Production of Low Activity Rhenium by Transmuting Tungsten Metal in Fast Reactors with Moderator

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Abstract
The feasibility of rhenium (Re) production by irradiating tungsten (W) metal in a medium size fast reactor was evaluated by using a Monte Carlo code. The irradiation of W with hydride zirconium moderator in a fast reactor blanket region can produce about 50 kilograms of Re per every 3 years, which corresponds 1% of Japanese domestic annual production. The specific activity of Re recovered shows below the exemption level, and furthermore, it is decreased to the level below the natural Re specific activity when deuteride zirconium moderator is used.

Keywords
Nuclear transmutation, Tungsten, Rhenium, Specific activity

Transmutation using Fast Reactors and Neutron Moderator
Nuclear transmutation is defined as the change of an isotope to another. Thus the form of nuclear transmutation shows many patterns including natural disintegrations of radioactive nuclides to nuclear reactions induced by charged particles by accelerators. The practical way of nuclear transmutation is usually conducted by neutron-induced reactions in nuclear reactors.

Figure 1 shows the layout and profile of a typical prototype fast reactor (FR) core, which is employed for the evaluation of the transmutation. Table 1 lists the major specifications of the core. The profile of the fuel assembly is shown in the left hand of Figure 2 and the detailed design parameters of core components employed are listed in Table 2. The fuel material is plutonium-uranium mixed oxide located at the inner core (lower enrichment zone) and the outer core (higher enrichment zone). Some neutrons leak out to the blanket region where depleted uranium is located to breed fissile fuel by capturing leaked neutrons in the conventional design [1].

An estimated neutron balance of the FR core, where liquid sodium is used as coolant, is listed in Table 3 with that of the light water reactors (LWRs).

The neutron energy spectrum of FR cores shows faster or harder one at the core region than that of LWRs because the coolant (liquid sodium) is much heavier nuclides relative to that of water (hydrogen). Thus the average number of emitted neutrons of FRs per absorption, where the main fissile nuclide is plutonium-239, is about 2.5, while...
### Table 1: Specification of fast reactor.

| Item                                                      | Unit | Value | Note                                      |
|-----------------------------------------------------------|------|-------|-------------------------------------------|
| 1. Reactor thermal power by fission                       | MW   | 710   |                                           |
| 2. Coolant                                                |      | Liquid sodium | Mass density: 0.9058                   |
| 3. Core                                                   |      |       |                                           |
| (1) Type                                                  |      |       |                                           |
| Configuration                                             |      | Homogeneous |                                           |
| No. of enrichment zone                                    |      | 2     |                                           |
| (2) Number of core components                             |      |       |                                           |
| Core total                                                |      | 198   |                                           |
| Inner core                                                |      | 108   | Enrichment of Pu fissile 16%              |
| Outer core                                                |      | 90    | Enrichment of Pu fissile 21%              |
| Control rod                                               |      | 19    |                                           |
| Radial blanket                                            |      | 174   |                                           |
| Radial neutron shield                                     |      | 324   |                                           |
| (3) Core dimension                                       |      |       |                                           |
| Active core height                                        | mm   | 930   |                                           |
| Equivalent diameter                                       | mm   | 1788  |                                           |
| Height/Diameter                                           |      | 0.52  |                                           |
| Core volume                                               |      | 2335  |                                           |
| (4) Blanket thickness                                     |      |       |                                           |
| Axial blanket (upper/lower)                               | mm   | 300/350 |                                           |
| Radial blanket equivalent thickness                       | mm   | 315   |                                           |
| (5) Assembly pitch                                        | mm   | 115.6 |                                           |
| (6) Pu isotope ratio                                       |      |       |                                           |
| $^{239}\text{Pu}/^{240}\text{Pu}/^{241}\text{Pu}/^{242}\text{Pu}$ | -    | 58/24/14/4 |                                           |
| (7) U isotope ratio                                        |      |       |                                           |
| $^{235}\text{U}/^{238}\text{U}$                          | -    | 3/97  |                                           |

### Table 2: Specification of core components.

| Item                        | Unit | Value | Note                                           |
|-----------------------------|------|-------|------------------------------------------------|
| 1. Driver fuel              |      |       |                                               |
| Core fuel material          |      | MOX   | Mixed oxide with PuO$_2$-UO$_2$                |
| Core fuel pellet OD         | (mm) | 5.4   |                                               |
| Core fuel density           | (%T.D.) | 85 |                                               |
| Axial blanket material      |      | depleted U | $^{235}\text{U}/^{238}\text{U} = 0.003$ | |
| Axial blanket pellet OD     | (mm) | 5.4   |                                               |
| Axial blanket density       | (%T.D.) | 93 |                                               |
| Fuel pin cladding material  |      | SS316 |                                               |
that of LWRs is 2.1 due to the difference of neutron spectrum [1]. Furthermore, the neutron loss of parasitic absorption of structure and coolant per fission neutron is 0.1 in FRs, while that of LWRs is 0.5. Thus more excess neutrons are available to utilize for transmutation if the system is designed appropriately. The studies on the transmutation using FRs are dedicated for the transmutations of minor actinides or long-lived fission products to short-lived or stable nuclides so far because these radioactive wastes are considered to be the main source of hazards in future when the geological disposal of radioactive waste is employed.
In recent years, the demand for rhenium (Re) is growing as an additive to super alloys for jet engines. However, rhenium is one of the rarest elements in earth. The abundance of Re is much smaller: $10^9$ times of Si and $10^{-4}$ times of tungsten (W). The price of Re is about 500 times that of W at present. Therefore, active technology for creation of Re that we advocate has a great value.

Après ORIENT research program, newly initiated in 2011, includes transmutation of stable elements to create rare metals/RE (rare earth) elements by (n,γ) reaction with subsequent beta decays in

| Items                                                                 | Thermal Reactor | Fast Reactor |
|----------------------------------------------------------------------|-----------------|--------------|
| Number of fission neutrons per one neutron capture                   | 2.1             | 2.5          |
| To sustain chain reactions                                          | 1.0             | 1.0          |
| To be captured by coolant and structure material                    | 0.5             | 0.1          |
| Maximum number of neutrons available to transmutation, which are used to conversion of $^{238}$U to $^{239}$Pu in conventional reactors | 0.6             | 1.4          |
| Total                                                               | 2.1             | 2.5          |

Table 3: Estimated neutron balance of thermal and fast reactor.

Figure 1: Core layout and profile of fast reactor.
In our study, we focused two points for setting the transmutation system in FRs, amount of produced Re for practical use and specific activity of Re for radiation protection. The exemption level of specific activity, that is a radioactivity level under that market use is approved, is defined by IAEA for each radioactive nuclide as Bq/gram-element [6].

Figure 3 illustrates the transmutation scheme of W to Re with other related reactions in reactors. The isotope abundance of W indicates that, two main paths for Re production are:

1. $^{184}$W (abundance: 31%) to $^{185}$W by neutron capture reaction.

The reactors [2-4]. Re can be produced by nuclear transmutation where W captures neutrons and disintegrates to Re [5].

The objective of this study is to clarify the feasibility of production of Re from W metal in fast reactors by using neutron moderator.

The target assembly used for the W-Re transmutation is shown at the right hand of Figure 2, which is similar to the radial blanket fuel assembly located at the peripheral of the driver fuel except pellets accommodated in the pin.

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Figure 4: Capture cross section of $W$ isotopes.

Figure 5: Cross section of hydrogen and deuteron.
capture to $^{185}$Re by beta disintegration;

(2) $^{186}$W (abundance: 28%) to $^{187}$W by neutron capture to $^{187}$Re by beta disintegration.

The residual radioactivity produced by W irradiation is β disintegration of $^{187}$Re and no γ ray emitted after a few years cooling time and the energy of emitted electron is as low as 2.64 KeV. But such feature may be troublesome if lot of Re is utilized worldwide as artificially produced material because the detection of no γ ray emitted material is hard to detect out. Thus we have focused on the specific activity of the produced Re in our proposed system.

As shown in Figure 4, lower energy neutrons react with more W isotopes. Figure 5 shows the scattering and absorption cross section of the typical neutron moderator nuclides, proton and deuteron. Proton has a larger scattering cross section than deuteron by 1 order while deuteron has much smaller absorption cross section. We have selected, thus, materials containing proton or deuteron as candidates for effective moderator, and zirconium hydride or zirconium deuteride are employed because zirconium can retain much hydrogen (1.7 times Zr or more at 600 °C) and have some experiences for the reactor materials in FRs.

### Analysis Method and Verification

The code system used in the analysis is shown in Figure 6. A continuous energy three dimensional Monte Carlo code, MVP [7] with its burn-up calculation routine MVP-BURN [8] where detailed configuration of the core components are input and the neutron energy spectra of each zone of reactors are exactly simulated to evaluate the transmutation rate of W, the effective neutron cross sections and the neutron fluxes of W pin region for the use in ORIGEN2 [9], in which the specific activity of Re is calculated. Japanese evaluated nuclear data library, JENDL-4.0 [10] is used for base neutron cross sections except Re isotopes, which cross sections are derived from ENDF/B-7.0.

The one-point model burn-up code ORIGEN2 with one group cross section system is used for evaluating the specific activity of each isotope by applying the effective cross section and flux. In the original ORIGEN2 data library, cross sections for typical nuclear reactors are prepared, though some particular cross sections such as tungsten mixed with neutron moderator are not provided. Thus we have evaluated them by using MVP code.

In the treatment of neutrons, the interaction between particles is ignored and only the reactions with nuclei or atoms are considered. The particle behavior in the reaction of neutrons with nuclei or atoms is determined on the basis of the information of evaluated nuclear data files. In the case of the continuous-energy method by the Monte Carlo codes MVP, which we have employed, use the continuous-energy form of cross sections processed from the evaluated nuclear data files. The energy range for nuclear reactions and transport of neutrons is from $10^{-5}$ eV to 20 MeV. All reactions given in the evaluated nuclear data files are treated explicitly in this energy range. The MVP cross section data files are generated for each nuclide from the evaluated nuclear data by using the LICEM code [11]. The data for the interpolation between temperatures are also included in the date files and thus cross sections at arbitrary temperatures are generated from the data. The microscopic cross sections are provided at fine energy mesh points in the generated libraries. These energy mesh points are selected so that the requested accuracy of linearized cross sections is satisfied (normally 0.1%). The cross sections in the resolved resonance region are generated by the resonance formula given in the nuclear data file with the resonance parame-

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The cross sections between the given energy points are determined by the linear-linear interpolation. The cross sections in the unresolved resonance region are determined by the probability table method. In this method, the sets of capture, elastic scattering and fission cross sections and the probabilities for the sets are given and the cross sections are determined by random numbers.

In order to evaluate the core characteristics of fast reactor, a computer code system has been developed by utilizing the advanced analysis code MVP. The validity of MVP was verified by analyzing FBR MONJU experimental data obtained in the core physics tests. The differences between the results of MVP and the experimental data for major core characteristics such as criticality or control rod worth were 2% or less at the maximum [12].

In order to confirm the reliability the burn-up routine MVP-BURN, it was applied to the burn-up benchmark problems for a high conversion LWR lattice and a BWR lattice with burnable poison rods. The results of MVP-BURN have shown good agreement with those of a deterministic code for burn-up changes of major fuel nuclides and number densities of major fuel nuclides. In the analysis, the results of these codes agreed with measured values within an error of 10% for most nuclides [13].

Target Assembly Design and Modeling of the Core for MVP Calculation

The core layout and the pin layout of the target assembly modeled for MVP calculation are shown in Figure 7.

We assumed five types of pin layout for the target assembly illustrated at the right hand in Figure 3 for studying the effect of neutron moderators on the transmutation for the difference of the cross sections between proton and deuteron will affect the neutron energy spectra at the tungsten pins.

The pin layout cases are listed in Table 4 and illustrated in Figure 8, Figure 9, Figure 10, Figure 11 and Figure 12. For Case 1 to Case 4, outer 43 pins contain tungsten (W) pellets, which axial stack length is 930 mm.

The pin layout with 18 zirconium hydride (ZrH$_{1.7}$) pins facing the core is tested for emphasizing strong neutron moderation effect in Case 1, while the pin layout with 18 zirconium deuteride
The location of the target assembly is just outside of the core because the neutron moderator in the target assembly will affect the core performances through the softer neutron spectrum, which may decrease the number of fission neutrons emitted.

At the modeling of the whole core for the MVP calculation, we employed three dimensional model as is except the peripheral region such as neutron shield. The detailed dimensions of each core components and the composition of materials included are listed in Table 1 and Table 2. The height of the active core is set at 930 mm; the upper/lower axial blanket thickness is set at 300 mm/350 mm; the length of the fission gas plenum is set at 1300 mm. Thus the upper boundary of the model is set at the top of the gas plenum. The bottom boundary is set at the bottom of the lower shield 650 mm in length, which is located just below the lower axial blanket. The radial outer boundary is set at 1800 mm in radius, which is locate at the sodium coolant pool flooding the whole core components. The neutrons passing out the outer boundary are assumed to be lost from the system. For the burn-up calculation, MVP-BURN, the thermal power of the core is set at 710 MWt for 3 year-burn-up cycles and each cycle is divided to two sub-cycles. Total neutron histories for each 6 steps are set at 1200000, which are divided to 120 batches with 20 skip batches that means 20 bathes are skipped before the tally is started for Monte Carlo calculation.

MVP or MVP-BURN does not evaluate specific activity while ORIGEN-2 code do by using capture cross section and neutron flux, then we have calculated the capture cross sections of the nuclides and fluxes of the tungsten pin, which are provided in the output of MVP. One group average cross section is calculated by dividing the total reaction rate of nuclide over the whole energy by the total number density of the nuclide in MVP.

Results and Discussion

Cross section and neutron flux at W region

Table 4 lists the one group effective capture cross sections and neutron fluxes at the W regions evaluated by MVP for the use of ORIGEN2, where specific reactivity is calculated. The effective cross sections of moderator applied cases, Case 1 to Case 4 increase by a few times that of no moderator case (Case 5), while the fluxes of these cases decrease.
The produced Re weight at 3 years irradiation will be more than 50 kg in prototype reactor, which corresponds to about 1% of Japanese annual production of Re at present. 

**Figure 13** illustrates the effect of moderators on the cross sections and production of Re isotopes. The scattering cross section of proton is much larger than that of deuteron. Meanwhile, the resonance by about 0.6 to 0.9 time that of Case 5 due to the neutron absorption by the protons or deuterons included in the moderators.

**Production of Re after 3 years irradiation**

The produced Re weights after 3 years irradiation in the core has been evaluated by MVP-BURN code. Table 5 lists the loaded W weights, produced Re weights and the ratio of isotope fractions.

| Case  | Number of pins | Pin layout | W load (kg) | Re weight (kg) | Re/W (%) | 185Re (kg) | 187Re (kg) | 187Re/185Re |
|-------|----------------|------------|-------------|----------------|----------|------------|------------|-------------|
| Case 1 | ZrH_{1.7} 18 pins W 43 pins | Figure 8 | 3.520 | 51.2 | 1.45 | 14.1 | 37.1 | 2.63 |
| Case 2 | ZrD_{1.7} 18 pins W 43 pins | Figure 9 | 3.520 | 40.3 | 1.14 | 23.6 | 12.7 | 0.54 |
| Case 3 | ZrH_{1.7} 9 pins ZrD_{1.7} 9 pins W 43 pins | Figure 10 | 3.520 | 44.4 | 1.26 | 17.6 | 27.8 | 1.58 |
| Case 4 | ZrD_{1.7} 9 pins ZrH_{1.7} 9 pins W 43 pins | Figure 11 | 3.520 | 45.6 | 1.30 | 17.3 | 27.2 | 1.57 |
| Case 5 | W 61 pins (no moderator) | Figure 12 | 5.010 | 49.1 | 0.98 | 29.1 | 19.9 | 0.68 |

Table 4: One group effective capture cross section and neutron flux at W region by MVP code.

| Case  | Number of pins | Pin layout | 182W (barn) | 183W (barn) | 184W (barn) | 186W (barn) | 185Re (barn) | 187Re (barn) | Neutron flux (n/cm^2/s) |
|-------|----------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|------------------------|
| Case 1 | ZrH_{1.7} 18 pins W 43 pins | Figure 8 | 0.574 | 1.203 | 0.237 | 0.580 | 9.348 | 4.823 | 7.57E + 14 |
| Case 2 | ZrD_{1.7} 18 pins W 43 pins | Figure 9 | 0.268 | 0.792 | 0.230 | 0.176 | 2.355 | 2.361 | 1.09E + 15 |
| Case 3 | ZrH_{1.7} 9 pins ZrD_{1.7} 9 pins W 43 pins | Figure 10 | 0.418 | 1.053 | 0.235 | 0.365 | 6.255 | 4.138 | 8.79E + 14 |
| Case 4 | ZrD_{1.7} 9 pins ZrH_{1.7} 9 pins W 43 pins | Figure 11 | 0.442 | 1.115 | 0.240 | 0.399 | 6.728 | 4.39 | 8.65E + 14 |
| Case 5 | W 61 pins (no moderator) | Figure 12 | 0.187 | 0.459 | 0.169 | 0.124 | 1.093 | 1.008 | 1.21E + 15 |

Table 5: Production weight of Re after 3 years irradiation.

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Table 6: Exemption level of Re isotopes [5].

| Isotope (Half life) | Bq/g   |
|-------------------|--------|
| $^{186}$Re (3.8 d) | $1 \times 10^3$ |
| $^{187}$Re (5 x $10^{10}$ y) | $1 \times 10^6$ |
| $^{188}$Re (17 h) | $1 \times 10^2$ |

Specific activity of Re

The specific activity of Re during irradiation and cooling has been evaluated by ORIGEN2 with the cross section and flux shown in Table 4.

Figure 14 shows the specific activities of the isotopes of W, Re, and osmium (Os) in Case 1, in which the produced Re is the maximum among the evaluated cases. The exemption levels of Re isotopes determined by IAEA [5] are listed in Table 7.

As shown in Figure 14, the main radioactivity of Re is that of $^{188}$Re, the daughter of $^{188}$W, during the cooling time if W and Re are not separated after the irradiation. The specific activity of $^{188}$Re is 6 decades higher than that of the exemption level. If W and Re is separated after the irradiation, radioactivity of most Re isotopes are negligible as shown in Figure 15.

Thus the exemption level of Re specific activity is easily achieved in a half year cooling in case the separation of W from Re is conducted.

Specific activity for different moderators

Figure 16 illustrates the specific activity of Re for different types of moderators when Re is separat-
Figure 14: Specific activity when Re is not separated from W.

Table 7: Specific activity of Re and natural Re.

| Case | Number of pins | Pin layout | Specific activity (Bq/g) | Produced Re weight (kg) | Re/W (%) |
|------|----------------|------------|-------------------------|-------------------------|----------|
| Case 1 | ZrH$_{1.7}$, 18 pins W 43 pins | Figure 8 | 1150 | 51.2 | 1.45 |
| Case 2 | ZrD$_{1.7}$, 18 pins W 43 pins | Figure 9 | 658 | 40.3 | 1.14 |
| Case 3 | ZrH$_{1.7}$, 9 pins ZrD$_{1.7}$, 9 pins W 43 pins | Figure 10 | 1004 | 44.4 | 1.26 |
| Case 4 | ZrD$_{1.7}$, 9 pins ZrH$_{1.7}$, 9 pins W 43 pins | Figure 11 | 1033 | 45.6 | 1.30 |
| Case 5 | W 61 pins (no moderator) | Figure 12 | 938 | 49.1 | 0.98 |
| Natural Re | - | - | 1050 | - | - |

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Figure 15: Specific activity when Re is separated from W and Os after irradiation.

Figure 16: Specific activity of Re vs. types of moderator.
ed from W and Os after the irradiation. The use of ZrD₁.₇ (Case 2) reduces the specific activity by half compared to that of ZrH₁.₇ (Case 1) or no moderator (Case 5) due to the decrease of the fraction of ¹⁸⁷Re (T₁/₂ = 4.3 × 10¹⁰ years).

The comparison of specific activity of each case and natural Re is listed in Table 7. The specific activities of Re for the mixed moderator cases (Case 3 and Case 4) are intermediate values between that of Case 1 and Case 2.

The specific activity of produced Re is less than that of natural Re (1050Bq/g-Re, the abundance of ¹⁸⁷Re: 62.6%), which suggests the no moderator case seems acceptable, though the production ratio (Re/W ratio) is lower than other cases as shown in Figure 17. This figure suggests that Case 2 is more preferable than Case 5 if the production efficiency of Re per loaded W is crucial if emphasizing the system economy.

**Reprocessing and the separation of Re from W**

After the completion of the irradiation of W in the fast reactor, Re, the main transmutation product of W, is discharged with the target assemblies, then will simultaneously be reprocessed with Spent Fuel (SF). In the PUREX reprocessing, Re and remained W may form possibly oxo anions ReO₄⁻ and WO₄²⁻ in the dissolver solution. These will be co-extracted with UO₂²⁺ and Pu⁴⁺ in replacing one NO₃⁻ anion. In the case of ReO₄⁻, for instance,

\[ \text{UO}_2^{2+} + \text{ReO}_4^{-} + \text{NO}_3^{-} + 2\text{TPB} = \text{UO}_2(\text{ReO}_4) \cdot \text{NO}_3^{-} \cdot 2\text{TPB}. \]

Since ReO₄⁻ and WO₄²⁻ are known to express almost the same distribution characteristic (D vs. HNO₃) as that of TcO₄⁻ for TBP, they might be distributed to the whole extraction cycles as the same manner as TcO₄⁻ [14], and finally be concentrated in the high-level liquid waste (HLLW). Therefore, it is obvious to investigate Re recovery from the HLLW. The typical electrode reactions with E° of Re, W and Tc in acidic solution are shown as follows;

\[ \text{WO}_4^{2-} + 4\text{H}_2\text{O} + 6\text{e}^- = \text{W} + 8\text{OH}^- \quad E^o = -1.05V \]
\[ \text{ReO}_4^{-} + 8\text{H}^+ + 7\text{e}^- = \text{Re} + 4\text{H}_2\text{O} \quad E^o = +0.362V \]
\[ \text{ReO}_4^{-} + 4\text{H}^+ + 3\text{e}^- = \text{ReO}_2 + 2\text{H}_2\text{O} \quad E^o = +0.510V \]
\[ \text{ReO}_4^{-} + 2\text{H}^+ + \text{e}^- = \text{ReO}_3 + 2\text{H}_2\text{O} \quad E^o = +0.732V \]
\[ \text{TcO}_4^{-} + 8\text{H}^+ + 7\text{e}^- = \text{Tc} + 4\text{H}_2\text{O} \quad E^o = +0.472V \]
\[ \text{TcO}_4^{-} + 4\text{H}^+ + 3\text{e}^- = \text{TcO}_2 + 2\text{H}_2\text{O} \quad E^o = +0.738V \]

The large ΔE° between ReO₄⁻ or TcO₄⁻ and WO₄²⁻ suggests the preferential deposition of Re or Tc by the electrolytic extraction (EE) method; When polarizing the electrode potential to CA. 0 to 0.3V (V vs. SHE) for instance, Re and Tc will

**Figure 17: Specific activity of Re and Re to W ratio vs. types of moderator.**

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Electrodes: smooth Pt; cathode (2cm²); anode (8cm²); RE: Ag/AgCl; Catholyte: 0.5M HCl; Tc_{conc}: 50ppm; Re_{conc}: 200ppm; Temp: 50°C; Ic: 2.5mA/cm² (1hr) → 75mA/cm² (2hr) → 100mA/cm² (4hr)

Figure 18: UPD effect on the deposition of Re and Tc by adding Rh³⁺ Galvanostatic electrolysis.

Figure 19 shows the distribution ratios (D) of the elements composing the HLLW on macro-cyclic B18C6 resin [16]. In this 5M HCl condition for instance, the high separation of PGM can be expected with SF_{Re/PGM} > 100 by the ion-exchange (IX) method.

Namely, the combinatorial separation by EE and IX processes will ensure the promising recovery and refining of Re from W, fission products and actinides in the HLLW. The mutual separation of Re and Tc must be the issue.

Conclusions

The feasibility of rhenium (Re) production by irradiating tungsten (W) metal in a medium size fast reactor was evaluated by using the Monte Carlo calculation code MVP and ORIGEN2. The prototype fast reactor can produce about 50 kilograms of Re per every 3 years, which corresponds to about 1% of Japanese domestic consumption. The specific activity of Re can be reduced below the exemption level or even the natural Re level if W and osmium (Os) are separated after the irradiation. The use of ZrD₁.₇ moderator reduces the specific activity to half that of ZrH₁.₇ moderator case, and even the no moderator case is acceptable if the specific activity of Re produced in fast reactors should be less than that of natural Re.
Figure 19: Relation between D and Surface charge density (Cr2) on metal ions for Macro-cyclic B18C6 resin-5MHCl-simu.

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