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 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, 2]. 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 [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 theory

1.1 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]. These parameters for a P1-type centrifuge are used to estimate the JCPOA-compliant IR-1 centrifuge.

Tab. 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

1.2 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 abondance (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 detailled 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 $\delta U(\theta)$, 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 abondance, 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, or the ratio of product flow to feed flow required to build an ideal cascade: β values and the feed assay, N_i:

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

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 operationnal paramter 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.

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

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.

1.3 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 [3] assumes the tails to product enriching factor remains constants ($\gamma = \alpha \times \beta$). Models behavior, and assumptions are summarized in Tab. 2.

Tab. 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

1.3.1 Case 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),

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.

1.3.2 Case 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.

1.3.3 Case 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).

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