's laws:

$$J_j(x,t) = -D_j(T(x,t)) \left[\nabla c_j(x,t) + \frac{c_j(x,t)Q^*}{kT(x,t)^2} \nabla T(x,t) \right] \quad (18)$$

and

$$\partial c_j(x,t)/\partial t = -\nabla J_j(x,t) + G_j(x) - \sum_i \partial c_T^{ij}(x,t)/\partial t \quad (19)$$

where $c_j(x,t)$ is the concentration of the j^{th} diffusing species, $c_T^{ij}(x,t)$ represents the concentration of the j^{th} species in the i^{th} trap, Q^* is the heat of transport, $G_j(x)$ is the implant (generation) source term for the j^{th} species, and all other terms have the standard meanings.

Solutions can be obtained for planar, spherical, and cylindrical geometries, where the spheres and cylinders can be hollow or solid. Trapping of the diffusing species can be modeled by DIFFUSE, a very convenient feature for modeling radiation trapping effects. For the i^{th} type of trap, the governing equations are:

$$\begin{aligned} \partial c_T^{ij}(x,t)/\partial t = & D_j(T(x,t)) c_j(x,t) G_T^i(x,t)/\lambda^2 \\ & - c_T^{ij}(x,t) \nu_o \exp[-(E_t^i + E_d)/kT(x,t)] \end{aligned} \quad (20)$$

and

$$C_{Te}^i(x,t) = C_{To}^i(x) - \sum_j f^i c_{Tij}(x,t) \quad (21)$$

where $C_{Te}^i(x,t)$ is the effective concentration of the i^{th} trap, $C_{To}^i(x)$ is the actual concentration of the i^{th} trap, λ is the jump distance, ν_0 is the detrapping attempt frequency, E_T^i is the i^{th} trap energy, E_d is the activation energy for diffusion, and f^i is the inverse trap saturability for the i^{th} trap.

Tritium decay to helium can also be modeled as a trap:

$$\partial c_{T1}(x,t)/\partial t = -\gamma c_1(x,t) \quad (22)$$

with γ the tritium decay constant and the resultant helium considered to be the first trap for diffusing tritium.

The source of the diffusing species can be modeled as an implantation, a diatomic gas permeation of surfaces, or an initial concentration. Two traps and/or two implantation profiles are allowed simultaneously. By using both the implantation and initial concentration provisions, homogeneous steady-state tritium generation can be modeled within the material. The initial conditions for diffusing and trapped species are given by:

$$c_j(x,0) = c_{j,0}(x) \quad (23)$$

$$\text{and } c_{Tij}(x,0) = c_{Toij}(x) \quad (24)$$

Five types of boundary conditions are available in DIFFUSE:

(1) a perfectly reflecting boundary:

$$J_j(x_s, t) = 0, \quad (25)$$

(2) zero concentration at the boundary:

$$c_j(x_s, t) = 0, \quad (26)$$

(3) Sievert's law which models bulk solubility due to gas pressure at the surface:

$$c_j(x_s, t) = S[T(x_s, t), P(t)] X_j(t), \quad (27)$$

with $S(T,P)$ the solubility, $P(t)$ the total pressure, and $X_j(t)$ the mole fraction of the j^{th} species in the gas phase;

(4) recombination of single atoms into a diatomic molecule at the surface prior to release:

$$J_j(x_s, t) = \sum_{j'} K_{jj'} [T(x_s, t)] [c_j(x_s, t) c_{j'}(x_s, t) - X_j(t) X_{j'}(t) S[T(x_s, t), P(t)]^2] \quad (28)$$

where

$$K_{jj'}(T) = \frac{4 \alpha c_1 \exp [(2E_s - E_x)/kT]}{\rho \sqrt{(M_j + M_{j'})} T^2 S_0^2} \quad (29)$$

$$\text{and } E_x = \text{MAX} (E_s + E_d, 0) \quad (30)$$

with $K_{jj}(T)$ is the recombination constant for the j^{th} and j^{th} species, α is a sticking coefficient, c_1 is a kinetic theory constant, E_s is the heat of solution, E_x is the surface barrier energy, ρ is the matrix density, and M_j is the mass of species j ;

(5) a simple interface between two materials which mandates continuity of flux and chemical potential of the diffusing species:

$$J_j(x_i^-, t) = J_j(x_i^+, t) \quad (31)$$

$$\text{and } \frac{c_j(x_i^-, t)}{S^-(T(x_i, t), P)} = \frac{c_j(x_i^+, t)}{S^+(T(x_i, t), P)} \quad (32)$$

Both diffusivity and solubility of the material are assumed to exhibit Arrhenius behavior, i.e.

$$D_j(T) = D_0 M_j^{-1/2} \exp(-E_d/kT) \quad (33)$$

$$\text{and } S(T, P) = S_0 P^{1/2} \exp(-E_s/kT) \quad (34)$$

with D_0 and S_0 the pre-exponential terms.

Additional features of DIFFUSE are provisions for different temperatures at each interface (and thus a linear temperature profile across each material), different partial pressures of the diffusing gas at the outer surfaces, and linear heating ramps at the interfaces and surfaces and linear pressure ramps at the surfaces.

The value of applying DIFFUSE to blanket tritium phenomena is its ability to analyze a variety of geometries, boundary conditions, and material parameters under different blanket conditions. This versatility gives both consistency in modeling and a convenient tool to approximate blanket inventories with a minimum of analytical modeling. DIFFUSE can approximate both experimental results and the inventory values of some BCSS and FINESSE models. Good agreement between DIFFUSE and the other models would encourage use of DIFFUSE for calculations of blanket inventory and release. The provisions for surface effects (recombination and solubility), trapping, and a variety of material and boundary conditions in DIFFUSE permit relatively straightforward analysis of these effects, unlike the analytical models presently employed which require a piecemeal approach to model each individual phenomenon.

Another significant advantage of DIFFUSE is the use of results from one time/temperature/generation step as the input to a new step using different input parameters. This feature makes DIFFUSE ideal for analyzing transient behavior in a straightforward and self-consistent manner, e.g. for the analysis of reactor start-up and shutdown effects on tritium behavior. The provision for temperature and pressure ramps over time is another major aid in transient modeling.

4. COMPARISON OF DIFFUSE RESULTS TO OTHER MODELS

Only limited numerical results are available in BCSS and FINESSE for given input parameters with which DIFFUSE outputs can be compared. Two analyses are given in FINESSE (22) directly amenable to DIFFUSE analysis. The first is an analysis of a Li_2O plate design, for input parameters of 10 micron grain radius, tritium generation rate of 1.85×10^{-5} wppm/s, 510°C minimum and 795°C maximum temperature, and the diffusion coefficient given by equation (2). FINESSE applied a value $\alpha = 0$ to equation (14) and converted equation (13) to the form:

$$I_d = [r_g^2 \dot{G} / 15 D_0] f \exp (Q/RT) \quad (35)$$

where

$$f = \int_0^1 \exp [(Q/RT)(T/T - 1)] d\xi \quad (36)$$

For $\alpha = 0$, both temperature and generation profiles are constant across the blanket, making the above equations amenable to a DIFFUSE analysis of a characteristic Li_2O grain for the given parameters.

The above equations were converted to the form:

$$I_d = \frac{r_g^2 \dot{G}}{15 D_0 \exp (-Q/RT)} \exp (-Q/RT) \int_0^1 \exp (Q/RT) d\xi \quad (37)$$

$$\text{for } T = T_{\min} + (T_{\max} - T_{\min})(1 - \xi^2) \quad (38)$$

Note that the first term on the right hand side of equation (37) is identical to the spherical grain model of equations (8) and (9). This term should correspond to the DIFFUSE output, and the following two terms can be evaluated numerically. The average temperature was calculated to be 700°C . FINESSE reported a result of 2.09×10^{-5} wppm inventory. The DIFFUSE-based evaluation gave an inventory of 2.05×10^{-5} wppm, differing 1.9% from the FINESSE value.

FINESSE also evaluated a LiAlO_2 plate using the same equations, a diffusion coefficient given by equation (14), and input values of 0.1 micron grain radius, a generation rate of 2.41×10^{-5} wppm/s, and 520°C minimum and 1000°C maximum temperatures. The average temperature was calculated to be 840°C . FINESSE reported a value of 0.0460 wppm inventory. The DIFFUSE-based result gave a value of 0.0440 wppm, a difference of 4.3% from FINESSE.

As another comparison, the same input values for Li_2O and LiAlO_2 were applied to the spherical grain model of equations (8) and (9). The DIFFUSE inventory results for a single grain were compared directly to calculated values obtained using:

$$I_d = r_g^2 \dot{G} / [15 D_0 \exp (-Q/RT)] \quad (39)$$

For Li_2O , equation (39) gave an inventory of 1.13×10^{-5} wppm while DIFFUSE gave an inventory of 1.11×10^{-5} wppm, a difference of only 1.8%. For LiAlO_2 , equation (39) gave a value of 1.58×10^{-3} wppm and DIFFUSE gave a result of

1.51×10^{-3} , a difference of 4.4%.

For all comparisons, DIFFUSE results agreed with the models well within 5%. These results are very compatible and support the conclusion that the DIFFUSE code can be used to provide valid results for diffusive tritium inventories within spherical grains comparable to those of other commonly used models.

5. STEADY-STATE TRITIUM INVENTORY

Having verified the DIFFUSE results to be comparable to other models, the code was then used to explore the effects of several of the relevant parameters on diffusive inventory. Having chosen LiAlO_2 as the candidate solid breeder, grains of this material were modeled using the diffusion coefficient obtained from TRIO and the arbitrary tritium generation rate of 2.41×10^{-5} wppm/s.

The effects of temperature and grain size on diffusive inventory were analyzed. The results are shown in Figures 8 and 9. The temperature range relevant to this blanket design, approximately 800 to 1400 °K, was used in these figures. Figure 8 indicates substantial inventory build-up as the temperature decreases below 800°K, encouraging design of higher temperature blankets. Figure 9 shows a rapid increase in inventory as the grain sizes become larger; this figure supports the BCS choice of 0.1 micron grain radii, the same size as chosen for this blanket design.

A parameter relevant to transient effects is the time to steady-state diffusive inventories as a function of temperature and grain size, shown in Figures 10 and 11. This steady-state condition represents a tritium release rate equal to the generation rate. For a 0.1 micron LiAlO_2 grain, Figure 10 shows time to steady-state varying from a few seconds at high temperatures to days at low temperatures. Figure 11 shows a similar increase in time to steady-state as the grain size increases.

In agreement with the results of early modeling efforts, the only component of ceramic tritium inventory used in this evaluation of steady-state inventory was the diffusive inventory within the grains. The other modes of transport, grain boundary diffusion, solubility and surface effects, and porosity/purge stream transport were all assumed negligible compared with the magnitude of the diffusive inventory. By considering only diffusive inventory within the grain, we can model the entire blanket inventory by a judicious choice of characteristic grains to represent different portions of each rod. By scaling up the steady-state inventories of these grains, we can obtain approximations for the entire blanket diffusive inventory.

To analyze the effect of diffusion coefficient on steady-state inventory, the two reported values for LiAlO_2 in equations (3) and (4) were used as input to DIFFUSE in modeling the diffusive inventory as a function of temperature for a typical grain. A major variation in results is obvious in Figure 12 across the entire temperature range, up to seven or eight orders of magnitude. Use of the larger diffusion coefficient reported by Brüning *et al.* would lead to insignificant inventories and remove one of the major advantages claimed

Figure 8

DIFFUSIVE INVENTORY IN LiAlO2 VS. TEMPERATURE

Figure 9

LiAlO₂ TRITIUM INVENTORY VS. GRAIN SIZE (1300 K)

Figure 10

LiAlO₂ TIME TO STEADY-STATE VS. TEMPERATURE

Figure 11

TC TIME TO STEADY-STATE VS. GRAIN SIZE (T=1300K)

Figure 12

EFFECT OF DIFFUSION COEFFICIENT ON INVENTORY

for Li_2O over LiAlO_2 as a tritium breeder. However, the TRIO value was obtained from an in-situ reactor experiment and may more accurately reflect actual operating conditions. For this reason, the TRIO value was chosen over the Brünig *et al.* value for modeling LiAlO_2 in BCSS, FINESSE, and in this study.

The input values for tritium generation rate were obtained from the results of neutronics analysis. The generation rate for each pin was taken to be its axial value in graphs of generation rate (in wppm/s) vs. distance into the module. Asymmetries in generation rate across the pin should largely average out from front to back. The largest error might come in the first row, where the generation profile is very steep. Previous thermal hydraulic analyses provided the average coolant temperature at each row of pins. Application of a standard heat transfer equation to the row by row volumetric heating rates gave the temperature profile within each pin. For steady-state conditions, the maximum central pin temperature approached 1150°C and the minimum outer temperature was slightly above 530°C . These relatively high temperatures played a major role in keeping total blanket inventory to a minimum.

Some question exists of the behavior of LiAlO_2 at the maximum temperatures, since this exceeds the 900°C experimental temperatures used in the detailed FUBR-1A experiments with LiAlO_2 (19). Concerns over grain growth at high temperature can be alleviated by extrapolation of FUBR results: no significant grain growth was observed over the range 500 to 900°C . Likewise, extrapolation of both FUBR results and thermodynamic calculations (18) indicate no significant ceramic vapor phase transport at high temperatures, unlike the case for Li_2O . Another concern might be the effect of high lithium burnup rates in the first row pins: all lithium-6 would likely be converted to tritium over the expected three year blanket lifetime. Although unexpected ceramic properties might become evident, no serious structural transformations can be foreseen. The final ceramic might be closer to Al_2O_3 in composition than to LiAlO_2 . If this severe burnup poses a problem, a lower percentage of lithium-6 enrichment for the first row would reduce both the burnup rate and the steep heat generation profile for this row, but at a cost of a greater parasitic neutron capture by the structural materials in this region of the module, and thus a lower overall tritium breeding ratio.

As mentioned before, the method of characteristic grains is used to model inventory within each rod. As a first approximation, the ceramic portion of each rod was divided into five concentric zones of equal width. Within each zone, the volumetrically-averaged position was determined and the temperature at that position calculated from the temperature profile across the pin. This temperature was used to represent a characteristic grain for each zone. DIFFUSE gave the diffusive steady-state inventory for each of these grains in wppm. This inventory was scaled up for the mass of each zone, and the inventories of the five zones added to give a total inventory for the pin. Knowing the number of pins per each row per module and the number of modules over the entire blanket, the total inventory for each row was determined and these values summed for the total blanket inventory. This method gave a total blanket inventory of 12.9 g.

Because diffusive inventory is heavily weighted toward the colder regions of the rods, the possibility of understating the inventory existed with this

method. As a better approximation, the outermost zone of each rod was divided into two smaller zones of equal thickness, a representative temperature for each zone determined as before, and the zonal inventories and total blanket inventory again extrapolated from the DIFFUSE results. This six-zone method resulted in a total blanket inventory of 13.3 g, only 3% greater than the 5-zone approximation.

To obtain a more precise determination of blanket inventory than these approximate methods could give, the governing analytical equations were manipulated into a form amenable to numerical analysis independent of DIFFUSE. Again, the spherical grain model of equation (39) was used as the basis. The average intragranular inventory within the pin can be calculated from:

$$\bar{I}_{gr} = \frac{\int_V I_d dV}{\int_V dV} \quad (40)$$

Using equation (39) to substitute for I_d and evaluating the volume integrals across the hollow cylinders, an equation amenable to numerical analysis was obtained:

$$\bar{I}_{gr} = \frac{2 r_o^2 \dot{G}}{15 D_o (r_o^2 - r_i^2)} \int_{r_i}^{r_o} \exp(Q/RT) r dr \quad (41)$$

After insertion of the temperature $T=T(r)$ obtained from the calculated profile across the ceramic pin, this equation provided the average grain inventories for each row of pins. A total blanket inventory of 13.2 g tritium was directly obtained from these results, independent of but in very good agreement with the DIFFUSE-based results. Figure 13 gives the total row-by-row inventories obtained with this numerical method, showing the predominance of inventory within the cooler small pins of rows 2 through 5. The inventories of rows 2 through 5 approach 0.6 wppm while rows 6 through 11 have less than 0.02 wppm and row 1 about 0.03 wppm tritium. If inventories are a major concern, this figure suggests tailoring the pin diameters in increasing size away from the plasma, to maintain consistently high ceramic temperatures for each row of pins.

The results of these three methods are plotted, row by row, in Figure 14. Significant agreement exists between all three methods, further supporting the validity of the DIFFUSE-based inventories. These results compare favorably with the GA model total of 38.3 g for a 522,000 kg $LiAlO_2$ blanket (14) vs. 129,000 kg for this blanket design. But the GA method (using the TRIT4 code) analyzes only one unit cell, with the uncertainties it implies for tritium diffusive inventories. The exact temperatures and other input parameters are never stated, preventing more detailed comparison.

Because of the large number of DIFFUSE runs needed to characterize the total inventory in the above methods (five to six runs per rod, eleven rows of rods over the blanket), a simpler approach was required to model each rod during transient and start-up/shutdown operations. Again, equation (39) was used as the starting point, but now an equation for an average temperature representative of the total pin inventory was desired:

Figure 13

TOTAL BLANKET INVENTORY, ROW BY ROW

Figure 14

$$I(\bar{T}) = \frac{r_g^2 \dot{G}}{15 D_o \exp(-Q/RT)} = \frac{\int_V I_d dV}{\int_V dV} \quad (42)$$

Manipulation of this equation gives:

$$\bar{T} = \frac{Q}{R \ln \left(\frac{2\xi}{r_o^2 - r_i^2} \right)} \quad (43)$$

where

$$\xi = \int_{r_i}^{r_o} \exp(Q/RT) r dr \quad (44)$$

Substitution of the pin temperature profile into equation (44) allows numerical evaluation of the diffusion-averaged temperature for each row of rods, and a DIFFUSE analysis was made at each of these temperatures for a single characteristic grain representative of an entire rod. The steady-state inventory for each grain was scaled up for the entire rod, then for each row, to give new values of total row-by-row blanket inventory. These results are also shown in Figure 14, and gave a total blanket inventory of 12.6 g. These results agree very well with the previous methods, with less than 5% variation from the results of the non-DIFFUSE numerical approximation method. Thus, reasonable inventory results can be obtained for an entire rod using only one DIFFUSE-analyzed characteristic grain at a temperature calculated from equation (43).

This result shows the single grain model to be ideal for transient analyses: by calculating the temperature profile for a rod under different power levels, an average temperature can be determined for each power level at which to analyze the characteristic grain with DIFFUSE. By assuming step changes in the power levels, the transient behavior of a rod can be simply modeled by a series of consecutive DIFFUSE runs for the same grain at different temperatures and generation rates, with the resultant diffusive concentration profile within the grain from one run used as an initial concentration profile for the next run. DIFFUSE is set up to perform exactly this kind of sequential analysis, thus making transient analyses very convenient.

6. TRANSIENT TRITIUM INVENTORY

Start-up

Reactor start-up was modeled for two different situations. The first considered helium coolant flow at 100% of full power status. The second considered significantly reduced helium flow during the transients to achieve higher operating temperatures and lower transient tritium inventories.

The transients modeled were at 10%, 20%, 50%, and 80% of full power, each lasting 3.5 days, followed by 100% power. The percentage of full power was

used to scale the volumetric heating rates for ceramic and cladding accordingly, and likewise for tritium generation rate. The rise in coolant temperature from module entrance (constant at 250°C) to each row of pins was taken as a corresponding percentage of the temperature rise at full power. The heat transfer coefficient from cladding to coolant was adjusted accordingly. These values were used to calculate the temperature profiles inside the pin for each row at each transient power level, and these results used to calculate a characteristic temperature for each rod during each transient, to use as DIFFUSE input as mentioned previously.

With each characteristic grain evaluated by DIFFUSE over several transients, the diffusive inventory can be obtained from the DIFFUSE output at any point during the two weeks prior to full power. After two weeks the input parameters were set at full power values, and the inventory soon returned to its steady-state values. Thus, after eleven DIFFUSE runs, each with several transients and each analyzing a characteristic grain for each row of pins, the results are scaled up for total blanket mass per row. The total transient inventories are obtained as a function of time for each row, and summed for the total blanket inventory.

The transient results involving 100% helium flow gave total blanket inventories of 226 g after 3.5 days at 10% power, 621 g after 3.5 days at 20% power, 429 g at 50% power, 61 g at 80%, and a short time at 100% returned the total inventory to the steady-state value of 12.6 g. These results are plotted in Figure 15, and the row by row results in Figures 16 and 17. The inventories are obviously much higher than steady-state during 10%, 20%, and 50% power levels, reaching several hundred grams with the biggest contribution from the first row and its dominant tritium generation rate. The characteristic temperatures ranged from 550 to 590°K at 10% power, 590 to 650°K at 20%, 680 to 830°K at 50%, 780 to 1010°K at 80%, and 840 to 1130°K at full power. The temperatures fall within the regime of very slow tritium diffusion for 10 to 50% power, leading to rapid build-up of the bred tritium within the pins.

These significant inventories could lead to safety-related concerns of large blanket inventory, especially for protracted start-up times at these temperatures. For this reason, the same start-up regime was re-analyzed under conditions of restricted helium flow, reducing the rate of cooling and allowing higher temperatures to be achieved within the ceramics. For the 10% and 20% power transients, the helium flow rate was set at 20% of that at full power. Thus, at 20% of full power the same coolant temperature should be obtained for each row as at 100% full power. Likewise, at 50% and 80% of full power the helium flow rate was set at 50% and 80% of full power, again giving the same coolant temperatures. For 10% of full power, with helium flow set at 20% the rise in temperature between blanket inlet and the row in question was taken to be one half that at full power. The volumetric heating rate and tritium generation rate were scaled down from full power according to the transient power level as mentioned previously. New temperature profiles across the pins were recalculated for each transient, characteristic temperatures evaluated for each transient at each row and the transient analyses rerun as before.

Due to considerably higher ceramic temperatures under these conditions of controlled coolant flow, the total blanket inventories were greatly reduced

Figure 15

TOTAL TRITIUM INVENTORY DURING STARTUP TRANSIENTS

Figure 16

Figure 17

INVENTORY AT END OF EACH TRANSIENT, ROWS 6 TO 11

from the uncontrolled flow transients. The results give total inventories of 153 g at 10% after 3.5 days, 40.2 g at 20%, 25.6 g at 50%, and 16.5 g at 80%. These results are also shown in Figure 15.

The results for these two cases clearly show the need for tailoring the helium flow rate to the transient power levels. An extended start-up could lead to massive inventories for uncontrolled conditions. Even with controlled flow, a gradual inventory build-up might be a concern for low power levels over an extended period of testing. In this case, supplemental pre-heating of the coolant would alleviate such concerns. Further study of the minimum practical helium flow rates is also warranted: the minimum of 20% of full power flow is a conservative estimate, to avoid problems with flow instabilities.

Shutdown

For shutdown, two different cases were analyzed: (1) coolant flow at 20% that for full power and (2) a combination of coolant flow reduction and heating such that the coolant temperature ranged from 470°C to 500°C across the pins. This second scenario can be thought of as "baking" the blanket to speed its purging of tritium inventory. Both scenarios assume afterheat volumetric generation of 1% that of full power and zero tritium generation.

For the first case, that of simply reducing the helium flow, the temperature of the coolant entering the blanket was again 250°C, and the temperature rise at each row of pins was taken to be 1/20 that of full power. These new coolant temperatures, 1% volumetric heating, and a corrected heat transfer coefficient were used to calculate new temperature profiles across the pins as before, and diffusion-averaged temperatures were again calculated for each pin. These temperatures were used as input to DIFFUSE along with zero generation rate as an additional step following the analysis for the three year run at 100% power. Thus, the characteristic grains start with their steady-state inventories, then instantaneous shutdown occurs at which no more tritium is generated but the steady-state concentration profiles within each grain are now subjected to the much lower temperatures at shut-down. As can be expected, tritium diffusion from the grains slows down drastically. The diffusive inventories are modeled for a year after shutdown, with total blanket inventory calculated as before.

Figure 18 shows that, after two weeks, the total inventory is reduced from the steady-state full-power inventory of 12.6 g to 12.4 g, only a 1.6% decrease in total inventory. At the end of six months at these shutdown conditions an inventory of 12.1 g still remains and after one year an inventory of 11.7 g, indicative of the almost negligible rate of diffusion at these cold shutdown temperatures. With all the characteristic temperatures near 540°K, only 7.1% of steady-state inventory is purged after one year.

In comparison, the characteristic grains are then modeled for hot shutdown, with the coolant temperatures mentioned before. Again, new row by row temperature profiles were calculated, average temperatures evaluated from these, and the previous analyses rerun at these higher temperatures. As could be expected, the result was a significantly accelerated tritium purge from the blanket. Figure 19 shows that, after only one week, the total inventory was reduced from 12.6 g to 0.45 g. After two weeks, inventory was reduced to an insignificant 0.02 g. Thus, with characteristic temperatures ranging from 750

Figure 18

TOTAL TRITIUM INVENTORY AFTER SHUTDOWN, NO HEATING

Figure 19

to 780°K and no tritium generation after shutdown, tritium purging can be considered complete after only two weeks.

For less than 13 g steady-state inventory, a question could arise whether such baking with the extra expense of heating the coolant is actually needed. However, if the final blanket is not as "clean" as our idealized model would indicate, this analysis shows that baking could rapidly clean out the major portion of the blanket inventory after shutdown. Such auxiliary heating should alleviate inventory concerns in a post-shutdown environment.

7. ADDITIONAL DIFFUSE MODELING

Completely Dense Pins

DIFFUSE was used to model a hypothetical case for steady-state inventory and release for this rod design, but using a ceramic pin of 100% theoretical density rather than 85% as assumed in this study. The purge channel was retained but the tritium was considered to be generated in and diffuse through one giant hollow cylindrical crystal of LiAlO_2 rather than a minute spherical grain. The boundary conditions were taken to be a perfectly reflecting outer surface (i.e. an inner oxide layer on the cladding) and zero concentration on the inside purge channel surface.

These 100% dense pins were analyzed for rows one, five, and eleven. The values for inner and outer surface temperatures were taken from the original 85% dense pins (although detailed analysis would require recalculation of temperature based on the changed thermal conductivity). DIFFUSE assumes a linear temperature profile rather than the actual parabolic design, slightly overestimating inventory and underestimating release. The same tritium generation rates were used as in the original pin design.

For row one, the minimum temperature is 1017°K and the maximum is 1410°K. After three years of steady-state operation, DIFFUSE evaluated the inventory of each pin to be 21.0 g of tritium, or over 350 kg for the first row over the entire blanket, an extremely high inventory. For row five, with temperatures from 809 to 891°K, the inventory for each pin was found to be 1.76 g and over the whole blanket nearly 30 kg. For row eleven, with temperatures from 900 to 1155°K, the single pin inventory was 6.30 g and the total blanket inventory about 40 kg. Obviously, the first row inventory will dominate the total due to the high generation rate.

The complement of high inventory is low release. Over three years, the entire first row would release 6.7 kg into the purge stream, or 1.7% of the total tritium generation. With their colder operating temperatures, rows five and eleven would release only a few hundredth of a percent of their total generation: all of row five would release a mere 1.0 g tritium, and row eleven only 6.9 g. Except for the relatively hot first row rods, tritium release over three years would be negligible.

The importance of these results is the lack of any significant release for most of the pins over the entire blanket lifetime, raising the possibility of using 100% dense LiAlO_2 pins and batch processing the retained tritium at the end of blanket life. Elimination of the purge channels as superfluous

would provide more breeder mass in the blanket and a higher breeding ratio. More significant is an increase of over 17% in breeder mass in using 100% vs. 85% density, with its major impact on tritium breeding ratio. With no purge channel, total release from the colder outer zones of the pins through the oxide barrier of the cladding would likely be insignificant. Structural integrity of the ceramic during burn-up would be enganged, considering the results of the FUBR-1A experiment (19). Actual permeation losses over lifetime would likely be less than with permeation through the purge system.

The main disadvantage to this concept is of course very high inventories, but this should not affect safety concerns as long as all pins remain intact over lifetime. Retention of tritium the entire three years would lead to enhanced decay to helium prior to extraction, but DIFFUSE indicates total decay to be 8% of all bred tritium, insignificant considering the 17.6% increase in breeder mass and breeding ratio with 100% vs. 85% dense LiAlO_2 . A major concern is the presence of any grain boundaries in the 100% dense pin, leading to more rapid diffusion than our ideal single grain cylinder. This problem would be alleviated by retaining the purge channels to handle such diffusion.

Although the inventory levels with these dense pins appears frightening, the structural integrity of the pins over blanket lifetime mitigates the safety concerns. The advantages obtainable from these dense pins might encourage future consideration.

Other Inventory Phenomena

All previous DIFFUSE analyses assumed a zero tritium concentration on the surface of a spherical grain, analogous to previous modeling efforts. However, TRIO (6) assumed a significant surface inventory under a pure helium purge stream to explain the experimental results. Solubility effects are known to be significant for Li_2O . Concern exists over irradiation effects and the possibility of production of traps for tritium which might significantly increase inventory.

As a very preliminary indication of the versatility of the DIFFUSE code, several analyses were made under different conditions. Using input parameters for LiAlO_2 felt to be reasonable (due to the lack of relevant experimental data), both Sievert's Law (solubility effects) and surface recombination boundary conditions were compared to zero surface concentration over a range of temperatures, all other parameters held constant. In addition, an analysis was made assuming a trap concentration of 1% atomic fraction and a trapping energy of 2 eV. Results are presented in Figure 20.

For all temperatures below 1100°K, these other phenomena show no effect on total inventory, indicating diffusive inventory to be overwhelming. However, at higher temperatures, measurable additions to diffusive inventory are apparent. Radiation trapping under these conditions is insignificant, but surface recombination becomes significant and solubility very significant as temperature becomes very high. However, with an ambient tritium gas pressure of one torr assumed, these solubility results may overstate actual operating concentrations.

These limited results are not significant without further analysis, but the potential of DIFFUSE for additional analyses into these phenomena is

Figure 20

obvious.

Radiation Trapping

Some parametric analysis using DIFFUSE has been done (23) to estimate significant tritium trapping regimes under irradiation, i.e. combinations of temperature, trap concentration, and trapping energy with which significant contributions are made to total inventory. The results are not presented here, but will be briefly summarized.

No experimental determination of tritium trapping energies in lithium ceramic breeders due to irradiation has been made. Trapping energies for helium in metals is known to be 1.5 to 2.5 eV, but the ionic nature of the diffusing triton prevents direct comparison. DIFFUSE analysis of tritium trapping in LiAlO_2 was made at two temperatures over a range of trapping energies from 1.5 eV to 4.5 eV, all other parameters held constant, and an assumed trap concentration of 1 appm. At 773°K, trapped inventory was insignificant, reaching only a few percent of diffusive inventory at a 4.5 eV trap energy. At 1273°K, diffusive inventory is greatly reduced, and trapped inventory equals diffusive at about 4 eV and greatly exceeds diffusive at 4.5 eV.

For an assumed trap energy of 3.5 eV and a temperature of 1273°K, the relative inventories were compared as a function of trap concentration. At 1 appm traps, trapped inventory is insignificant. At a trap concentration of about 10^{-4} atom fraction, the two inventories are equal. At higher trap concentrations, the trapped inventory rapidly increases.

Finally, given a trap concentration of 1% atomic fraction, trapped and diffusive inventories were compared between 700 and 1475°K for trap energies of 2.5 eV and 3.5 eV. For 2.5 eV the trapped inventory is predominant at 750°K, equals diffusive at about 825°K, and rapidly becomes insignificant to that of diffusive at higher temperatures. For 3.5 eV, the trapped inventory is overwhelming at all but the highest temperature, where it is still an order of magnitude above the diffusive inventory.

Lack of experimental analysis of radiation damage effects in LiAlO_2 prevents direct application of DIFFUSE results to blanket design and engineering. These limited results suggest trapping energies approaching 3 eV are significant for high trap concentrations i.e. at high lithium burn-up fraction. For low trap concentrations (1 appm) the trapped inventory becomes significant at higher temperatures, while an inverse temperature effect occurs for 1% atomic fraction of traps. Much more analysis is required to determine the significance of radiation effects on tritium inventory. Hypotheses of tritium trapping mechanisms remain rudimentary at best (24,25).

8. SUMMARY AND RECOMMENDATIONS

This section of the pin-type solid breeder blanket study is the first detailed attempt at modeling tritium inventory and release within a fusion reactor blanket based on actual tritium generation and thermal hydraulic profiles, rather than a simple average unit cell extrapolation or some assumed exponential profiles.

The DIFFUSE 83 code was found to give inventory results consistent with previous modeling efforts and with the general spherical grain model.

The inventories for this blanket design calculated using DIFFUSE were found to be very satisfactory, less than 14 g at steady-state for a 129,000 kg LiAlO_2 blanket. This result is reasonable compared with a BCSS LiAlO_2 blanket inventory calculated by GA Technologies.

DIFFUSE was found to be very useful in approximating tritium inventories during transient start-up/shutdown modes. The evaluations of transient inventories in this study appear to be the most detailed to date. The results suggest the need for controlling coolant flow during start-up to maintain high breeder temperatures and low tritium inventory, and the use of pre-heated coolant to "bake" out tritium inventory after shut-down.

DIFFUSE modeling of breeder pins of 100% theoretical density indicates very limited tritium release from the LiAlO_2 ceramic, suggesting batch processing of the pins for tritium extraction at the end of blanket lifetime.

Preliminary analysis of other surface and radiative trapping effects shows DIFFUSE to be potentially a very useful tool in approximating and evaluating experimental results. Additional DIFFUSE analysis of these effects given the available experimental data is warranted.

Another logical area for DIFFUSE analysis is tritium permeation of the pin cladding and structure within the blanket. This area will be pursued in the future.

A real need for modeling of tritium behavior in ceramic breeders is a broader experimental data base. Order of magnitude approximations and unknown diffusive and trapping mechanisms for tritium are inappropriate for detailed modeling of tritium behavior and accurate estimates of tritium inventory, permeation, and release within fusion reactor solid breeder blankets.

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