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

Baptiste Mouginot[1], Kathryn Mummah[1], Paul P.H. Wilson[1]

[1]*Department of Nuclear Engineering and Engineering Physics, University of Wisconsin-Madison*

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 to design more effective and efficient international safeguards 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, those methods evaluate the cut, the feed to product, feed to tail and the product to tail enrichment ratio, respectively, alpha, beta and gamma, as a function of the cascade feed assay. As those four parameters depends on each other, determining two of them allows to compute the other. The first approach consists of fixing the cut and alpha recomputing the corresponding assays at each stages of the cascade. The second one maintains the ideal condition of the cascade (alpha and beta fixed across the whole cascade), modifying the cut value at each stage accordingly. Both approaches have been implemented into the Cyclus fuel cycle simulator[1, **?**]. The third fixes the cut and gamma, using both alpha and beta at each stage as free parameters. The third method has been investigated in [2].

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 ideal manner, with no losses in separative work, the most effective way. 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 fix 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 amount of High Enricht Uranium (HEU).

The present work investigates the performance of a enrichment cycle when chaining gas enrichment cascade 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 takes also advantage of the Cyclus[1] fuel cycle capabilities to evaluate the assay blending equilibrium.

2 Theory

2.1 Centrifuge properties

The present work uses the analytical solution by Räetz [3] of the differential equation for the gas centrifuge as described in [4]. 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 [4] and [2]. These parameters for a P1-type centrifuge are used to estimate the JCPOA-compliant IR-1 centrifuge.

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	$1e3$	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 stage of the cascade, where α and β respectively represent the feed to product and the feed to tail 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 [5] 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 $\delta U(\theta)$, 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:

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

From equation (2) and (3) it is possible to determine the cut, θ, or the ratio of product flow to feed flow required to build an ideal cascade: β values and the feed assay, N_i:

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

Since α_i and β_i remain constant, only the value of the cut, θ_i, changes in each stage i 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... 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 than or equal to than the desired assay, and the tails assay is similarly less than or equal to the desired tails 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 how to populate the cascade with the user-defined maximum number of centrifuges.

One solves the linear flow equation, (5), to determine the theoretical flow in the cascade.

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

Once the relative flow of each stage has been determined, the cascade can be populated with actual machines up the stages until the maximum number available of machines is reached.

2.3 Miss-use 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, the second one, assumes that the cut value at each stage is retuned to maintain the ideal state of the cascade, the last one, described in [2] assumes the tails to product enriching factor remains constants ($\gamma = \alpha \times \beta$). Models behavior, and assumptions are summarized in Tab. 2.

2.3.1 Model A

The tuning method A does not re-optimize θ_i based on the true flow enrichment. As δU and α do not depend on the stage feed assay (N'), they do not change from stage to stage. According to equation (3),

Table 2: Summary of miss-use model properties.

Model	A	B	C
Constant parameters	α_i, θ_i	$\alpha_i = \beta_i$	$\gamma_i = \alpha_i * \beta_i, \theta_i$
Optimised parameters	β_i	θ_i	α_i, β_i
Assays determination	blended	ideal	blended
Flow	unchanged	scaled	unchanged

when α and θ are fixed, when the feed assay (N) changes, then 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 respectively the next and the previous stage must be blended in order to determine the correct stage feed assay. As this is a obvious cycling problem, an iterative solution has been chosen: all feed assays are iteratively updated, blending the proper product and tails, then using the updated feed assay, the new product and tail assays are recomputed. This process is repeated until the change in assays is smaller than the set precision (1e-8 by default). As the cut remain fixed at each stage the different flow do not need to be recomputed.

2.3.2 Model B

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. As the cascade remains ideal, the product and tail assay at each stages (and for the overall cascade) is easily determined using equations (1).

As the cuts values change, the flow rate between the different stage has to be recomputed. Because the cascade is not reorganised (the number of cascade per stage remain the same as the original design). The new flow rate are computed as the flow rates of the reconfigured cascade scaled down by the possible flows of the original one: the flow rates of a reconfigured cascade are computed, the ratios of the flow stage by stage with the original are determined, the smaller ratio is used to scale down all the flow rates.

2.3.3 Model C

The last model assumes that the tail 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 as 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):

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

The only solution allowing product assay values ranging between 0 and 1 is the following :

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

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

Similarly as 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 miss use 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.

3.1 The cascade configuration

3.1.1 reference

As mentioned previously, 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 tail assay close to $0.3w\%$ uranium. 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 $3.5w\%$. This cascade will be layered and fed with uranium at higher enrichment to evaluate the possibility to used them, with few 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	Feed	$0.71w\%$	$0.71w\%$
Assays	Product	$90w\%$	$4.0w\%$
	Tail	$0.3w\%$	$0.3w\%$
Effective	Product	$90.35w\%$	$4.13w\%$
Assays	Tail	$0.28w\%$	$0.28w\%$
Stages	Enriching	4	4
Number	Stripping	39	10

3.2 scenarios

Seven different simulations have been simulated:

- one as the reference calculation, with a single centrifuges designed to produce directly HEU from natural uranium,

- three calculations (one per miss-use model) were default cascade are chained to produce HEU, without recycling the tails of each cascade, the cascade tails are directly sent to the waste,
- three calculations (one per miss-use model) were default cascade are chained to produce HEU, the tails of each cascade are recycled, blending the tail of one level in the feed of the previous level of cascades (see Figure 1.

In the following, cascades can be connected in tandem, where each set of cascade in parallel is called a "level", as illustrated on Figure 1.

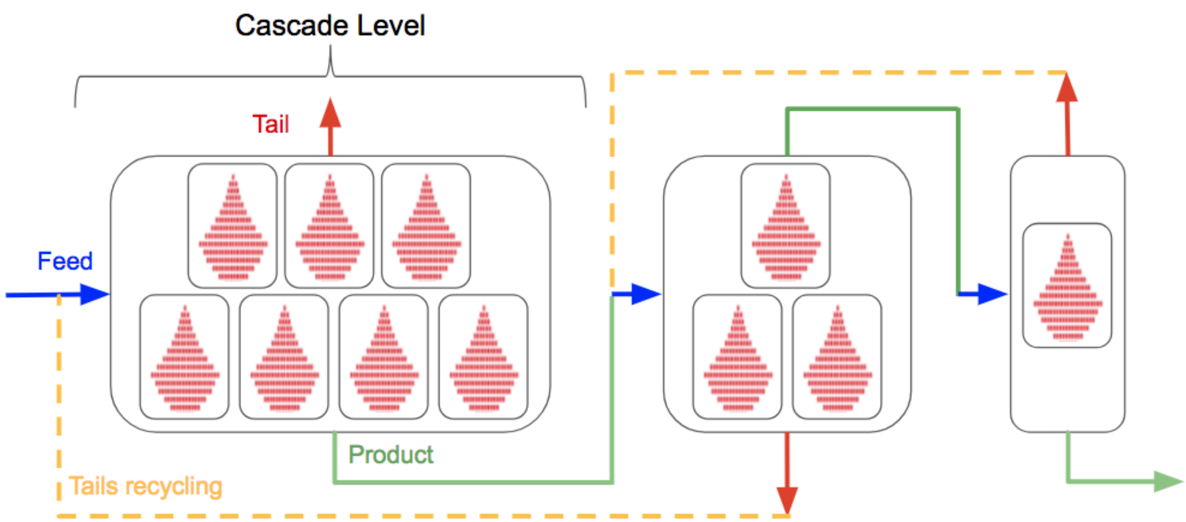


Figure 1: Schematic representation of the chained cascades with three levels, with the feed, product and the tail flows, respectively in blue, green and red. The dashed orange line represent the alternative tail flow with recycling them.

3.3 Level population

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

$$\theta_i^v = \frac{F_i - T_i}{P_i - T_i}, \tag{8}$$

where, i represents a level of cascade and F_i, P_i and T_i respectively the feed, product and tail assay of the cascades at this level.

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

3.4 Timestep effect

As it can be observed on Figures 2, 3 and 4, the different cascade levels required up to $2n+1$, with n the level number to start enriching uranium. This corresponds to the time required for the material to propagate from the natural uranium source to the level, regardless of the duration of the timestep (hour, day, month,...). This is also true for the number of timestep required to reach the equilibrium assays value in the tail reprocessing cases. This is why one will only consider equilibrium values.

4 Results

4.1 Miss-use modeling

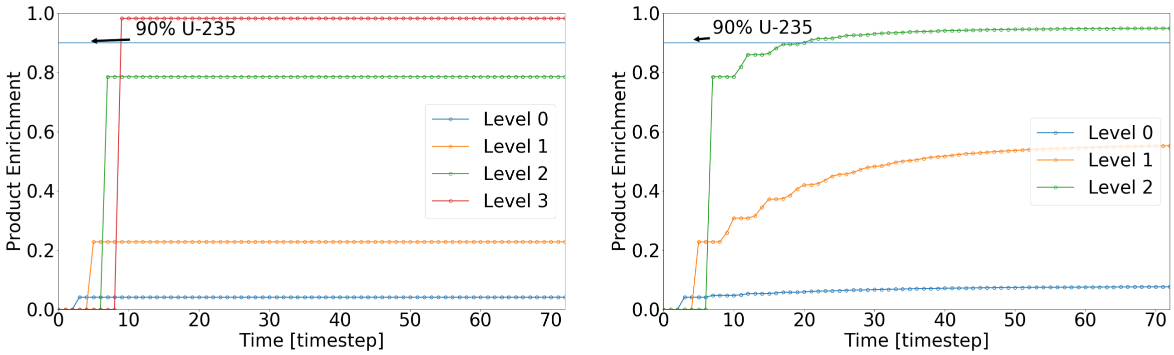
Table 4: Summary of cascades level population.

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	$4.13w\%$	$7.7w\%$	$4.13w\%$	$5.43w\%$	$4.13w\%$	$9.53w\%$
		Tail	$0.29w\%$	$0.5w\%$	$0.29w\%$	$0.39w\%$	$0.29w\%$	$0.69w\%$
	Cascades		26.73	26.45	26.6	25.8	26.73	26.45
		Feed	$4.13w\%$	$11.9w\%$	$4.13w\%$	$6.84w\%$	$4.13w\%$	$13.0w\%$
Level 1	Assay	Product	$22.8w\%$	$55.7w\%$	$20.6w\%$	$30.7w\%$	$22.9w\%$	$69.8w\%$
		Tail	$1.8w\%$	$6.6w\%$	$1.72w\%$	$2.91w\%$	$1.81w\%$	$9.43w\%$
	Cascades		2.92	3.20	2.91	3.41	2.92	3.20
		Feed	$22.8w\%$	$55.7w\%$	$20.6w\%$	$34.3w\%$	$22.9w\%$	$72.6w\%$
Level 2	Assay	Product	$78.5w\%$	$95.0w\%$	$61.0w\%$	$75.8w\%$	$82.0w\%$	$98.4w\%$
		Tail	$4.12w\%$	$50.9w\%$	$9.56w\%$	$17.5w\%$	$15.7w\%$	$69.4w\%$
	Cascades		0.31	0.35	0.37	0.64	0.32	0.35
		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.
		Tail	$76.1w\%$	N.A.	$79.3w\%$	$56.1w\%$	$80.3w\%$	N.A.
	Cascades		0.03	N.A.	0.080	0.18	0.03	N.A.

As illustrated on 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... The same effect is observed when recycling the tails...

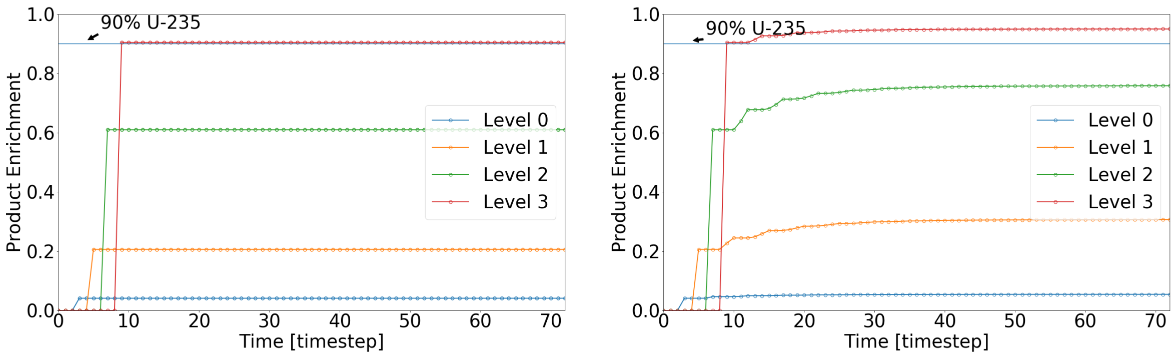
4.2 Tails recycling

As demonstrated on Figures 2b, 3b and 4b, recycling the tails increases the overall product assay at all the different levels. As shown on Table 4, the tail assay of level n is always higher than the product assay of level $n-2$, recycling the tails of level n will consequently increase the feed assay of level $n-1$. Moreover, as the feed assay of level $n-1$ increases, its tail and product assays increase as well, increasing de facto the feed assays of respectively cascade levels $n-2$ and n... This effect allow to reduce the number of cascade levels required to reach HEU in case A and C.



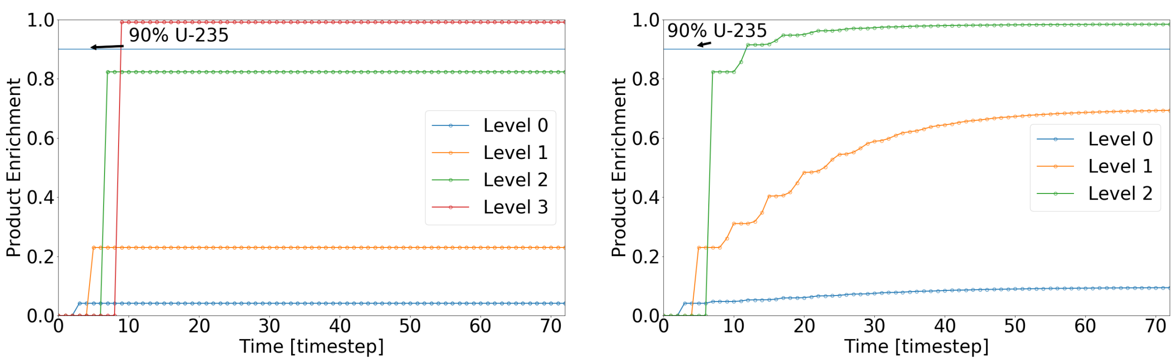
(a) No tail recycling (b) Tail recycling

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



(a) No tail recycling (b) Tail recycling

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



(a) No tail recycling (b) Tail recycling

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

4.3 HEU Production

As shown Figure 5, recycling increases the final HEU production rate, from 2 to almost 20 kg/y when using model 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 Model A and C, relies on maintaining the cut values at each stages of the cascade and share the same number of levels, both the same repartition of cascades across the different levels and then the same HEU production rate.

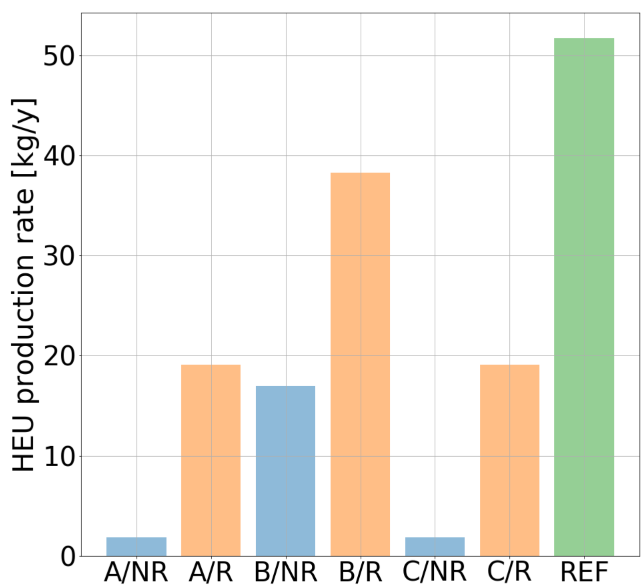


Figure 5: Production rate for the different model configuration, with in blue the case without tail recycling, in orange with tail recycling, and in green the reference one. Where A-B-C represent the model used, and NR-R respectively the case without tail recycling and the case with tail recycling

5 Discussion

It is really interesting to observe that when the cascade is left completely untouched (Model A) or when it is slightly retuned to maintain the tail to product enrichment factor as well as the cut of each centrifuges, 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 while chaining them, the HEU production rate is favored over the enrichment gain.

The tail recycling allows for each model a huge gain in productivity, even for then model B for which it does not change the number of levels required to reach 90$w\%$ of ^{235}U in the uranium. Even if no cascades chaining also to retrieve the same production rate as a direct enrichment, the model B with reprocessing reach about 80% of an optimum production, which is far from being negligible…

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 miss-use 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 miss-use tuning methods implemented and are welcoming any insight on the matter.

7 Acknowledgments

This work was funded by the Consortium for Verification Technology under Department of Energy National Nuclear Security Administration award number DE-NA0002534

References

[1] K. HUFF, M. GIDDEN, R. CARLSEN, R. FLANAGAN, M. MCGARRY, A. OPOTOWSKY, E. SCHNEIDER, A. SCOPATZ, and P. WILSON, "Fundamental concepts in the Cyclus nuclear fuel cycle simulation framework," *Advances in Engineering Software* (April 2016).

[2] M. E. WALKER and R. J. GOLDSTON, "Timely Verification at Large-Scale Gas Centrifuge Enrichment Plants," *Science & Global Security*, **25**, *2*, 59–79 (2017).

[3] E. RÄTZ, *Analytische Lösungen für die Trennleistung von Gaszentrifugen zur Urananreicherung*, PhD dissertation, echnical University of Berlin (21983).

[4] A. GLASER, "Characteristics of the Gas Centrifuge for Uranium Enrichment and Their Relevance for Nuclear Weapon Proliferation," *Science & Global Security*, **16**, *1-2*, 1–25 (2008).

[5] D. G. AVERY and E. DAVIES, *Uranium enrichment by gas centrifuge [by] D. G. Avery, E. Davies*, Mills and Boon London (1973).