# THERMODYNAMIC SIMULATION OF OXIDATIVE PROCESSES

# AT THE REPROCESSING OF SPENT NUCLEAR FUEL

# IN THE LiCl-KCl MELT

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**Abstract**

The initial material composition of the nitride spent nuclear fuel (SNF) was calculated by the methods of thermodynamic modeling. The process of interaction of nitride SNF with CdCl2 and with PbCl2 in molten LiCl-KCl eutectic is studied. It is shown that the chlorination process takes place in two stages. Both the rate of the process and the composition of the resulting products significantly depend on temperature.

## INTRODUCTION

At present, in Russia, within the framework of the Breakthrough project, an intensive development of a pyrochemical (anhydrous) method for reprocessing nitride spent nuclear fuel (SNF) is underway. The pyrochemical method is devoid of the disadvantages inherent in the hydrometallurgical method, such as prolonged exposure of fuel before processing, a large volume of liquid radioactive waste, etc. [1-4].

The process of mild chlorination of spent nuclear fuel with its simultaneous transfer to a dissolved state can be considered as the head operation of the pyrochemical reprocessing scheme. Mild chlorination refers to chlorination without the use of chlorine gas. Instead, it is technologically more convenient to use chlorinating agents - for example, CdCl2 or PbCl2.

The aim of this work is to thermodynamically simulate the process of dissolution of components of nitride SNF in molten LiCl-KCl eutectic using CdCl2 or PbCl2 as chlorinating agents.

Spent nuclear fuel is a complex, multicomponent system. It is difficult to study both because of the complexity of its composition, as well as because of its high radioactivity. Thermodynamic modeling methods make it possible to assess the composition and properties of spent nuclear fuel, compare various processing methods, and select optimal conditions.

## BASIS OF CALCULATIONS

Thermodynamic modeling was carried out using the HSC Chemistry 9.9 software package [5]. The calculation of the thermodynamic equilibrium of systems is carried out by solving a mathematical problem to find the minimum of Gibbs free energy. The extremum is found taking into account some restrictions and assumptions in the mathematical model. The initial conditions are the amount of substance of the compounds, the temperature of the process and the pressure in the system. A detailed description of the calculation methodology is described in [6].

By default, the activity coefficients of all compounds are taken equal to 1. But when modeling the equilibrium composition of mixtures in molten LiCl-KCl eutectic, we set many activity coefficients ourselves, using the literature data. Activity coefficients of (CdCl2) = 0.03; (PbCl2) = 0.4 [7], trichlorides of rare earth elements 0.01 [8]. As for actinide chlorides: γ(UCl3) = 0.001, γ(UCl4) = 10-4 [9]. Activity coefficient of PuCl3 was taken similar to UCl3.

## RESULTS OF THERMODYNAMIC SIMULATION

### SNF material composition

The first step in modeling the SNF reprocessing processes is to calculate the material composition of the nitride SNF. As the initial data, we used the model elemental composition of spent nitride nuclear fuel given in TABLE 1, combined from the data [10-12].

TABLE 1. MODEL ELEMENTAL COMPOSITION OF SPENT NITRIDE NUCLEAR FUEL COMPILED FROM DATA [10-12].

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| № | Compound/element | Amount of substance, mol. % | № | Compound/element | Amount of substance, mol. % |
| 1 | N | 47.9 | 23 | Y | 0.0722 |
| 2 | U | 37.6 | 24 | I | 0.0710 |
| 3 | Pu | 6.67 | 25 | Rb | 0.0632 |
| 4 | Xe | 0.872 | 26 | Ag | 0.0555 |
| 5 | Mo | 0.826 | 27 | Cd | 0.0448 |
| 6 | Ru | 0.745 | 28 | Sn | 0.0352 |
| 7 | Zr | 0.719 | 29 | Pm | 0.0234 |
| 8 | Cs | 0.716 | 30 | Eu | 0.0200 |
| 9 | Nd | 0.624 | 31 | Gd | 0.0186 |
| 10 | Pd | 0.578 | 32 | Np | 0.0141 |
| 11 | Ce | 0.389 | 33 | Se | 0.0124 |
| 12 | Ba | 0.282 | 34 | Sb | 0.0106 |
| 13 | C14 | 0.244 | 35 | Cm | 0.0073 |
| 14 | Rh | 0.230 | 36 | He | 0.00538 |
| 15 | La | 0.215 | 37 | In | 0.00447 |
| 16 | Tc | 0.204 | 38 | Br | 0.00396 |
| 17 | Pr | 0.200 | 39 | Tb | 0.00117 |
| 18 | Sm | 0.174 | 40 | Dy | 0.00105 |
| 19 | Sr | 0.133 | 41 | H3 | 0.00054 |
| 20 | Te | 0.126 | 42 | Ge | 0.000360 |
| 21 | Am | 0.0888 | 43 | As | 0.000110 |
| 22 | Kr | 0.0736 |  |  |  |
| Сумма |  |  |  | 99.999 |

The main elements are nitrogen, uranium, plutonium. Among the fission products, it is worth noting the noble metals - ruthenium, palladium and rhodium; rare earth elements, cesium and zirconium. The behavior of these elements will be given special attention in this article.

Based on the data on the elemental composition, the material composition of the nitride SNF was calculated at 700 °C. This temperature was chosen on the basis of data on the diffusion coefficients of elements in nitride fuel [13] and estimates of fuel rod temperatures during reactor operation, which are 1200 - 1500 °C. Also, for completeness of the calculation, the missing thermodynamic parameters of some nitrides of actinides and lanthanides were estimated using the data [14, 15].

Table 2 shows the material composition of the nitride SNF according to the results of thermodynamic modeling. Here are 68 compounds out of 1018 formed. The total content of compounds not listed here does not exceed 0.002 mol. %.

TABLE 2. MATERIAL COMPOSITION OF NITRIDE SNF AT 700 °C BASED ON THE RESULTS OF THERMODYNAMIC MODELING

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| № | Compound/element | Amount of substance, mol. % | № | Compound/element | Amount of substance, mol. % |
| 1 | (U0.8Pu0.2)N | 44.9 | 35 | GdN | 0.0384 |
| 2 | UN | 34.6 | 36 | EuTe | 0.0378 |
| 3 | PuN | 4.81 | 37 | BaC2 | 0.0346 |
| 4 | U2N3 | 3.09 | 38 | NpN | 0.0292 |
| 5 | Xe(g) | 1.80 | 39 | Cd(g) | 0.0280 |
| 6 | ZrN | 1.49 | 40 | SrTe | 0.0253 |
| 7 | NdN | 1.29 | 41 | MoC | 0.0249 |
| 8 | CeN | 0.804 | 42 | SrSe | 0.0244 |
| 9 | Mo | 0.781 | 43 | SrC2 | 0.0244 |
| 10 | Cs(g) | 0.497 | 44 | LaSb | 0.0201 |
| 11 | URu3 | 0.467 | 45 | CmN | 0.0150 |
| 12 | Cs | 0.428 | 46 | Sr3N2 | 0.0121 |
| 13 | LaN | 0.425 | 47 | He(g) | 0.0111 |
| 14 | Tc | 0.422 | 48 | In | 0.00924 |
| 15 | PrN | 0.412 | 49 | Cs2(g) | 0.00763 |
| 16 | UPd3 | 0.398 | 50 | Mo3C2 | 0.00731 |
| 17 | Ba | 0.391 | 51 | RbI | 0.00563 |
| 18 | SmN | 0.361 | 52 | Rh | 0.00488 |
| 19 | Mo2C | 0.346 | 53 | EuN | 0.00351 |
| 20 | Cs2Te | 0.198 | 54 | CsBr | 0.00328 |
| 21 | MoN0.5 | 0.187 | 55 | Ba3N2 | 0.00272 |
| 22 | AmN | 0.181 | 56 | TbN | 0.00242 |
| 23 | Sr | 0.164 | 57 | CsI(g) | 0.00218 |
| 24 | Rh3U | 0.157 | 58 | DyN | 0.00217 |
| 25 | Kr(g) | 0.152 | 59 | PrSb | 0.00183 |
| 26 | YN | 0.149 | 60 | BaBr2 | 0.00166 |
| 27 | Ru | 0.140 | 61 | CsRb(g) | 0.00165 |
| 28 | CsI | 0.137 | 62 | CsBr(g) | 0.00121 |
| 29 | Ag | 0.115 | 63 | BaSe | 0.00104 |
| 30 | Ba2Sn | 0.0727 | 64 | C | 0.000979 |
| 31 | Cd | 0.0645 | 65 | BaI2 | 0.000752 |
| 32 | Rb | 0.0635 | 66 | Ge | 0.000744 |
| 33 | Rb(g) | 0.0597 | 67 | BaH2 | 0.000488 |
| 34 | PmN | 0.0484 | 68 | BaTe | 0.000452 |
| Total | 99.998% |

Actinides and lanthanides are found in their mononitrides - AmN, CmN, PuN and LaN, CeN, PrN, NdN, PmN, SmN, EuN, GdN. The main phase (U0.8Pu0.2)N, in which the nitrides of the remaining actinides and lanthanides are dissolved.

Noble metals are mainly found in the form of intermetallic compounds URu3, UPd3 and URh3. Their formation is noted in [16]. A small part of noble metals is in free form.

Almost all iodine is combined with cesium and rubidium, CsI and RbI. And since there is little iodine in the system, the remaining cesium and rubidium, apparently, remain in free form.

Zirconium is in the form of its ZrN nitride. Molybdenum also partially forms nitrides, but due to their instability it remains in a free form with a small impurity of MoN0.5.

### Soft chlorination of SNF in LiCl-KCl eutectic

#### Chlorinating agent: CdCl2

The SNF chlorination process with its simultaneous transformation into a dissolved state can be considered as the first stage in the technology of SNF nitride reprocessing. A molten mixture of LiCl - KCl of eutectic composition (58.8 mol% LiCl and 41.2 mol% KCl) was chosen as a solvent. It is technologically more convenient to use for chlorination not gaseous chlorine, but softer chlorinating agents, for example, *p*-metal chlorides. Soft chlorination is a technologically convenient method for the initial opening of nitride SNF, and in our case, a method for its dissolution in the LiCl-KCl melt.

During chlorination, the following reactions take place:

|  |  |
| --- | --- |
| $$AnN+1.5CdCl\_{2}=AnCl\_{3}+1.5Cd+0.5N\_{2}\uparrow $$ | (1) |
| $$LnN+1.5CdCl\_{2}=LnCl\_{3}+1.5Cd+0.5N\_{2}\uparrow $$ | (2) |

Where An are actinides and Ln are lanthanides.

The main element of spent nuclear fuel is uranium. Its chlorination proceeds according to reaction (3).

|  |  |  |
| --- | --- | --- |
| $$ UN+1.5CdCl\_{2}=UCl\_{3}+1.5Cd+0.5N\_{2}\uparrow $$ | $$∆G= -61 kJ at 500°C$$ | (3) |

However, simultaneously with reaction (3), reactions of the formation of UNCl, U2N3, UN2 and nonstoichiometric nitrides of the UN1.55, UN1.69, UN1.73 type always proceed.

|  |  |  |
| --- | --- | --- |
| $$UN+0.5CdCl\_{2}=UNCl+0.5Cd$$ | $$∆G= -71 kJ at 500°C$$ | (4) |
| $$UNCl+CdCl\_{2}=UCl\_{3}+Cd+0.5N\_{2}\uparrow $$ | $$∆G= 10 kJ at 500°C$$ | (5) |
| $$UN+0.612CdCl\_{2}=0.591UN\_{1.69}+0.612Cd+0.408UCl\_{3}$$ | $$∆G= -59 kJ at 500°C$$ | (6) |
| $$UN+0.5CdCl\_{2}=0.667UN\_{1.5}+0.5Cd+0.333UCl\_{3}$$ | $$∆G= -56 kJ at 500°C$$ | (7) |

In [17], it was experimentally demonstrated that at 500 °C only ~ 30% UN interacts with CdCl2 according to reaction (3) with the formation of UCl3. The rest of the uranium was found as a black precipitate consisting of a mixture of insoluble stoichiometric and non-stoichiometric nitrides and nitride UNCl. Fig. 1 shows the temperature dependences of the Gibbs free energy of formation of reactions 3 - 5.



*Fig. 1. Temperature dependence of the Gibbs energy change for reactions 3 - 5.*

Up to 600 °C, the reactions with the formation of UCl3 and UNCl proceed in parallel and the chlorination products of uranium nitride will be these two compounds, as well as a mass of non-stoichiometric uranium nitrides. However, at temperatures above 615 °C, UNCl and other insoluble nitrides begin to interact with an excess of CdCl2 to give the target product, UCl3.

|  |  |  |
| --- | --- | --- |
| $$UN\_{1.69}+1.5CdCl\_{2}=UCl\_{3}+1.5Cd+0.845N\_{2}\uparrow $$ | $$∆G≈0 kJ at 500°C$$ | (8) |
| $$UN\_{1.69}+1.5CdCl\_{2}=UCl\_{3}+1.5Cd+0.845N\_{2}\uparrow $$ | $$∆G= -23 kJ at 650°C$$ | (9) |
| $$UN\_{1.5}+1.5CdCl\_{2}=UCl\_{3}+1.5Cd+0.75N\_{2}\uparrow $$ | $$∆G≈0 kJ at 500°C$$ | (10) |
| $$UN\_{1.5}+1.5CdCl\_{2}=UCl\_{3}+1.5Cd+0.75N\_{2}\uparrow $$ | $$∆G= -25 kJ at 500°C$$ | (11) |

 Thus, it can be concluded that there are two stages in the chlorination process. At temperatures below 615 °C, only the first stage takes place with the formation of UNCl, U2N3, UN2 and nonstoichiometric nitrides UN1.55, UN1.69, UN1.73. Above 615 °C, the second stage becomes thermodynamically possible, in which all intermediate products react with an excess of CdCl2. Note that at 615 °C the Gibbs energy of the reactions only changes sign from plus to minus. It is possible that in order to achieve reaction rates sufficient for practice, a higher temperature will be needed. For example, in [2, 18] it was demonstrated that at 750 °C and some excess of CdCl2, the interaction of UN and CdCl2 proceeds according to the overall reaction (3). No insoluble products were found.

 FIG. 2 shows the result of thermodynamic modeling of the chlorination process of 1 mol of UN at 750 °C in a simplified form that is easy to understand. The figure shows the stages through which the process goes. The abscissa shows the amount of CdCl2 added to the system.

 

*Fig. 2. Equilibrium composition of the UN + CdCl2 system depending on the amount of CdCl2 added to the system at 750* °C*.*

Looking at FIG. 2, two stages of the soft chlorination process can be distinguished. The first stage with the formation of UNCl and nonstoichiometric uranium nitrides occurs in the region of a lack of cadmium chloride in the system with respect to the stoichiometry of reaction (3). When cadmium chloride is added to the system, the formed non-target products are chlorinated with the formation of UCl3 and partially UCl4.

For visual clarity of the calculation, we will take the amount of the substance of the compounds equal to their molar percentages from TABLE 1. Thus, the calculation will be carried out for 100 mol of SNF. We will choose argon in the amount of 50 mol as the atmosphere. The amount of the eutectic substance will be taken as 100 mol (58.8 mol LiCl and 42.2 mol KCl). We’ll take a twofold excess of the chlorinating agent (300 mol). The calculation results are presented in TABLE 3.

TABLE 3. COMPONENTS FORMED AFTER SOFT CHLORINATION OF NITRIDE SNF USING CdCl2 IN LiCl-KCl EUTECTIC AT 750 °C BASED ON THE RESULTS OF THERMODYNAMIC MODELING

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| № | Compound/element | Amount of substance, mol. % | № | Compound/element | Amount of substance, mol. % |
| 1 | UCl3(l) | 70.9 | 25 | SmCl2 | 0.149 |
| 2 | PuCl3(l) | 13.0 | 26 | MoC | 0.147 |
| 3 | UCl4(l) | 2.18 | 27 | Kr(g) | 0.144 |
| 4 | Xe(g) | 1.70 | 28 | YCl3(l) | 0.141 |
| 5 | Ru | 1.46 | 29 | RbCl(l) | 0.123 |
| 6 | CsCl(l) | 1.40 | 30 | Sn | 0.0669 |
| 7 | ZrN | 1.36 | 31 | Li3Cl3(g) | 0.0662 |
| 8 | NdCl3(l) | 1.22 | 32 | C(g) | 0.0605 |
| 9 | Mo | 0.892 | 33 | MoN0.5 | 0.0597 |
| 10 | CeCl3(l) | 0.760 | 34 | ZrCl4(g) | 0.0432 |
| 11 | Rh | 0.448 | 35 | LiCl(g) | 0.0416 |
| 12 | Tc | 0.399 | 36 | EuCl2(l) | 0.0390 |
| 13 | UPd3 | 0.376 | 37 | GdCl3(l) | 0.0362 |
| 14 | BaCl2 | 0.356 | 38 | Ag3I3(g) | 0.0318 |
| 15 | LaCl3 | 0.271 | 39 | Li2Cl2(g) | 0.0318 |
| 16 | SrCl2(l) | 0.259 | 40 | PmCl2 | 0.0307 |
| 17 | CdTe | 0.247 | 41 | Mo3C2 | 0.0294 |
| 18 | PrCl3 | 0.215 | 42 | NpCl3 | 0.0276 |
| 19 | Mo2C | 0.211 | 43 | CdSe | 0.0241 |
| 20 | BaCl2(l) | 0.195 | 44 | KCl(g) | 0.0239 |
| 21 | SmCl3(l) | 0.192 | 45 | CdI(g) | 0.0230 |
| 22 | PrCl3(l) | 0.176 | 46 | Li2Cl2 | 0.0204 |
| 23 | AmN | 0.157 | 47 | PmCl3 | 0.0150 |
| 24 | LaCl3(l) | 0.150 | 48 | AmCl3 | 0.0144 |
| Total | 99.89% |

For clarity, only some of the compounds are shown. The sum of the amount of the substance of the compounds not included in the table does not exceed 0.11 mol.%.

The main compounds, as expected, were the chlorides of uranium and plutonium, as well as the chlorides of rare earth elements and other actinides and lanthanides.

#### Chlorinating agent: PbCl2

The Pb2+/Pb potential is much more positive than the Cd2+/Cd potential. Hence PbCl2 is a stronger chlorinating agent than CdCl2. The chlorination process will also proceed according to reactions 1-11, where instead of CdCl2 there will be PbCl2, and metallic lead will be formed, not cadmium. As follows from FIG. 3 process in this case can be carried out at lower temperatures, because chlorination of UNCl occurs at a lower temperature.



*Fig. 3. Dependence of Gibbs energy on temperature for chlorination reactions of UN with lead chloride.*

 FIG. 3 shows that already starting from a temperature of 323 °C, the chlorination reaction of the formed UNCl to UCl3 becomes possible. Therefore, presumably, the process can be carried out at temperatures only slightly higher than the melting point of lead chloride (501 °C).

 For thermodynamic modeling of the chlorination process using PbCl2, we use the same initial data as for the chlorination of CdCl2. Since theoretically the process can be carried out at relatively low temperatures, we will choose 650 °C as the working temperature. The result of calculating the equilibrium composition of the mixture formed during the chlorination of nitride SNF with lead chloride in the LiCl-KCl melt is presented in TABLE 4.

TABLE 4. COMPONENTS FORMED AFTER SOFT CHLORINATION OF NITRIDE SNF USING PbCl2 IN LiCl-KCl EUTECTIC AT 750 °C BASED ON THE RESULTS OF THERMODYNAMIC MODELING

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| № | Compound/element | Amount of substance, mol. % | № | Compound/element | Amount of substance, mol. % |
| 1 | UCl3(l) | 67.5 | 25 | YCl3(l) | 0.141 |
| 2 | PuCl3(l) | 13.0 | 26 | MoC | 0.139 |
| 3 | UCl4(l) | 5.25 | 27 | RbCl(l) | 0.123 |
| 4 | Xe(g) | 1.70 | 28 | PrCl3(l) | 0.117 |
| 5 | Ru | 1.45 | 29 | LaCl3(l) | 0.0957 |
| 6 | CsCl(l) | 1.39 | 30 | CdCl2(l) | 0.0818 |
| 7 | Mo | 1.38 | 31 | Sn | 0.0682 |
| 8 | NdCl3(l) | 1.22 | 32 | SmCl2 | 0.0625 |
| 9 | ZrN | 1.21 | 33 | PmCl3 | 0.0425 |
| 10 | Rh | 0.447 | 34 | EuCl2(l) | 0.0389 |
| 11 | BaCl2 | 0.399 | 35 | GdCl3(l) | 0.0361 |
| 12 | Tc | 0.397 | 36 | Ag3I3(g) | 0.0351 |
| 13 | CeCl3(l) | 0.757 | 37 | Mo2C | 0.0322 |
| 14 | UPd3 | 0.374 | 38 | NpCl3 | 0.0275 |
| 15 | LaCl3 | 0.323 | 39 | PbSe | 0.0233 |
| 16 | C | 0.298 | 40 | Sb | 0.0202 |
| 17 | SmCl3(l) | 0.277 | 41 | CmCl3 | 0.0141 |
| 18 | PrCl3 | 0.273 | 42 | MoN0.5 | 0.0118 |
| 19 | SrCl2(l) | 0.259 | 43 | He(g) | 0.0105 |
| 20 | PbTe | 0.241 | 44 | PbCl(g) | 0.00935 |
| 21 | ZrCl4(g) | 0.188 | 45 | PbI2(g) | 0.00800 |
| 22 | AmCl3 | 0.171 | 46 | PbCl2(g) | 0.00780 |
| 23 | BaCl2(l) | 0.149 | 47 | Li3Cl3(g) | 0.00524 |
| 24 | Kr(g) | 0.143 | 48 | TeI2(g) | 0.00477 |
| Total | 99.95% |

The sum of the amount of the substance of the compounds not included in the table does not exceed 0.05 mol.%. In both cases, during chlorination, the main products are UCl3, UCl4, and PuCl3. Inert gases Xe, Kr are released from the fuel.

Noble metals form intermetallic compounds for example UPd3, but they are also present in the form of Ru, Rh metals. Silver forms silver iodide.

Lanthanides are chlorinated and are present in the form of chlorides LaCl3, CeCl3, NdCl3, etc. Actinides are also chlorinated (AmCl3, CmCl3).

During chlorination, zirconium remains in the form of its nitride ZrN and a small amount of ZrCl4. Molybdenum remains partly in the form of its nitride MoN0.5, but most of it is in free form.

## Conclusions

The material composition of the nitride SNF was calculated by the methods of thermodynamic modeling. The equilibrium composition of mixtures, which are formed during the chlorination of SNF using CdCl2 or PbCl2 in molten LiCl-KCl eutectic, has been calculated. It is shown that in both cases chlorination proceeds in two main stages through several parallel reactions. The results obtained can be used to select the technological parameters of chlorination operations.

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