Evaluating computational methods for modeling off-normal operation of gas centrifuge cascades

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Abstract

This work compares and evaluates different computational approaches for modeling off-normal operation of a gas centrifuge enrichment cascade.

The goal of this work focuses on developing the necessary understanding of potential misuse of enrichment cascades. The latter would allow more effective international safeguards designs and approaches. While it is straightforward to design an enrichment cascade under ideal conditions as a function of the theoretical feed, product and tails assays, it is very difficult to find reliable information about the behavior of a given cascade when the feed assay does not match the design value. Several methods have been developed to assess the behavior of an enrichment cascade in such circumstances. In addition of the cut (θ) those methods evaluate the feed to product, feed to tails and the product to tails enrichment ratio, respectively, α, β and γ, as a function of the cascade feed assay. As those four parameters depend on each other, determining two of them fully defines the other. The first approach consists of fixing θ and α recomputing the corresponding assays at each stages of the cascade. The second one maintains the ideal condition of the cascade (α and β fixed across the whole cascade), modifying θ value at each stage accordingly. Both approaches have been implemented into the Cyclus fuel cycle simulator[1, 2]. The third fixes θ and γ, using both α and β at each stage as free parameters. The third method has been investigated in [3].

Following a description of each method and an evaluation of differences between each approach, this work compares the results produced by these methods within scenarios involving misuse of enrichment cascades simulated using the dynamic nuclear fuel cycle simulator, Cyclus.

1 Motivation

Gas centrifuge cascades are usually designed to operate in an ideal manner, with no losses in separative work. To achieve such ideal configuration, the cascade is designed to be fed with a specific feed assay and produce the target enrichment while rejecting tails at a fixed assay.

With the current international tensions regarding enrichment capabilities, this work aims to measure the effectiveness of an enrichment cascade when used outside of its designed scope and quantify the attractiveness of such way to build up significant quantity of High Enriched Uranium (HEU).

The present work investigates the performance of an enrichment cycle when chaining gas enrichment cascades tuned for low enrich uranium production from natural uranium. As literature on the mater is for obvious reason limited, three behavior models have been implemented and used to evaluate the response of an enrich cascade when fed with different assays than the design one. This work also takes advantage of the Cyclus[1] fuel cycle capabilities to evaluate the assay values at equilibrium.

2 Theory

2.1 Centrifuge properties

The present work uses the analytical solution by Räetz [4] of the differential equation for the gas centrifuge as described in [5]. Centrifuge parameters, such as average gas temperature, T, peripheral speed, v, height, h, diameter, d, pressure ratio, x, feed flow rate, F, counter-current flow ratio, L/P, and efficiency, e have been chosen (Table 1) to match the cascade design describe in [5] and [3] using P1-type centrifuges.

Table 1: Summary of the centrifuge parameters.

T[K]	v[m/s]	h[m]	d[m]	x	F[mg/s]	L/F	e
320	320	1.8	0.105	10^3	13	2	1.0

2.2 Cascade Design

The cascade is built as an ideal cascade, with no losses in the separative work, which corresponds to $\alpha = \beta = const$ for all stages of the cascade, where α and β respectively represent the feed to product and the feed to tails enrichment factors. α and β can be expressed as function of the abundance (R) or the enrichment (N) of respectively the product (R', N') and the feed (R, N) and the feed and the tails (R'', N'') such as:

$$\alpha = \frac{R'}{R} = \frac{N'}{1-N'}\frac{1-N}{N} \tag{1a}$$

$$\beta = \frac{R}{R''} = \frac{N}{1-N}\frac{1-N''}{N''} \tag{1b}$$

As detailed in [6] it is also possible to derive α from the first principle, and express it as a function of the feed rate F, the separative performance $\delta U(\theta)$ and the cut θ:

$$\alpha = \sqrt{\frac{2\delta U}{F}\frac{1-\theta}{\theta}} + 1 \tag{2}$$

From the mass conservation, $N = \theta N' + (1-\theta)N''$, and equations (1) it is possible to express β as a function of the feed abundance, R, the cut θ and α:

$$\beta = R\left(\frac{1-\theta}{\frac{R}{R+1} - \theta\frac{\alpha R}{1+\alpha R}} - 1\right) \tag{3}$$

From equation (2) and (3) it is possible to determine the cut, θ required to build an ideal cascade:

$$\theta_i = \frac{N_i - \frac{1}{1+\beta/R_i}}{\frac{\alpha R_i}{1+\alpha R_i} - \frac{1}{1+\beta/R_i}} \tag{4}$$

As α_i and β_i remain constant, only the value of the cut, θ_i, changes across the different stages of a cascade. This algorithm assumes that the corresponding separative power δU (not re-computed) can be achieved with the chosen centrifuge design, tuning other operational parameter such as the rotation speed, the counter-current flow ratio, etc. Once θ_i is determined, it is possible to compute the product and the tail assay.

The design of the cascade is performed through 2 steps. First one determines the configuration and number of stages, adding stages until the product assay of the final stage is greater or equal the product targeted assay, and similarly the tails assay is less or equal the tails desired assay. This determines the number of enriching and stripping stages as well as their enrichment properties (N_i, N_i', N_i'',θ_ii).

The second step determines the relative flows at each stages, solving the linear flow equation, (5). The cascade can then be populated with actual machines until the maximum number available of machines is reached.

$$\begin{bmatrix} -1 & 1-\theta_{S+1} & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ \theta_S & -1 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 \\ & & & & & & \dots & & & & & \\ 0 & 0 & 0 & \dots & \theta_{-2} & -1 & 1-\theta_0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & \theta_{-1} & -1 & 1-\theta_1 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & \theta_0 & -1 & 1-\theta_2 & 0 & \dots & 0 \\ & & & & & & \dots & & & & & \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & -1 & 1-\theta_E \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 & \dots & \theta_{E-1} & -1 \end{bmatrix} \times \begin{bmatrix} F_S \\ F_{S+1} \\ \cdots \\ F_{-1} \\ F_0 \\ F_1 \\ \cdots \\ F_{E-1} \\ F_E \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 0 \\ F \\ 0 \\ \cdots \\ 0 \\ 0 \end{bmatrix} \quad (5)$$

2.3 Misuse models

Little information is available about optimising an existing enrichment cascade that is being fed with a feed enrichment that does not match the design one. So far 3 different methods have been investigated.

The first one assumes that no change are been made on the cascade, i.e δU, F and θ are fixed across all stages. The second one assumes the cut value at each stage is retuned to maintain the ideal state of the cascade, α and β remain fixed. The last one, described in [3] assumes the tails to product enriching factor and the cut remain constants ($\gamma = \alpha \times \beta$). Models behaviors and assumptions are summarized in Tab. 2.

Table 2: Summary of misuse model properties.

Model	A	B	C
Constant parameters	α_i, θ_i	$\alpha_i = \beta_i$	$\gamma_i = \alpha_i.\beta_i, \theta_i$
Varying parameters	β_i	θ_i	α_i, β_i
Assays determination	blended	ideal	blended
Flow	unchanged	reduced	unchanged

2.3.1 Model A

The tuning method A does not re-optimize θ_i keeping the same flow as the ideal configuration. From equation (2), maintaining δU, F and θ unchanged implies α remains unchanged as well. According to equation (3), when α and θ are fixed, if the feed assay (N) changes, β will change accordingly. This breaks the ideal status of the cascade, i.e. $N_i \neq N'_{i-1} \neq N''_{i+1}$.

In order to compute the proper product and tails assay at each stage, the tails and the product from the next and the previous stage respectively must be blended in order to determine the correct stage feed assay. All feed assays are iteratively updated, blending the proper product and tails, then using the updated feed assay, the new product and tails assays are recomputed. This process is repeated until the sum of the square difference in assays is smaller than 10^{-8}. As the cut remain fixed at each stage the flows do not need to be recomputed.

2.3.2 Model B

Using the second method, the cut value at each stage θ_i, is retuned in order to maintain the α_i and β_i at their original values (equation (4)). The cascade remaining ideal, the product and tails assay at each stages are easily determined using equations (1).

As the cut values change, the relative flow rates between the different stage are recomputed using equation (5). The flow rates are determinted as the largest flow rates allowed by the cascade design, number of centrifuges limiting the flow at each stage.

2.3.3 Model C

The last model assumes that the tails to product enrichment factor remains constant regardless to the feed assays. To compute the response of the cascade one need to determine α and β such that their product and θ remain fixed. From equations (1) and the assay conservation equation $N = \theta N' + (1-\theta)N''$ it is possible to express the product N' as a function of the feed assay N, γ and the cut θ as one solution of the second order equation (6):

$$\theta(\gamma-1)N'^2 + ((N+\theta)(\gamma-1)+1)N' - N\gamma = 0 \tag{6}$$

The only solution allowing product assay to range between 0 and 1 is the following :

$$N' = \frac{N+\theta}{2\theta} + \frac{1-\sqrt{\gamma^2(N-\theta)^2 + 2\gamma(N^2+N-\theta^2+\theta) + (N+\theta+1)^2}}{2\theta(\gamma-1)} \tag{7}$$

Once the product assay is known, one can trivially determine the tails assay, α and β using equations (1) and mass conservation.

Similar to model A, because the cut values remain constant, the flows don't need to be recomputed, and the correct assays, α and β are determined through iterative blending of the product assays of the previous stage and the tails assay of the next stage using equation (7).

3 The experiment

This works focuses on comparing the different misuse models to a reference calculation in which a single large cascade is build and designed to directly produce HEU from natural uranium. This works uses the Cyclus fuel cycle simulator to allow material exchange between facilities. The enrichment cascade algorithm have been implemented in the *mbmore* package [2]. In each cases, 5060 centrifuges have been used and spread across up to 30 different gas enrichment cascades.

3.1 The cascade configuration

3.1.1 Reference

As mentioned, all the further calculations will be compared to the most favorable configuration to produce HEU, where all the available centrifuges are used in a single large cascade designed to directly produce HEU from natural uranium, with a tails assay close to $0.3w\%$. The design characteristic of the reference cascade are summarized in Table 3.

3.1.2 Default cascade

The default cascade is the cascade design for normal civilian enrichment operation, enriching natural uranium to about $3.5w\%$, with a tails assay close to $0.3w\%$. This cascade will be layered and fed with uranium at higher enrichment to evaluate the possibility to use them, with little or no tuning, to produce HEU. The characteristics of the default cascade are summarized in Table 3.

Table 3: Summary of cascade design.

Cascade Design		Reference	Default
Targeted Assays	Feed	$0.71w\%$	$0.71w\%$
	Product	$90w\%$	$3.5w\%$
	Tails	$0.3w\%$	$0.3w\%$
Effective Assays	Product	$90.35w\%$	$4.13w\%$
	Tails	$0.29w\%$	$0.29w\%$
Stages Number	Enriching	4	4
	Stripping	39	10

3.2 Scenarios

In the following, cascades can be connected in tandem, where each set of cascade in parallel is called a “level“, as illustrated in Figure 1. Seven different simulations have been simulated, to evaluate the effectiveness of an enrichment cascade when used outside of its designed scope :

- one as the reference calculation, with a single cascade designed to directly produce HEU from natural uranium,
- three calculations (one per misuse model) where default cascade are chained to produce HEU, without recycling the tails of each cascade sending their tails to the waste,
- three calculations (one per misuse model) where default cascade are chained to produce HEU, and the tails of each cascade are recycled, blending the tails of one level in the feed of the previous level of cascades (see Figure 1).

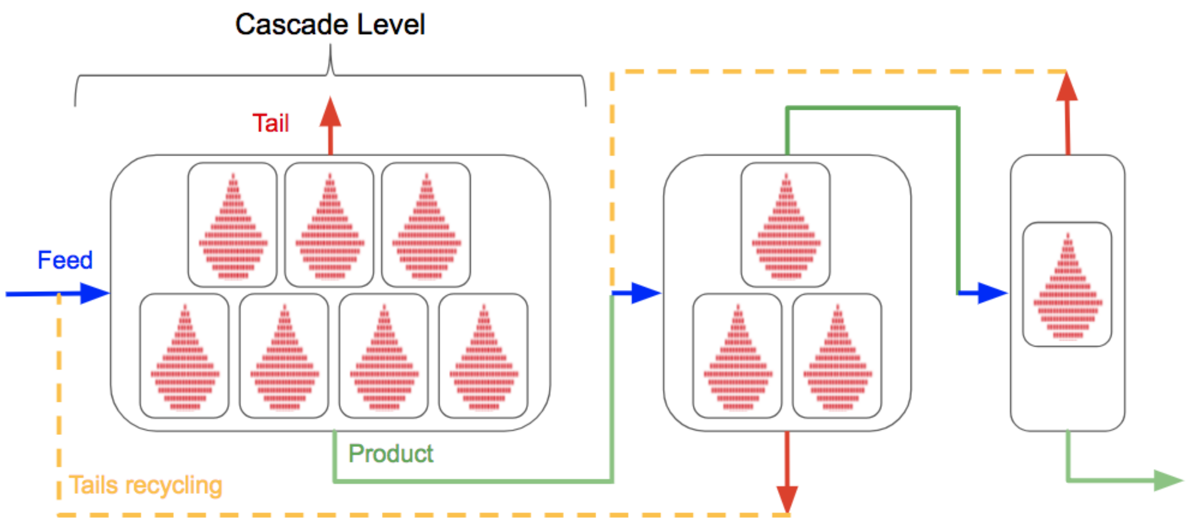


Figure 1: Schematic representation of the chained cascades with three levels, with the feed, product and the tails flows, in blue, green and red, respectively. The dashed orange line represent the alternative tails flow when tails recycling is considered.

3.3 Level population

In order to assign the optimum number of cascades to each level, a virtual cut as been computed as:

$$\theta_j^v = \frac{F_j - N_j''}{N_j' - N_j''}, \tag{8}$$

where, j represents a level of cascade and N_j, N_j' and N_j'' the feed, product and tails assay, respectively, of the cascades at this level.

A flow equation similar to (5) is then solved to obtain the optimum number of cascade per level. When the tails are not recycled, the $(1-\theta)$ terms are removed from the flow equation. The results of the level population are summarized in Table 4.

As it is not possible to assign a fraction of an enrichment cascade, cascade per level are rounded up for each level but the first one. The remaining available cascades is attributed to the first level.

3.4 Timestep effect

As it can be observed in Figures 2, 3 and 4, the different cascade levels required up to $2n+1$ timesteps before it starts to enrich uranium, where n corresponds to the level number. This corresponds to the number of timesteps required for the material to propagate from the natural uranium source to the n-th level, regardless of the duration of the timestep (hour, day, month, etc.). This is also true for the number of timesteps required to reach the equilibrium assays value in the tails reprocessing cases. As timestep can be artificially small or large, one will only be considering equilibrium values of flow rates and assays in the following analysis.

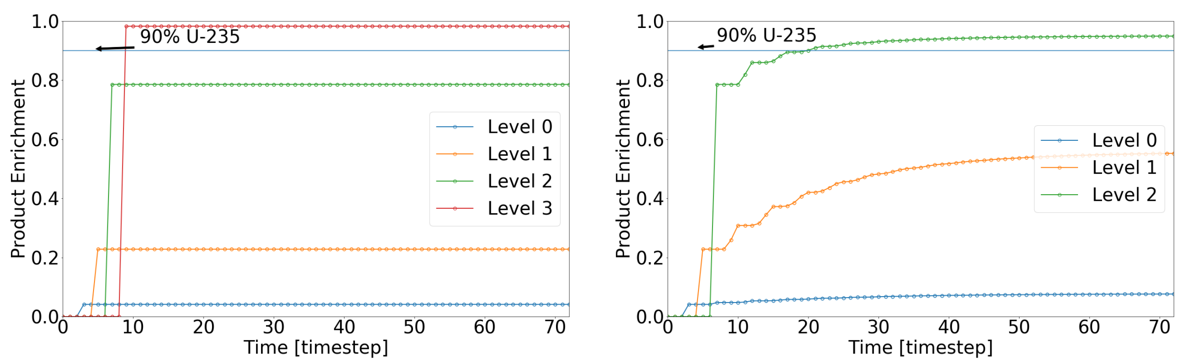
4 Results

4.1 Miss-use modeling

Table 4: Summary of cascades level population.

Model			A/NR	A/R	B/NR	B/R	C/NR	C/R
		Feed	$0.71w\%$	$1.3w\%$	$0.71w\%$	$0.94w\%$	$0.71w\%$	$1.66w\%$
Level 0	Assay	Product	$4.13w\%$	$7.7w\%$	$4.13w\%$	$5.43w\%$	$4.13w\%$	$9.53w\%$
		Tails	$0.29w\%$	$0.5w\%$	$0.29w\%$	$0.39w\%$	$0.29w\%$	$0.69w\%$
	Cascades		25	25	25	24	25	25
		Feed	$4.13w\%$	$11.9w\%$	$4.13w\%$	$6.84w\%$	$4.13w\%$	$13.0w\%$
Level 1	Assay	Product	$22.8w\%$	$55.7w\%$	$20.6w\%$	$30.7w\%$	$22.9w\%$	$69.8w\%$
		Tails	$1.8w\%$	$6.6w\%$	$1.72w\%$	$2.91w\%$	$1.81w\%$	$9.43w\%$
	Cascades		3	4	3	4	3	4
		Feed	$22.8w\%$	$55.7w\%$	$20.6w\%$	$34.3w\%$	$22.9w\%$	$72.6w\%$
Level 2	Assay	Product	$78.5w\%$	$95.0w\%$	$61.0w\%$	$75.8w\%$	$82.0w\%$	$98.4w\%$
		Tails	$4.12w\%$	$50.9w\%$	$9.56w\%$	$17.5w\%$	$15.7w\%$	$69.4w\%$
	Cascades		1	1	1	1	1	1
		Feed	$78.5w\%$	N.A.	$61.0w\%$	$75.8w\%$	$82.3w\%$	N.A.
Level 3	Assay	Product	$98.2w\%$	N.A.	$90.4w\%$	$95.0w\%$	$99.1w\%$	N.A.
		Tails	$76.1w\%$	N.A.	$79.3w\%$	$56.1w\%$	$80.3w\%$	N.A.
	Cascades		1	N.A.	1	1	1	N.A.

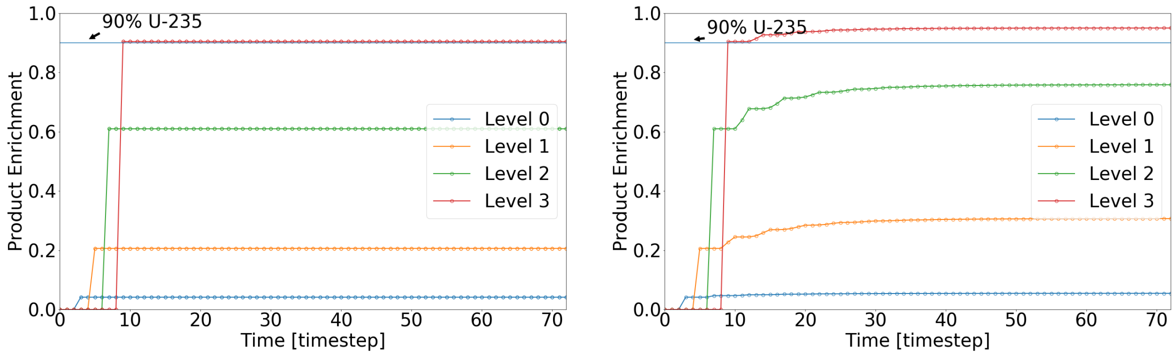
As illustrated in Figures 2a, 3a and 4a and summarized on Tab 4, the different model don't have the same effect on the cascade behavior. While the models A and C, allow a quick enrichment gain, with the cascades chaining, respectively 4/23/78/98 and 4/23/82/99, the model B, the enrichment gain is only 4/21/61/90.



(a) No tails recycling

(b) Tails recycling

Figure 2: Evolution of the product assays at each level with considering misuse model A, with (right) and without recycling (left).

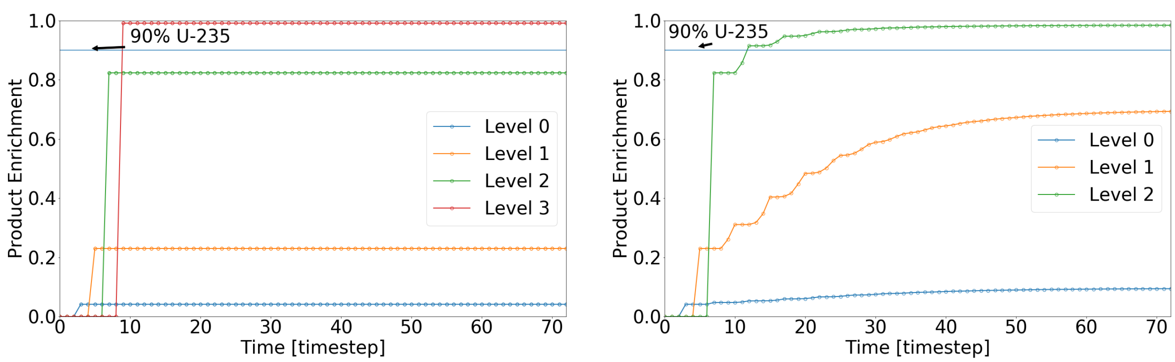


(a) No tails recycling (b) Tails recycling

Figure 3: Evolution of the product assays at each level with considering misuse model B, with (right) and without recycling (left).

4.2 Tails recycling

As shown in Figures 2b, 3b and 4b, recycling the tails increases the overall product assay at all the different levels. As the tails assay of a level $n+1$ is always higher than the product assay of the level $n-1$, recycling the tails of level $n+1$ will consequently increase the feed assay of level n (see Table 4). Moreover, with an increased feed assay, tails and product assays increase as well, increasing de facto the feed assays of respectively cascade levels $n-1$ and $n+1$, etc. This effect reduces the number of cascade levels required to reach HEU in case A and C.



(a) No tails recycling (b) Tails recycling

Figure 4: Evolution of the product assays at each level with considering misuse model C, with (right) and without recycling (left).

4.3 HEU Production

As shown in Figure 5, recycling increases the final HEU production rate, from 2 to almost 20 kg/y when using models A and C, and from 17 to 38 kg/y with the model B. For the reference calculation where all the available cascades are used within a single large cascade design for direct HEU production, the HEU production rate is slightly over 50 kg/y.

As models A and C, rely on maintaining the cut values at each stages of the cascade and share the same number of levels, have the exact same cascade repartition across the different levels and the same HEU production rate.

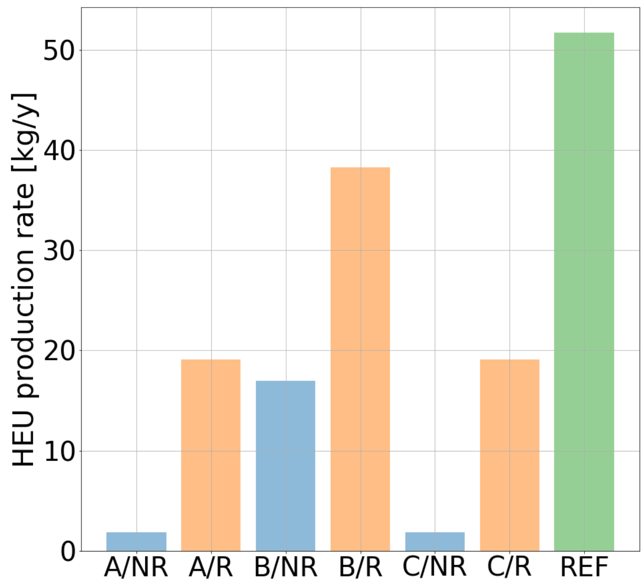


Figure 5: Production rate at equilibrium for the different model configurations, the case without tails recycling (blue), with tails recycling (orange), and the reference one (green). A-B-C represent the model used, and NR-R the case without tails recycling and the case with tails recycling, respectively.

5 Discussion

We can observe that when the cascade is left completely untouched (Model A) or when it is slightly retuned to maintain the tails to product enrichment factor as well as the cut of each centrifuges (Model C), chaining the cascade we can observe high increase of the enrichment at each level. On the contrary, when retuning the cut of each centrifuges to maintain the ideal state of the cascades (Model B) while chaining them, the HEU production rate is favored over the enrichment gain.

The tails recycling allows each model to achieve a large gain in productivity, even for then model B in which the number of levels required to reach $90w\%$ of ^{235}U in the uranium does not change. Even if no cascade chaining options achieves the same production rate as direct enrichment, the model B with tail recycling reached about 80% of the optimum production rate. Such production rate would allow the build up of a Significant Quantity of HEU in less than 8 months. . .

6 Conclusion and future works

This works has investigated and quantify the difference between potential retuning of a gaseous enrichment cascade in order to chain them to produce HEU initially tuned to produce uranium enrichment for commercial reactors. One of this tuning method allows up to 80% of the production rate of a single large enrichment cascade designed specifically for HEU production using the same number of centrifuges.

This works will be extended to the near future with additional misuse method, allowing for example the reconfiguration of the centrifuges in the cascades.

For this study, the usage of the Cyclus fuel cycle simulator was not really required, it only allows a quick determination of the blending equilibrium. It is planned to make use of the Cyclus Dynamical Resource Exchange full capability in order to automatically assign the different cascades to the different level as function of the resources availability, optimising the productions rates in each cases.

While mathematically correct, the authors do not guaranty the feasibility different misuse tuning methods implemented and are welcoming any insight on the matter.

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