Fuel cycle studies of Generation IV reactors with the SITON v2.0 code and the FITXS burn-up scheme

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Abstract. Due to the high computational cost of detailed burn-up calculations, most scenario codes use burn-up tables or parametrized few group cross-sections to calculate fuel depletion in reactors. As a special parametrization approach, a fast and flexible burn-up scheme called FITXS was developed at the BME Institute of Nuclear Techniques, which is based on the fitting of one-group cross-sections as polynomial functions of the detailed fuel composition. The scheme was used to develop burn-up models for the Generation IV Gas-cooled Fast Reactor (GFR), Lead-cooled Fast Reactor (LFR) and Sodium-cooled Fast Reactor (SFR), which are able to calculate spent fuel compositions with high accuracy for a wide range of initial compositions in very short computational time. The models were also integrated into the nuclear fuel cycle simulation code SITON v2.0, developed at the HAS Centre for Energy Research, and several fuel cycle scenarios were investigated and compared with the different fast reactor models concerning the reduction of transuranium inventories and the stabilization of the plutonium inventory.

Key Words: fuel cycle, Generation IV, fast reactor, transmutation

1. Introduction

The Generation IV International Forum has identified six systems which merit development to achieve the goals of sustainability, proliferation resistance, economics and improved safety [1]. Three of these systems are fast-spectrum reactors, which have the ability to generate their own fuel from fertile ^{238}U and burn minor actinides (MAs) to reduce the long-term radiotoxicity of nuclear wastes [2]. Strategic decisions about the deployment of fast reactors and the transition from open to closed fuel cycle need scenario codes, which are capable of modelling the most important facilities of the nuclear fuel cycle and the material flows between them. Most scenario codes use burn-up tables or burn-up dependent cross-sections to calculate fuel depletion in reactors, which may not provide accurate results if multiple recycling of the spent fuel is considered. In order to cope with this difficulty, a fast and flexible burn-up scheme called FITXS was developed at the BME Institute of Nuclear Techniques (BME NTI). Based on the parametrization of the one-group cross-sections as functions of the detailed isotopic composition of the fuel, the scheme can provide accurate results in very short computational time even when multiple recycling of the fuel is performed.

The FITXS scheme was used to develop burn-up models for the Generation IV Gas-cooled Fast Reactor (GFR), Lead-cooled Fast Reactor (LFR) and Sodium-cooled Fast Reactor (SFR), of which the GFR burn-up model was also integrated into the fuel cycle simulation code SITON v2.0, developed at the Hungarian Academy of Sciences Centre for Energy Research (MTA EK). Using the burn-up models we analyzed the closed fuel cycle equilibrium breeding and transmutational capabilities of the reactors. A more complex scenario investigating the transition from a European Pressurized Reactor (EPR) fleet to a Gas-cooled Fast Reactor fleet was also simulated with the SITON v2.0 code. In the present paper we discuss the calculational methods and the developed burn-up models, as well as the results of the different fuel cycle simulations.

2. The FITXS burn-up scheme

The determination of the spent fuel composition in the reactors is an inseparable part of fuel cycle simulations. The composition of the spent fuel can be calculated with the solution of the Bateman-equation system, which consists of balance equations regarding the atomic densities of nuclides in the fuel [3]:

$$\frac{dN_i}{dt} = \sum_j (\sigma_{j\to i}\Phi + f_{j\to i}\lambda_j)N_j - (\sigma_i^{tot}\Phi + \lambda_i)N_i \qquad (1)$$

where N_i is the atomic density of nuclide i in the examined region, σ_i^{tot} is the total microscopic cross-section and λ_i is the decay constant of nuclide i, respectively. The average microscopic one-group cross-section of the reaction from nuclide j to nuclide i is denoted by $\sigma_{j\to i}$, while $f_{j\to i}$ is the branching ratio of the decay from nuclide j to nuclide i. Finally, Φ is the space and energy integrated neutron flux in the examined region.

The difficulty in solving the (1) equation system is that both the one-group cross-sections and the neutron flux depend on the neutron spectrum (and consequently on the composition) in a complicated way. The determination of the neutron spectrum requires detailed core calculations which cannot be integrated into dynamic fuel simulations due to their high computational cost. At the BME NTI we have developed a fast and flexible burn-up scheme called FITXS, which we first applied for the analysis of the Generation IV Gas-cooled Fast Reactor (GFR) [4]. Based on the fitting of the k_{eff} and one-group cross-sections in function of the detailed fuel composition, the developed burn-up models are able to calculate spent fuel composition with high accuracy for a wide range of initial compositions in less than one second computational time. The application of the FITXS burn-up scheme can be divided into three main steps:

1. selection of the fitting parameters: the chosen nuclides should thoroughly describe the one-group cross-sections, and the multiplication factor;
2. preparation of the cross-section database: detailed transport calculations have to be performed for numerous different isotopic compositions;
3. cross-section parametrization: based on the prepared database the cross-sections and the k_{eff} are approximated with the following second-order polynomial of the atomic densities of the selected nuclides:

$$\sigma(\underline{N}) = a_0 + \sum_{j=1}^{n} a_j N_j + \sum_{j=1}^{n}\sum_{k=j}^{n} a_{j,k} N_j N_k \qquad (2)$$

The detailed description of the individual steps can be found in Halász et al. [5].

3. The SITON v2.0 fuel cycle simulation code

SITON v2.0 is a discrete facilities/discrete materials and discrete events fuel cycle simulation code designed to model transient fuel cycles. The code is developed in MTA EK, and its detailed presentation is given in [6]; here we only summarize its main features. The physical model of SITON includes the most important facility types from the point of view of natural uranium utilization and waste generation, i.e.: reactor, fuel fabrication plant, enrichment plant, spent fuel reprocessing plant, material stock and spent fuel interim storage facility.

The reactor in SITON operates in cycles; it is commissioned and shut down according to its user-defined energy demand, which is the electrical energy demanded from the reactor to be

produced. The reactor is fuelled during its lifetime with the same type of fuel having the same parameters: discharge burn-up, effective full power days and number of cycles spent in the reactor. Fresh fuel can be produced from several materials each having fixed mass fraction. However, it is homogeneous just like the discharged fuel, which has one discharge burn-up and discharged composition. Discharged composition is determined from burn-up tables except for the GFR2400, for which the FITXS burn-up model is used.

The front-end plants in SITON work on-demand and have infinite capacity. They can have losses and a processing time, which is the period that a plant needs to produce output from its input. For the enrichment plant, the user can set the enrichment level and the ^{235}U content of the enrichment tailings. In contrast to the front-end plants, the spent fuel reprocessing plant works autonomously according to its user-defined capacity. It can have a processing time and the user can set the separation efficiency of each chemical element. Reprocessing takes into account the cooling time of the spent fuel and the user can set the mass fraction of different spent fuel types in the plant's input stream.

Routing of front-end material streams in SITON is flexible since connections of the front-end facilities can vary in time. Material transfer between the facilities is represented by transfer of discrete packages, the composition of which is stored by nuclide. SITON tracks 25 fission products and 27 actinides that contribute to the long-term impact of nuclear waste. Finally, the driver of SITON is the electrical energy demanded from each reactor to be produced, while the result is the time-dependent material flow between facilities by nuclide.

4. Burn-up models

Following the steps described in Section 2, we developed three different fast reactor burn-up models for the Generation IV GFR, LFR and SFR. The burn-up models consist of the corresponding fitted coefficient database and a Bateman-equation system solver. The core configurations selected for the analyses as well as the preparation of the cross-section databases are discussed in the following two subsections.

4.1. Reference cores

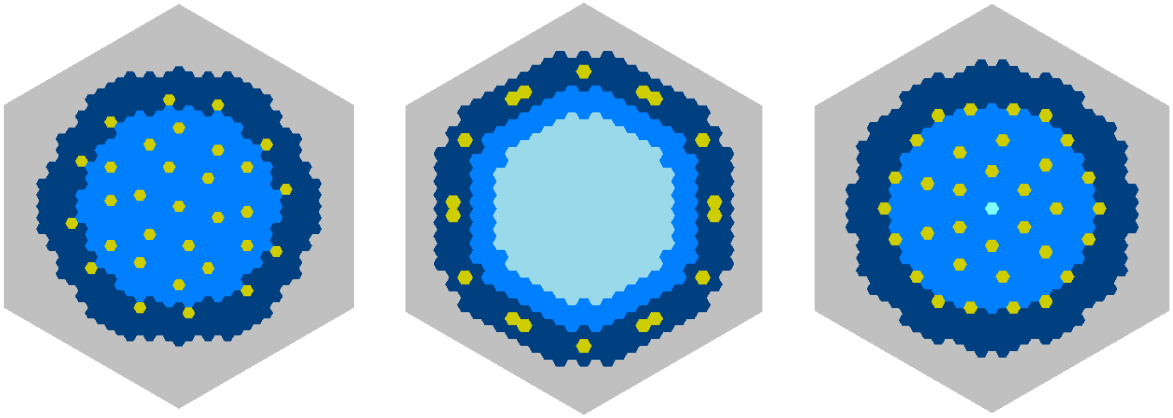
We have selected the following reference cores for the development of the burn-up models of the three Generation IV fast reactors:

- the 2400 MW_{th} reference design GFR2400 for the GFR [7]
- the 1500 MW_{th} ELSY (European Lead-cooled SYstem) core for the LFR [8]
- the 3600 MW_{th} ESFR working horse concept for the SFR [9]

The main parameters of the reference cores are listed in Table I, and the core layouts are depicted in Figure 1. Each one of the selected core configurations consist of multiple fuel regions with different Pu content in order to flatten the power distribution inside the cores. Besides the fuel assemblies, the core layouts contain control and shutdown assemblies with rod followers, as well as radial reflectors, and the axial structures include upper and lower plenums and axial reflectors without any fertile blankets.

TABLE I: Main parameters of the reference core configurations [7,8,9]

Parameter	GFR2400	ELSY	ESFR
Thermal power	2400 MW	1500 MW	3600 MW
Fuel material	(U,Pu)C	$(U,Pu)O_2$	$(U,Pu)O_2$
Cladding material	SiC	T91 steel	ODS steel
Fuel temperature	990°C	950°C	1227°C
Coolant	He	liquid Pb	liquid Na
Avg. coolant temperature	665°C	440°C	470°C
Active core volume	24 m^3	21 m^3	18 m^3
Actinide mass	67.7 t	50 t	71.4 t
Fuel assembly type	15x15 hexagonal	13x13 hexagonal	17x17 hexagonal
Nr. of fuel assemblies	252+264	163+102+168	225+228
Nr. of fuel pins in FA	217	169	271
Active length	165 cm	120 cm	100.56 cm
Fuel assembly pitch	17.83 cm	21.6 cm	21.22 cm
Fuel pin lattice pitch	1.157 cm	1.55 cm	1.19 cm
Average burn-up	50 MWd/kg	60 MWd/kg	60 MWd/kg
Fuel management	3x481 EFPD	3x547.5 EFPD	5x410 EFPD



a) GFR2400 *b) ELSY* *c) ESFR*

Figure 1. Core layouts of the reference core configurations

4.2. Preparation of the cross-section databases

The core calculations were performed with the SCALE 6.0 sequence [10] depicted in Figure 2. The preparation of the cross-section database required a few thousand core calculations, therefore in order to reduce computational time a two-step homogenization was used. In the first step we homogenized the elementary cell, then the fuel assembly containing the homogenized elementary cells, the assembly wrapper and the inter-assembly coolant. The three-dimensional models of the reactors were built from the homogenized fuel assemblies, rod followers and structural elements (axial and radial reflectors, fission gas plenums). Transport calculations were done with the KENO-VI 3D Monte Carlo module of the SCALE 6.0 code system, whose results were the reaction rates and fluxes in the different fuel regions, as well as the k_{eff} for the different fuel compositions.

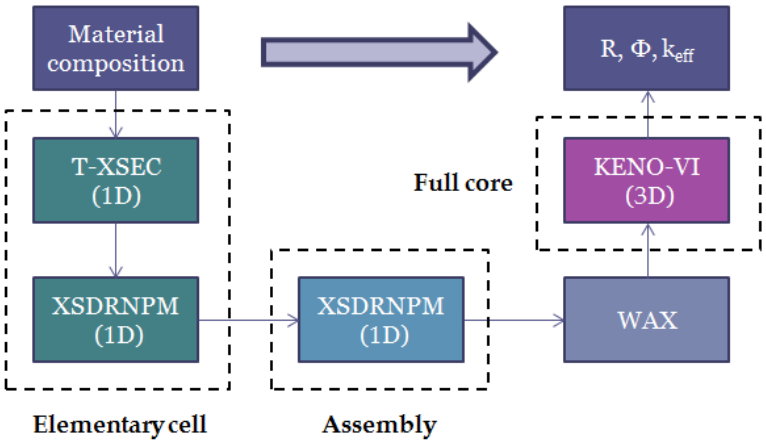


Figure 2. SCALE 6.0 sequence used for the core calculations.

The set of nuclides used for the cross-section parametrization (as well as average fission product compositions) were determined with assembly-wise TRITON burn-up calculations performed for an assembly with average fuel composition until the burn-up specified for the reference cores (see Table I). Fuel compositions used in the preparation of the cross-section database were randomly sampled taking into account the following constraints:

- Pu fraction was sampled between 10-25% and MA fraction between 0-10% of the total actinide mass. The rest of the actinide content was U.
- Fission products were considered with average compositions, and their total quantity was directly related to the sampled fuel burn-up.
- The ratio of the Pu content in the core regions was kept at constant value of respective Beginning-Of-Life conditions.

The isotopic compositions of elements were also determined by random sampling between specific lower and upper limits, allowing a wide range of possible compositions, and considering the results of prior fuel cycle analyses for the Generation IV Gas-cooled Fast Reactor [4]. As the FITXS models calculate average core composition instead of individual fuel region compositions, therefore we used correction factors to obtain correct total reaction rates which correspond to the volume-weighted average atomic densities. The flux ratios required for the calculation of the correction factors were also fitted as functions of the atomic densities. A detailed description of the method which was used to account for different core regions can be found in [5].

5. Closed fuel cycle equilibrium analyses

The FITXS burn-up models were integrated into the fuel cycle model depicted in Figure 3 in order to investigate the closed cycle equilibrium parameters of the reactors. The initial fuel loadings of the fast reactors were covered with Pu from the spent fuel of Light Water Reactors (LWRs), which was reprocessed after 5 years cooling time and was considered with constant composition throughout the simulation. The fast reactors were operated in multi-batch cycles with number of batches specified in Table I. After every cycle, one fuel batch of the reactors was replaced; the refueling time was 30 days. The fresh fuel was fabricated from the recycled U, Pu and MAs of the fast reactor, while the required fuel mass was reached by adding depleted uranium, as well as Pu from spent LWR fuel if needed in order to set the excess reactivity. Fresh fuel loading was determined iteratively based on Beginning-Of-Cycle (BOC) and End-

Of-Cycle (EOC) k_{eff} calculated from the polynomial fitting of the multiplication factor with respect to the fuel composition. Reprocessing losses were considered zero in order to obtain the maximal fuel utilization capabilities of the reactors.

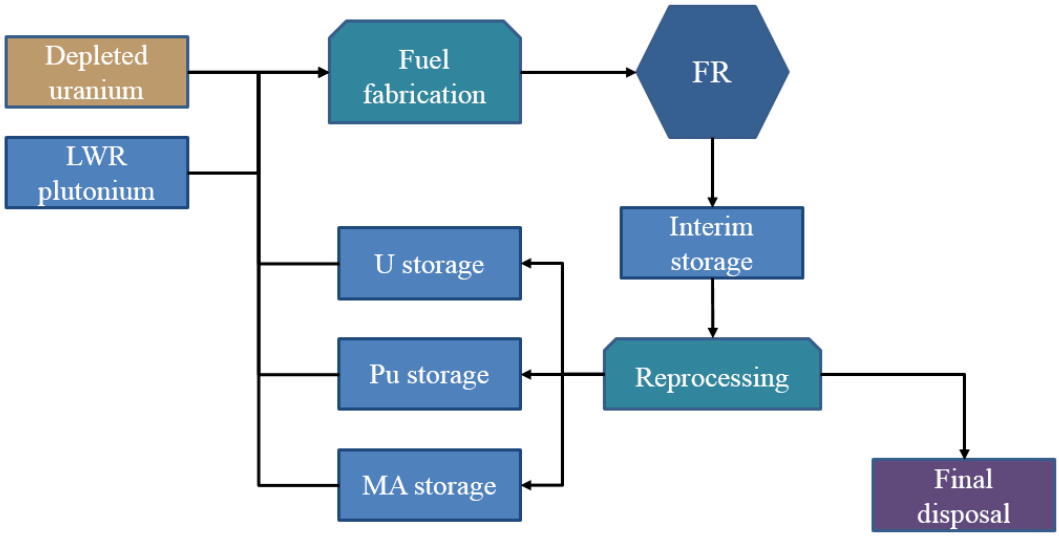


Figure 3. Schematic view of the closed fuel cycle models

As seen in Figure 4 the Beginning-Of-Cycle (BOC) Pu content increases in every core, which is mainly caused by the decay of fissile ^{241}Pu during interim storage and the accumulation of ^{240}Pu in the spent fuel. Each of the three investigated reactors reach break-even breeding: Figure 4 shows that the Pu feed of the FRs from the spent LWR fuel diminishes in the equilibrium. Other simulations performed with only U-Pu multirecycling showed that the reactors are iso-breeders only if the MA content of their spent fuel is also recycled. Results shown in Figure 5 confirm that the reactors are capable of operating in a fully closed fuel cycle, as the MA content of the cores also stabilizes, and there is no Cm accumulation in contrast with thermal reactors. The approximately 1% equilibrium MA content improves the breeding capabilities due to fertile and fissile MAs, enough that in the equilibrium no Pu feed is needed by either reactors. Consequently, the equilibrium feed consists only of depleted uranium, it equals the actinide mass lost due to fission, and the final waste is reduced to reprocessing losses (considered zero in these investigations) and fission products.

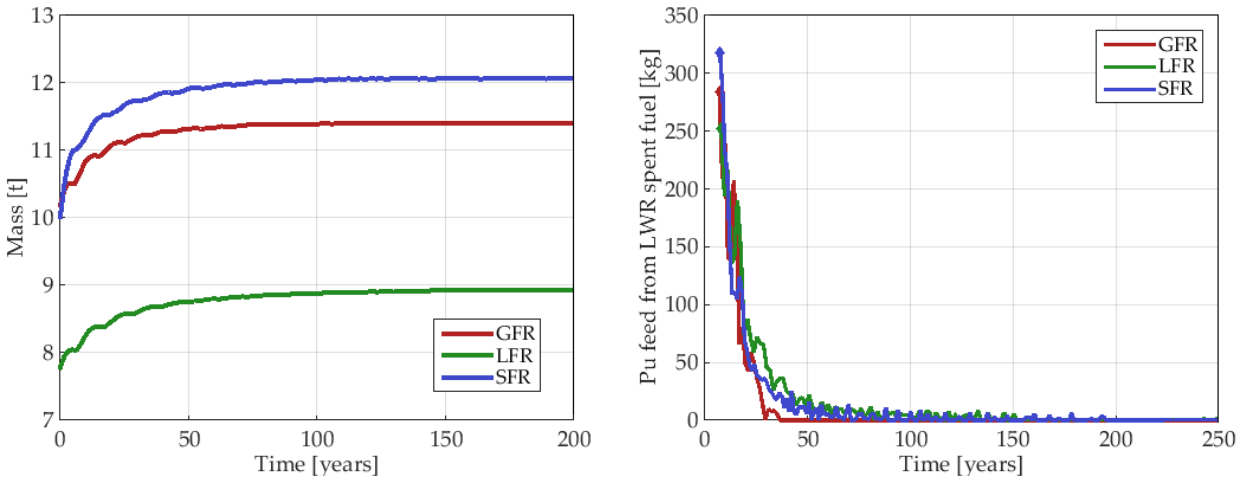


Figure 4. Beginning-Of-Cycle Pu content (left) and LWR Pu feed (right) of the fast reactor cores in the closed fuel cycle

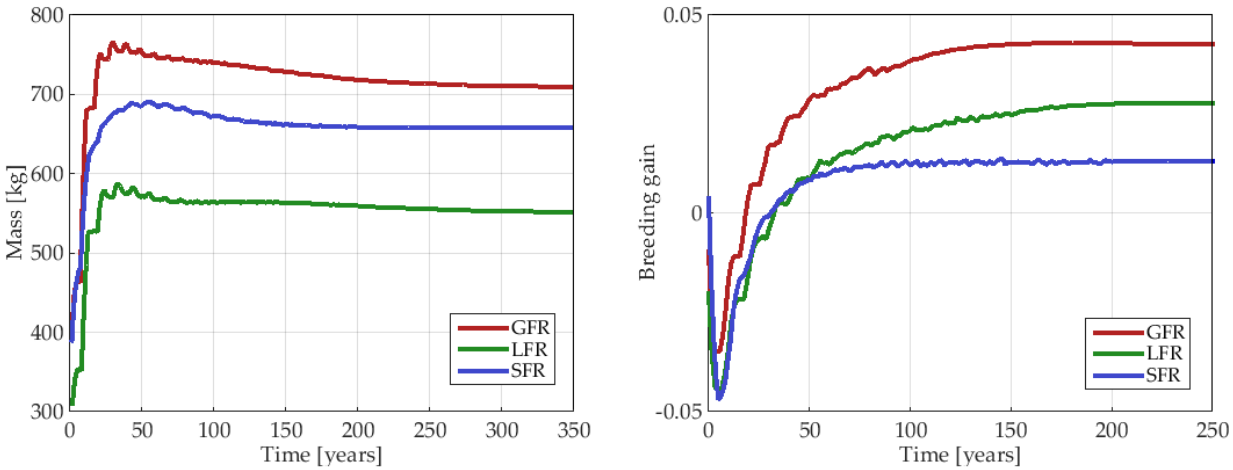


Figure 5. End-Of-Cycle MA content (left) and breeding gain (right) of the fast reactor cores in the closed fuel cycle

The equilibrium values of some important core parameters of the three fast reactors are listed in Table II. The results show good agreement with those of Krepel et al. [11], which were calculated with the EQL3D equilibrium procedure developed at the Paul Scherrer Institute. The approximately 1% equilibrium MA content of the cores, as well as iso-breeding due to the combined effect of slight breeding and ^{241}Pu decay during interim storage are also confirmed by EQL3D results.

TABLE II: Closed cycle equilibrium core parameters for the GFR, LFR and SFR reactors

Parameter	GFR	LFR	SFR
BOC Pu content (%)	17.7	18.1	17.1
EOC MA content (%)	1.03	1.14	0.99
(^{239}Pu+^{241}Pu)/Pu mass ratio	0.609	0.599	0.602
$k_{\text{eff,BOC}}$	1.0055	1.0050	1.0445
$k_{\text{eff,EOC}}$	1.0046	1.0081	1.0048
Breeding gain	0.0426	0.0274	0.0131
^{239}Pu/^{238}U mass ratio	0.121	0.129	0.122
MA/^{239}Pu mass ratio	0.107	0.108	0.097

6. EPR-GFR2400 transition scenario study

In this section, we study a hypothetical transition fuel cycle in which an EPR fleet was replaced by a single GFR2400 that recycled its own spent fuel. For the study, we used the SITON v2.0 fuel cycle simulation code with the integrated FITXS burn-up model for the GFR2400. The fresh fuel compositions of the GFR2400 were determined with preliminary FITXS calculations.

6.1. Description and model of the EPR-GFR2400 transition fuel cycle

Figure 6 shows the scheme of the model of the fuel cycle while parameters of reactors and their front-end and back-end facilities are summarized in Table III. In the first part of the fuel cycle EPRs operated until their designed lifetime. At the moment of shutting down the EPRs a GFR2400 was commissioned and it operated until its designed lifetime. The GFR2400

was started with reprocessed Pu and MAs originating from the spent EPR fuel; the reprocessing capacity was set to 400 t/y. Reprocessing of the spent GFR2400 fuel started as soon as the first discharged batch was available. Reprocessing capacity was set to 23.1 t/y; a bit higher than the mass of one batch. The first fuel batch with recycled material was loaded into the GFR2400 in year 70, in its 8th cycle. Both the initial and the recycled fuel had the same MA content (t_{MA}). However, as previous FITXS calculations showed, the Pu content of the initial and recycled fuel ($t_{\mathrm{Pu}}^{\mathrm{ini}}$ and $t_{\mathrm{Pu}}^{\mathrm{rec}}$) is different. Therefore, in SITON we used the GFR_ini and the GFR_recyc reactors to represent the initial GFR2400 core and the one with recycled fuel. Sum of the energy production of the reactors was equal to that of the GFR2400.

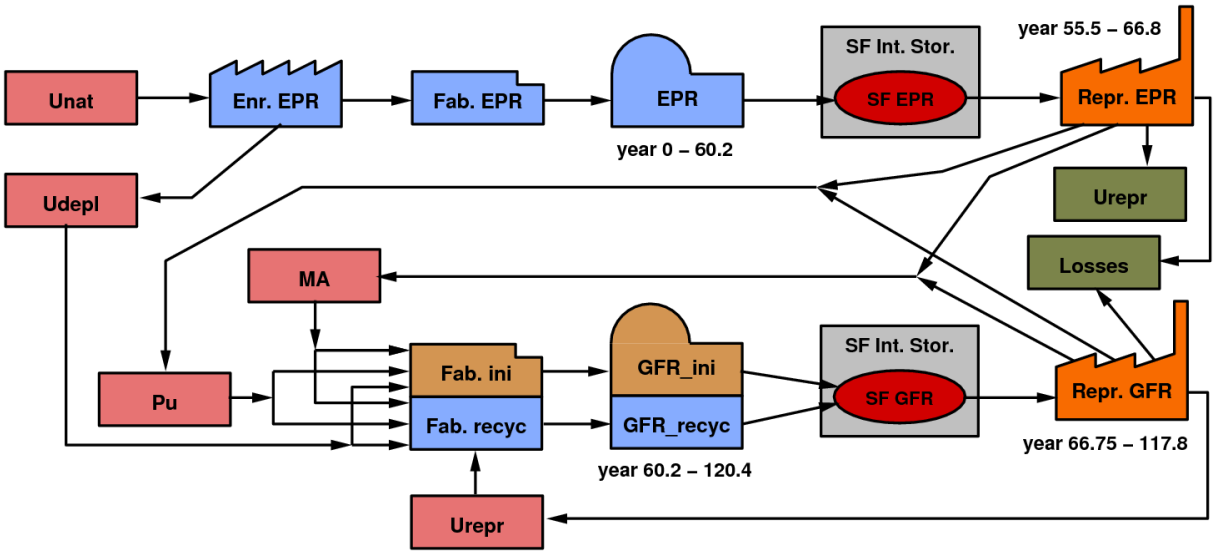


Figure 6. Scheme of the model of the EPR-GFR2400 transition fuel cycle with the operation period of reactors and reprocessing plants

TABLE III: Parameters of the reactors and their corresponding fuel cycle facilities

	EPR	GFR2400		EPR	GFR2400
Reactor parameters			**Enrichment parameters**		
Thermal power	4500 MW	2400 MW	^{235}U in DU	0.25%	–
Electrical power	1550 MW	1080 MW	Time	0 y	–
Thermal efficiency	34.44%	45.00%	Losses	0%	–
Capacity factor	81.76%	94.13%	**Fuel fabrication parameters**		
Cycle length	1.23 y	1.4 y	Time	1 y	1 y
Core refueling	4-batch	3-batch	Losses	0%	0%
Core mass, h.metal	120.12 t	69.26 t	**Reprocessing parameters**		
Fuel parameters			Cooling time	5 y	5 y
Type	UOX	(U,Pu)C	Method	adv.PUREX	advanced
Discharge burn-up	55 MWd/kg	50 MWd/kg	Time	1 y	1 y
Enrichment	4.5%	–	Efficiency	99.9% for U, Pu, MA	

6.2. Results of the EPR-GFR2400 transition scenario

First, we determined the number of EPRs the spent fuel of which contains enough Pu to start one GFR2400. Detailed FITXS calculation showed that as t_{MA} increases $t_{\mathrm{Pu}}^{\mathrm{ini}}$ increases slightly while $t_{\mathrm{Pu}}^{\mathrm{rec}}$ decreases significantly, therefore we set t_{MA} to the closed cycle equilibrium value 1%. According to our results if the power of the EPR fleet was 1.8 or 1.9 times that of an EPR there was lack of Pu shortly before or few cycles after the start of the recycle, respectively. Therefore, the EPR fleet must contain at least two EPRs in order to accumulate enough Pu for the start-up and for the operation of one GFR2400.

Secondly, we investigated whether the GFR2400 can consume all MAs originating from two EPRs. In order to see the dependence on t_{MA}, we changed it between 1.0% and 2.5%. Figure 7 shows the results. In the scenarios with $t_{\mathrm{MA}} > 2.3\%$ there was lack of MAs since the GFR2400 consumed all MAs before the end of its lifetime. In the scenario with $t_{\mathrm{MA}} = 2.3\%$ only 0.2 t MAs left in stock. However, because of the MA content of the spent fuel altogether 4.4 t MAs remained in the scenario, which is 59% of the mass of the reprocessed MAs from the EPR spent fuel. The electrical energy production of the EPR fleet was 1339.7 TWh while the EPR-GFR2400 coupled fleet produced 1.4 times more energy. The specific MA accumulation in the two fleets was 5.55 kg/TWh and 2.35 kg/TWh.

According to Figure 7, the Pu content of the spent GFR2400 fuel determines the total amount of Pu left in the scenario. Amount of Pu left in the scenario behaves in opposite way than amount of MAs since as t_{MA} increases $t_{\mathrm{Pu}}^{\mathrm{rec}}$ decreases. If $t_{\mathrm{MA}} = 2.3\%$ altogether 38.2 t Pu remains in the scenario which is 1.12 times higher than the mass of Pu originating from the spent EPR fuel. The specific Pu accumulation in the coupled fleet is 20.4 kg/TWh which is 80% that of the EPR fleet. However, this reduction is the result of the increased energy production only.

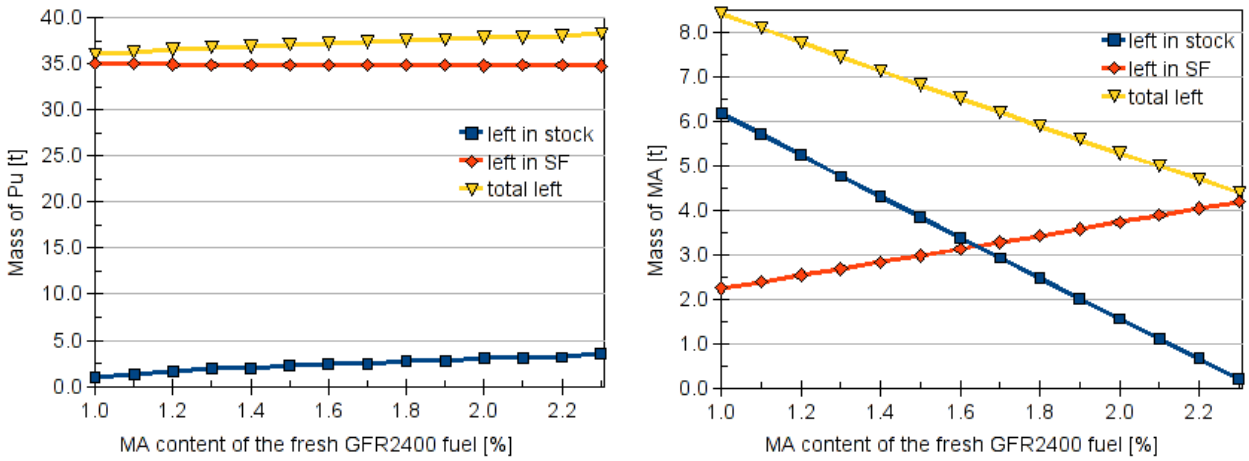


Figure 7. Mass of Pu (left) and MA (right) remained at the end of the scenario. SF: spent fuel.

7. Summary

The deployment of fast reactors, as well as strategic decisions concerning the closure of the nuclear fuel cycle demands detailed models, which are capable of modelling the most important facilities of the fuel cycle and the material flows between them. At the BME NTI a fast and flexible burn-up scheme called FITXS was developed based on the parametrization of one-group cross-sections as functions of the detailed fuel composition. The scheme was used to develop burn-up models for the Generation IV GFR, LFR and SFR reactors. The models

were integrated into fast reactor fuel cycle models and the closed cycle equilibrium parameters of the reactors were investigated. Results showed that the reactors are capable of breeding their own fissile material if both Pu and MAs are recycled from the spent fuel. Equilibrium core parameters showed good agreement with the results of the EQL3D procedure given in Krepel et al., confirming the accuracy of the developed burn-up models.

The FITXS burn-up model of the GFR2400 was integrated into the SITON fuel cycle simulation code developed at MTA EK. With this code, we analyzed an EPR-GFR2400 transition fuel cycle and found that the GFR2400 needed Pu from two EPRs to start and operate. The GFR2400 can consume all MAs originating from the spent EPR fuel however MAs left in the last discharged batches limit the MA reduction. In addition, the Pu left in the fuel cycle increases slightly due to improved breeding caused by fertile and fissile MAs.

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