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# Bias identification and estimation based on data reconciliation and first-principle model – application to nuclear fuel recycling process

Amandine Duterme[a*], Marc Montuir[a], Binh Dinh[a], Julia Bisson[b], Nicolas Vigier[c], Pascal Floquet[d], Xavier Joulia[d]

[a]*CEA Marcoule, Nuclear Energy Division, Research Department on Processes for Mining and Fuel Recycling, 30207 Bagnols-sur-Cèze, France*

[b]*ORANO, La Hague Plant, Technical Department, 50444 Beaumont-Hague, France*

[c]*ORANO, La Défense, Technical Department – R&D, 92400 Courbevoie, France*

[d]*Laboratoire de Génie Chimique, Université de Toulouse, CNRS, INP, UPS, Toulouse, France*

*amandine.duterme@cea.fr*

## Abstract

This work comes within the scope of a state estimation tool built on a simulation code for the nuclear fuel treatment process. The first step is to reduce the uncertainty of simulation code input data in order to estimate key performance indicators accurately. This paper focuses on the data reconciliation technique (DR). DR improves the degree of confidence in available information and generates consistent data. The inventory and analysis of the plant data (position and type of sensors …) enable an evaluation of the process redundancy. When many biases are present in the data, classical Gross Error Detection and Identification (GEDI) techniques delete the biased variables, decreasing the redundancy. This leads to information loss and possibly an inability to apply DR. The methodology proposed here combines DR and simulations to locate and estimate multiple biases and to make data consistent in case of inter-connected flows.

**Keywords**: simulation, nuclear fuel treatment, data reconciliation, bias estimation.

## 1. Introduction

A measurement intrinsically possess uncertainty that prevents straightforward closure of mass and energy balances. In the data reconciliation (DR) methodology, accuracy is given to the measurements by exploiting redundancies in process data and physical constraints, from steady-state mass balances (Simpson et al., 1991) to nonlinear dynamic constraints (Liebman et al., 1992).

There are two main approaches to dealing with gross errors that impact DR. The first uses Gross Error Detection and Identification (GEDI) methods (Narasimhan and Jordache, 2000) and sequentially deletes the biased variables from the DR. The redundancy, which implies the ability of DR to correct the measurements in order to satisfy the process constraints, is reduced. However, performances of DR and GEDI are still limited in disrupted cases, such as multiple flows between two units, numerous gross errors, and the position and magnitude of gross errors (Corderio do Valle et al. 2018). The second

approach, not discussed in this study, modifies the objective function of DR to mitigate the effect of gross errors (Fuente, M.J. et al. 2015).

A new methodology for a nonlinear system, combining the DR approach and a first-principle model, is proposed here. It prevents the removal of the biased variables from the measurement set. The bias estimation is performed by the model, which enables the maximum redundancy to be kept. With a set of consistent input data generated by DR, the simulation can precisely estimate key indicators.

## 2. System description

The PUREX process (Dinh et al., 2008) carries out the treatment of spent nuclear fuel. Spent fuel contains the elements of interest, uranium and plutonium, and the waste, i.e. fission products. TBP (tributyl-phosphate) is the extractive molecule used to recover and purify uranium and plutonium through interconnected liquid-liquid extraction steps. For the final products, very specific features in terms of purity as well as extraction efficiency are required. In order to reach the necessary high performances, the metal loading of the solvent (metal mass flowrate in the solvent for a specific TBP mass flowrate) must be precisely controlled. This ratio is a sensitive parameter which deeply impacts the process state (Bisson et al., 2016). Therefore, DR aims to reduce uncertainty on this key process indicator by giving reliable input data to the simulator of the PUREX process.

This study deals with an extraction-stripping step of the PUREX process where many sensors are implemented, and can be separated into two categories. Major consideration is given to a specific set of sensors essential for operation, control, and to respect the safety regulations (multiple sensors, regular checking, preventive maintenance, etc.). They are listed as reference information for the industrial plant. The secondary sensors are not used for process control or for industrial safety. They give additional information, increasing redundancy, which can help process state estimation. Some of this additional data can have biases non-detectable with previously-acquired data. A scenario is defined in order to encounter identified causes of GEDI performance loss (Corderio do Valle et al., 2018): the biases concern flows connecting the same two units, and their suppression leads to the system being non-redundant.

The initial graph of the PUREX process (Figure 1a) contains information about flows (directed arcs) and units (nodes). The redundancy graph (Figure 1b) is free of internal non-measured physical quantities: arcs depict constraints linking measurements of interest from one unit to the other. The measured variables used in the DR problem are volumetric flowrates, densities for each arc, temperature, and uranium, plutonium, nitric acid and TBP composition for specific arcs. The identified biases are all located on internal and output flowrates measured by secondary sensors.

For the classical GEDI methodology, each time a bias is detected, the redundancy decreases (Narasimhan and Jordache, 2000). The bias removal graph (Figure 1c) shows this loss of redundancy: DR cannot be applied on the aggregated node (IV+V+VIII+X+XI+XII), as only the calculation of the biases on output flowrates is possible in this scenario. In addition, classical GEDI techniques cannot locate a bias within two-way arcs between two units, such as between IV and VIII.

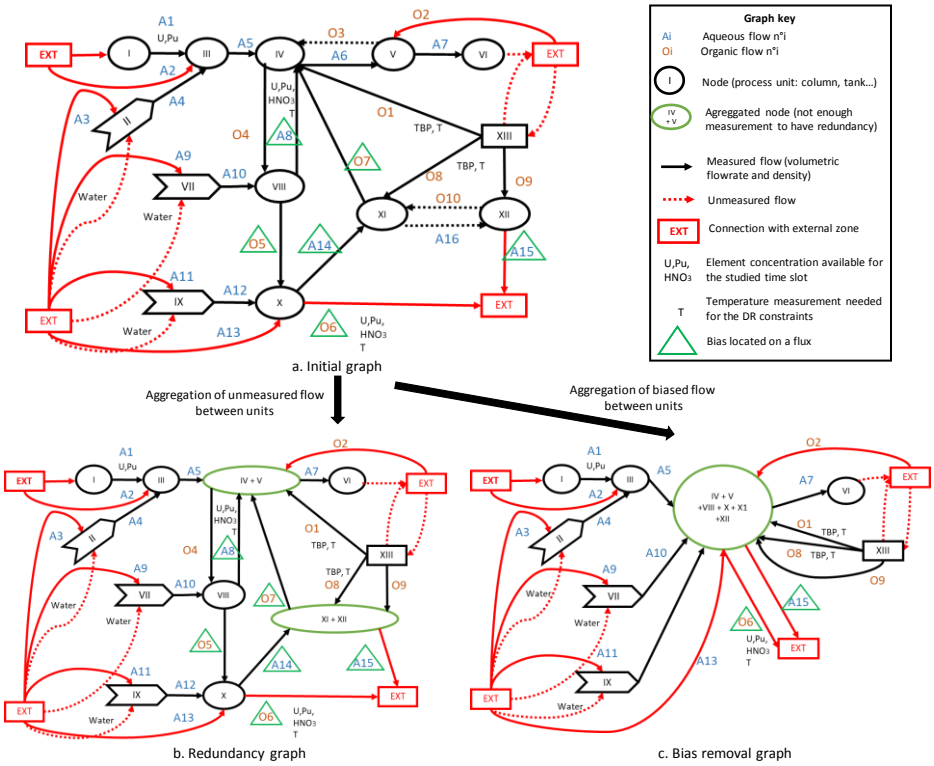


Figure 1: Graphs of an extraction-stripping step of the PUREX process.

The methodology proposed in this paper benefits from the PAREX simulation code developed and validated by the CEA (Dinh et al., 2008). It is based on first-principle models to simulate the PUREX process, notably taking into account the partitioning of the species, the transfer, and chemical kinetics.

## 3. Methodology

Graph theory can be used to classify data in order to distinguish observable (measured or calculable) data from non-observable data. Among observable data, three categories can be defined: redundant data (deleting this measurement does not change the system observability), non-redundant and measured data, non-measured data. The redundant data are reconciled.

The $n$ measurement vector $X^B$ is linked to the true value of the measured variables $X^T$, the random error $\varepsilon^B$ (assumed to be independent, with a zero mean and normally distributed), and the gross error $B$, here, the bias, by the following equation:

$$X^B = X^T + \varepsilon^B + B \tag{1}$$

Data reconciliation consists of minimizing an objective function ($OF$) constrained by a set of constraints $f$:

$$\underset{X^R,B}{Min}((X^B - B) - X^R)^T V^{-1}((X^B - B) - X^R)$$
$$s.t. f(X^R, \theta) = 0 \tag{2}$$

where $X^R$ is the $n$ reconciled values vector, $V$ the $(n,n)$ covariance matrix of the measured data, and $\theta$ the parameters of the system. $X^R$ are the best estimates of process variables, in the sense of the maximum likelihood. A study of the redundant variables, depending on the process topology and the number of independent equations, enables the determination of the ability of the DR to calculate a consistent set of reconciled data.

Because the entire PAREX model cannot be directly used as the constraints $f$ for the DR, a simplified model was built. It was made up of a selection of PAREX nonlinear equations specially chosen in order to exploit all information available from the measurements (flowrates, densities, temperatures, and compositions). In particular, it contains the total and partial mass balances (uranium and plutonium), density models, and nitric acid dilution equations.

The difficulty lies in simultaneously estimating biases $B$ and reconciling redundant data $X^R$. A new methodology is proposed (Figure 2) to perform bias estimation outside the DR by an iterative strategy. First, a map of the process (list of fluxes, units, sensors, uncertainties etc.) is built offline to generate the redundancy graph (Figure 1b). The second step makes use of process expertise to detect and identify biases located on secondary sensors, concerning measurements on internal or output fluxes. An initial PAREX simulation with raw measurements $X_e{}^B$ as input data gives a first estimation for the biases $B^{C(0)}$. As regards the vector of the calculated bias $B^C$, each element is null except for the identified biased output variables. These elements are equal to the difference between the biased measurements $X_s{}^B$ and the PAREX calculated outputs $X_s{}^C$.

The DR is then solved iteratively with respect to $X^R$ only, the values of biases $B^{C(i)}$ being considered fixed:

$$\begin{aligned} &\underset{X^R}{Min}((X^B - B^{C(i)}) - X^R)^T V^{-1}((X^B - B^{C(i)}) - X^R) \\ &s.t.\, f(X^R, \theta) = 0 \end{aligned} \tag{3}$$

Therefore, the process redundancy is unreduced by biases. To solve the nonlinear steady-state DR problem, this study uses the Fmincon function of Scilab software. The uncertainty for reconciled values is estimated at each DR solution by uncertainty propagation (Narasimhan and Jordache, 2000).

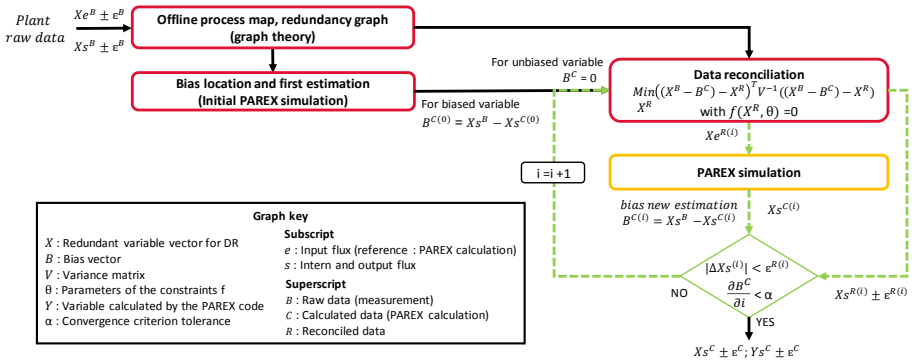


Figure 2: Bias identification and estimation methodology

At iteration i, the reconciled values of the input fluxes $X_e{}^{R(i)}$ are transferred to PAREX. The reconciled and calculated output flow information, $X_s{}^{R(i)}$ and $X_s{}^{C(i)}$ respectively, are compared. If the difference $|\Delta X_s{}^{C\text{-}R(i)}|$ between them is smaller than the uncertainties of

reconciled data, the DR gives consistent values for PAREX model equations in the case of Lipschitz continuity around the solution. New bias values $B^{C(i)}$ are estimated with the last PAREX calculation. The best estimation of the bias values is reached when the biases between two iterations are constant. If these two criteria are not respected, bias information given to the DR is not satisfactory. The new bias values $B^{C(i)}$ are given to the DR for the next step. The iterations continue until the bias value estimation enables consistent data to be reached. The final DR is performed with fully known bias information, and has a minimal objective function value $OF^{(i)}$.

## 4. Results

The first bias estimation $B^{C(0)}$ was obtained by the comparison between measured internal and output flow-rates and the initial PAREX calculation. Four iterations were needed to obtain consistent bias estimations $B^C$ and the minimum of the objective function $OF^{(i)}$. As soon as all biases can be considered constant, the iterations stop ($|B^{C(4)} - B^{C(3)}| < \alpha$, with $\alpha = 10^{-4}$ the tolerance of the convergence criterion). Note that the bias values are considerably higher than the measurement uncertainty in this scenario; therefore their contribution must be isolated.

All redundant data, biased and unbiased, are reconciled. Figure 3 displays the differences $\Delta X_s^{B-R}$ between the measured $X_s^B$ and reconciled $X_s^R$ values and their corresponding uncertainties. The differences $\Delta X_s^{B-C(0)}$ and $\Delta X_s^{B-C}$ between the measured $X_s^B$ and, respectively, initial $X_s^{C(0)}$ and final $X_s^C$ PAREX values, are also laid out.

The differences $\Delta X_s^{B-C(0)}$ result from input measurement uncertainty. For flowrate A7, flowrate O4, and density A8, the reconciled values are closer to the PAREX calculations than the measured values, highlighting the consistency of the final data set. Moreover, the uncertainty of the reconciled values is smaller than the measurement uncertainty.

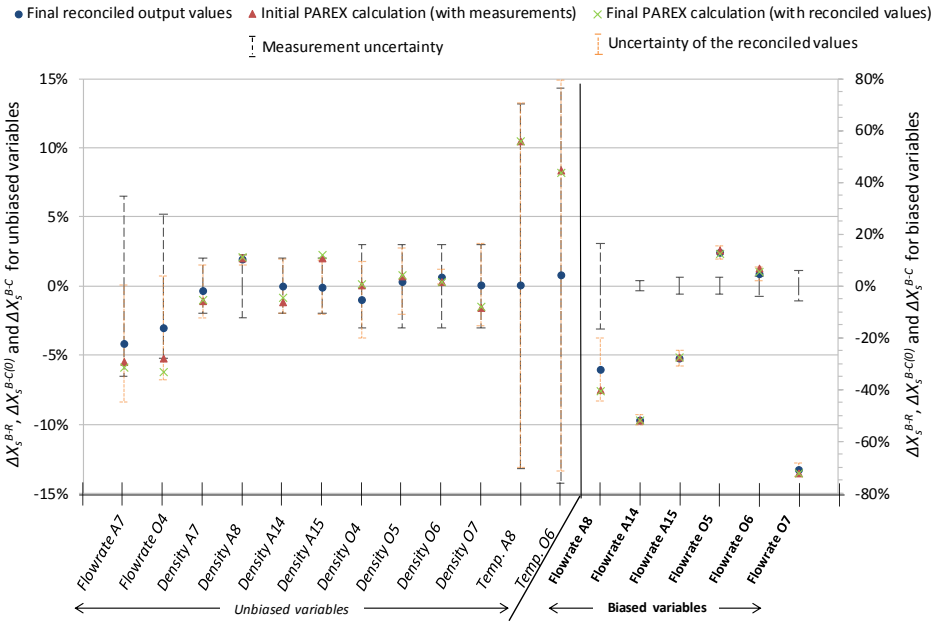


Figure 3: Comparison between measured, reconciled, and PAREX calculated outputs.

Concerning density A8 and density O6, the uncertainties of the reconciled values are very small and surround the reconciled and calculated values. These densities are linked to uranium and plutonium concentrations through a density equation. The analytical concentration measurement methods are more precise than the density sensors. Thus, the uncertainty propagation through the constraints enables the $X_s^R$ to be more precise.

Concerning the other unbiased variables, mostly linked by mass balances, the reconciled $X_s^R$ values are only slightly different from the measured $X_s^B$ values. The two PAREX simulations give very similar results. This reflects the low sensitivity of these physical quantities to the change in the inputs from measured to reconciled values.

As PAREX input data are reconciled, accuracy is given to process indicators estimation. For instance, the uncertainty of the TBP mass flowrate is reduced by half (measurement uncertainty: 5.26%, uncertainty of the reconciled value: 2.81%). The uncertainties of uranium and plutonium mass flowrates are also reduced (from 2.8% to 2.0%), which leads to a better estimation of the metal loading in the solvent.

## 5. Conclusions

Data Reconciliation (DR) and Gross Error Detection and Identification (GEDI) were performed on a spent nuclear fuel treatment process. As a tool to reduce uncertainty in nuclear matter management within the plant, combining data reconciliation and the PAREX code could help in process monitoring and control.

In classical GEDI methods, each bias decreases the redundancy of the system. The new methodology is based on nonlinear DR in which the biases are fixed and estimated by a first-principle model, the PAREX code, with the reconciled values as input data. Therefore, the redundancy is not modified. For the bias estimation to be precise, the PAREX code and the DR iterate until the bias values offer a consistent set of reconciled data. This methodology enables explicit and inexplicit constraints for a DR problem to be addressed.

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