Process operation and monitoring aided by a qualified model

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INTRODUCTION

The context

- **Online analysis** is a powerful tool to monitor process operations in a plant (ensures operation margins, increases final product quality…)

- **State indicators** can be defined but not always measurable (position of the sensor: difficult / impossible).

➢ How to get the maximum information from existing measurements?

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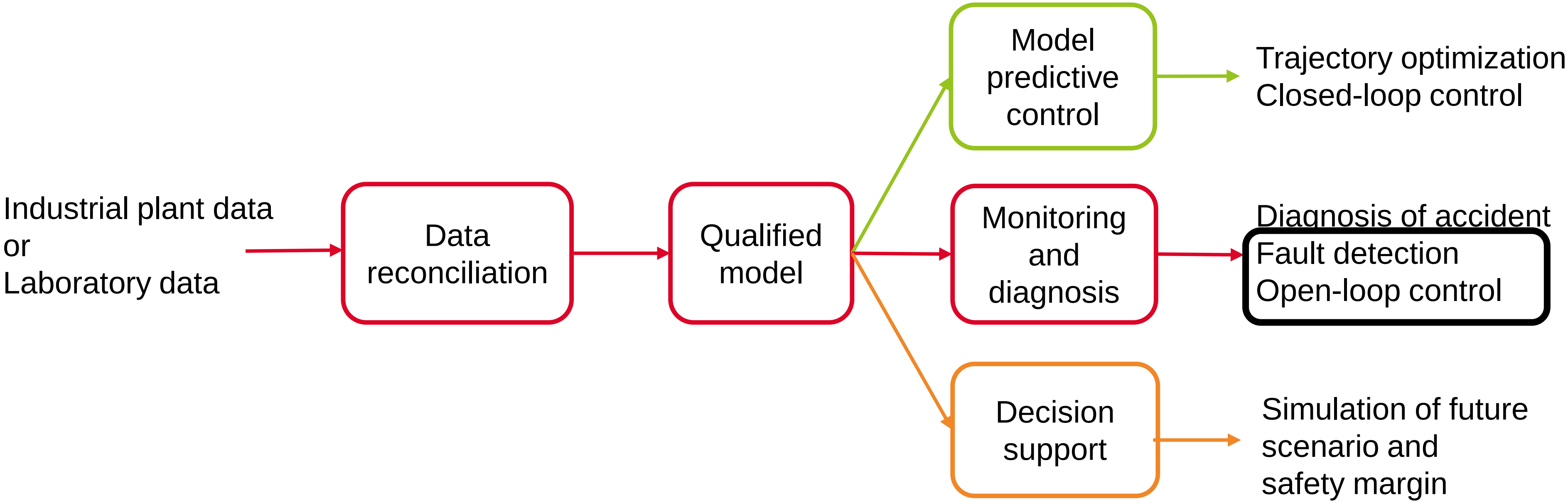
A qualified model for monitoring and control

- A **qualified model** can take part in many ways in the field of process engineering: from design and safety studies to monitoring and control.



Use of a qualified model in monitoring and control.

- In each case, **data reconciliation** is a compulsory step in order to exploit data from an industrial plant or from a laboratory.

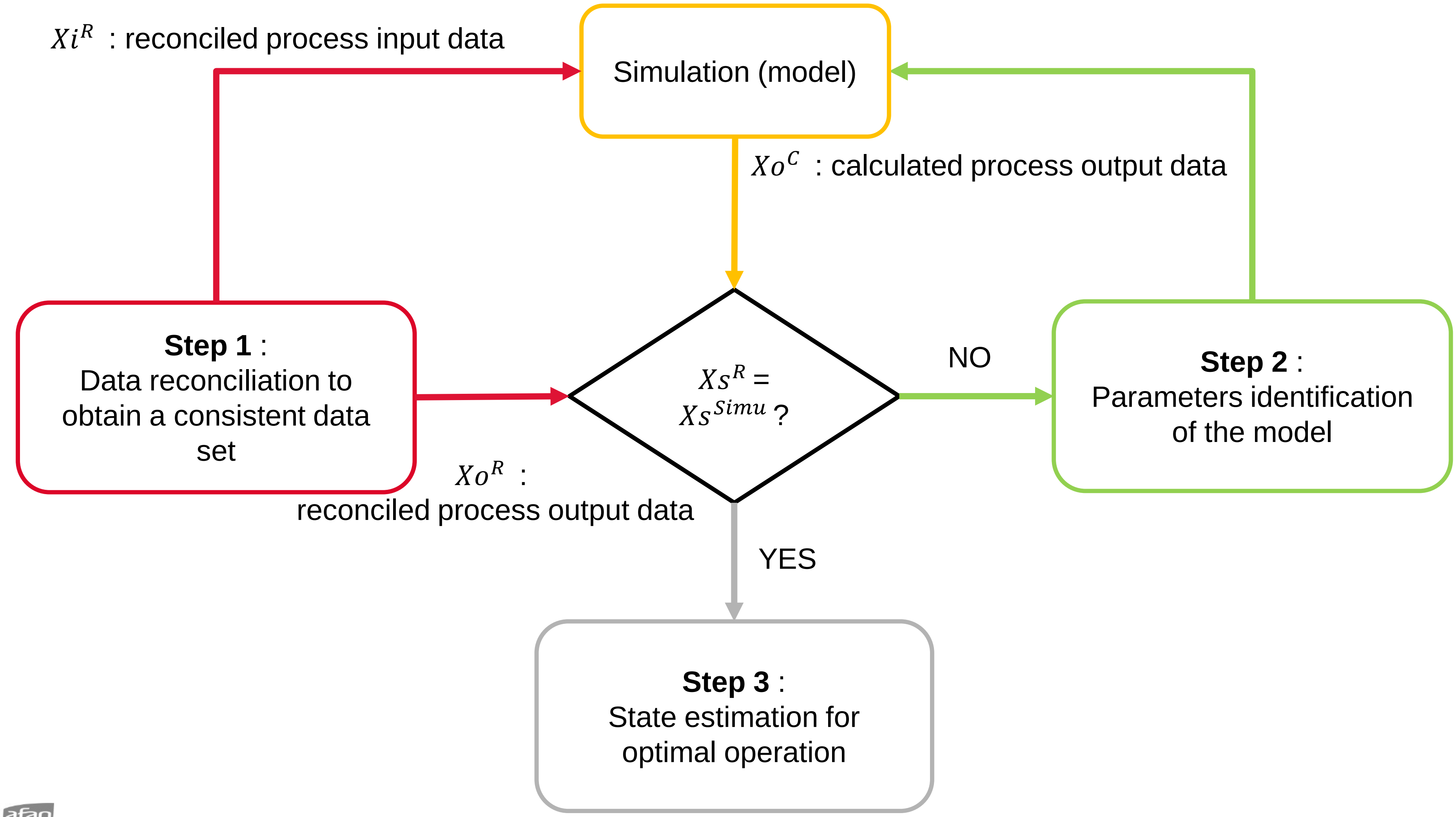
➢ Data reconciliation is the first step of the strategy.

A MONITORING TOOL EXAMPLE:

A SOFTWARE SENSOR FOR STATE ESTIMATION

A software sensor for state estimation

- Three main steps:



A qualified model: the PAREX code

- PAREX [1] is a **dynamic simulator** of liquid-liquid extraction processes, developped and validated by the CEA for more than 30 years.

- It is currently used:
  - for industrial process design or laboratory experiment design (unit sizing, operational condition tests etc.);
  - for determining and optimising the operational parameters of a plant according to the composition of the feed and the requirement on the final product quality
  - as an aid for plant operation (to understand the interaction of different physical and chemical phenomena in the process);
  - as a training tool for the operators to understand the process operation (sensibility of a parameter on the process, determining the best pathway for recovering a steady state after a perturbation);
  - as a tool for safety and security analysis (operating margin determination, discuss appropriate corrective actions in case of a malfunction).

- It is based on **first-principle models** for the chemistry and mass and energy balances; hydrodynamics is represented by a **parametric model**.

[1] PAREX, a numerical code for plant operation assistance, B. Dinh, M. Montuir, C. Sorel, J. Bisson, C. Huel, Procedia Chemistry, Vol. 32, 2016, pp 117-124.

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A qualified model: the PAREX code

- The user can create its own chemistry model.

→ Chemistry model validated

- Mass and energy balance: several equations used by PAREX to evaluate fluxes throughout the process.

→ Mass and energy balance

- Hydrodynamics: parametric models whose parameters value are determined for a specific state (retention rate, axial dispersion, transfert parameter).

→ Hydrodynamic parameters known for a specific range of input values → If state differs, need to reavaluate the hydrodynamic parameters

Complexity of building this tool

- Numerous researchs are already published: application of data reconciliation and qualified model to metal processing industries is not new.

- Still many difficulties to accurately build an integrated device: gap between theory and industrial processes. Many work are still **in progress;**

- Recent publications in mineral and metal processing industries, for instance:

  Selecting proper uncertainty model for steady-state data reconciliation – Application to mineral and metal processing industries, Amir Vasebi, Eric Poulin, Daniel Hodouin, Minerals Engineering 65 (2014) 130-144;

- The online use as well as non-linear parameter estimation from dynamic plant data are two main difficulties in the development of model-based tool.

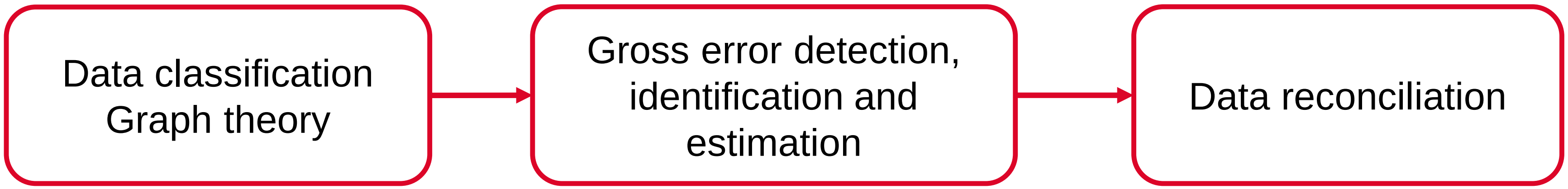
  The online use of first-principles models in process operations: Review, current status and futurs needs, C.C. Pantelides, J.G. Renfro, Computers and Chemical Engineering 51 (2013) 136-148;

A COMPULSORY STEP TO MONITOR PROCESSES:

DATA RECONCILIATION

Data reconciliation

- The goal of data reconciliation is to find values that verify a set of constraints (mass and energy balances…), as close as possible to measured data: **consistency** and **accuracy**.



Overall treatment of plant data

- Problem formulation:

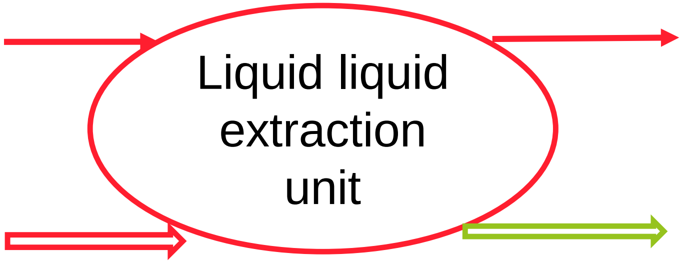
$$\begin{cases} Min \ \|X - X_m\|^2_{R^{-1}} \\ f(X, \theta) = 0 \end{cases}$$

X : reconciled variables
X_m : measured variables
R : Variance/covariance matrix
Θ : model parameters

Data reconciliation theory: a simple example

$Q_1^B = 100{,}4 \pm 0{,}8$

$Q_3^B = 95{,}3 \pm 1{,}1$



$Q_2^B = 60{,}8 \pm 0{,}9$

$Q_4^{not\ measured}$

Case n°1 :
Flow 1, 2 and 3 measured. Flow 4 can be calculated.

Observability : Mass flow rate for each flow is measures or calculated.

$$Q_1 + Q_2 = Q_3 + Q_4$$

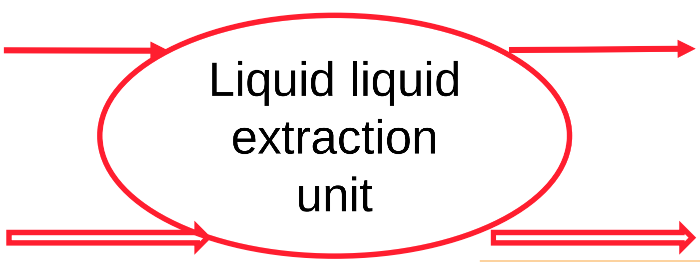
$Q_4^R = 65{,}9 \pm 2{,}8$

$Q_1^R = 101{,}01 \pm 0{,}71$

$Q_3^R = 94{,}15 \pm 0{,}86$

$Q_1^B = 100{,}4 \pm 0{,}8$

$Q_3^B = 95{,}3 \pm 1{,}1$



$Q_2^R = 61{,}57 \pm 0{,}78$

$Q_4^R = 68{,}43 \pm 0{,}64$

$Q_2^B = 60{,}8 \pm 0{,}9$

$Q_4^B = \mathbf{68{,}9} \pm 0{,}7$

Case n°1 :
Flow 1, 2, 3 and 4 measured.

Observability and Redundancy : the values can be reconciled.

$$Q_1 + Q_2 = Q_3 + Q_4$$

Mass balance not satisfied.

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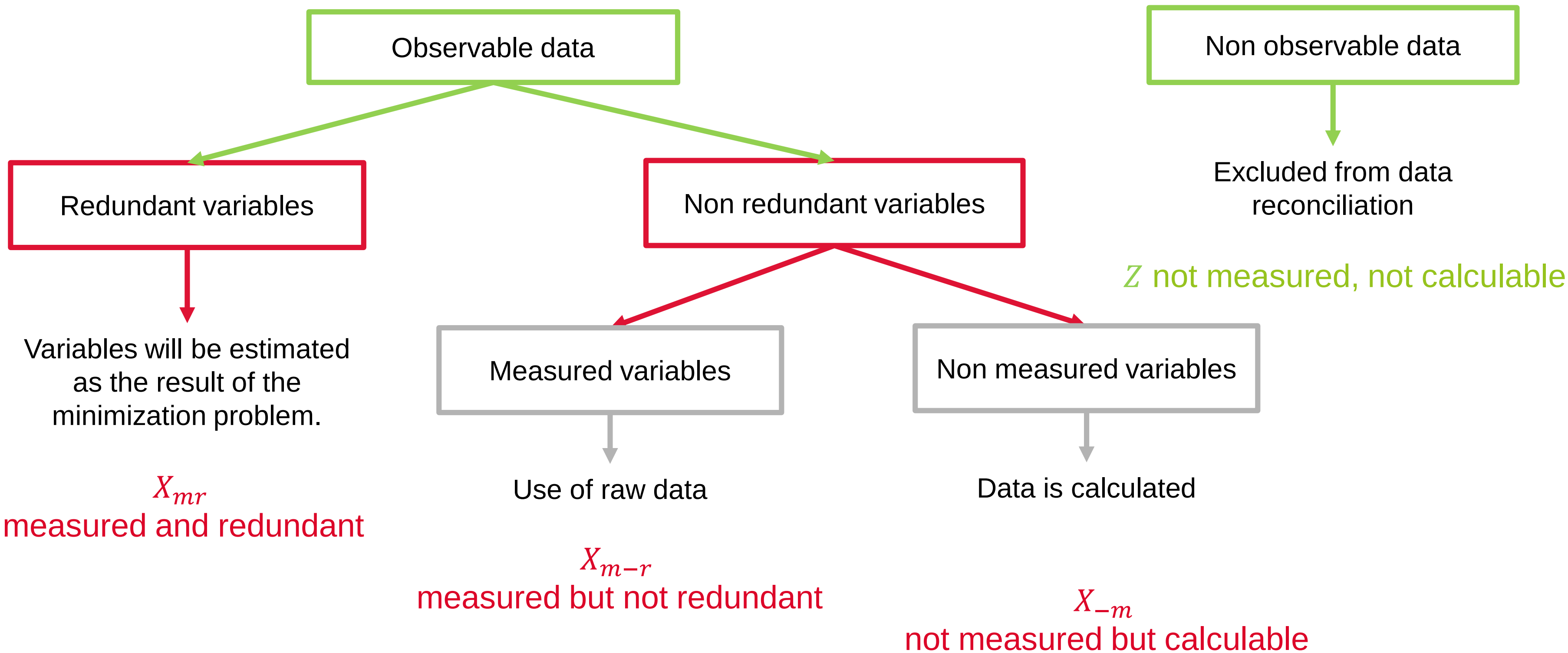
1st step : Data classification

- Data can be separated in input (Xi) or output variables (Xo).
- For data reconciliation, they can be classified in different categories:

Observable variables X : measured or calculated
Redundant variables : measured and calculated.



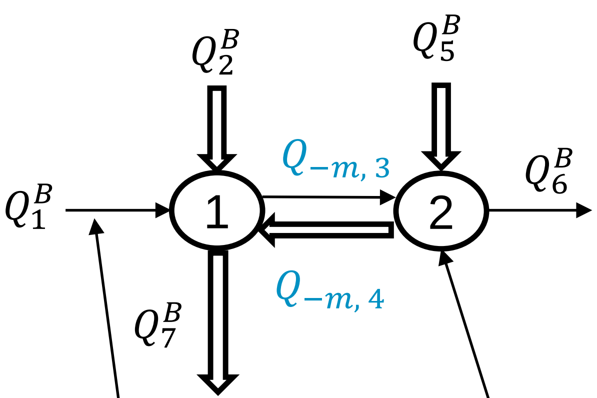
- These data can also be classified as raw data (X^M), reconciled data (X^R) or calculated data by simulation (X^C).

1st step : Data classification
Graph theory

- Graph theory is a graphic method that allows observable data to be distinguished from non observable data, as well as redundant data from non redundant data.

- Application to multiphase flow process:

Data classification ?
Initial graph

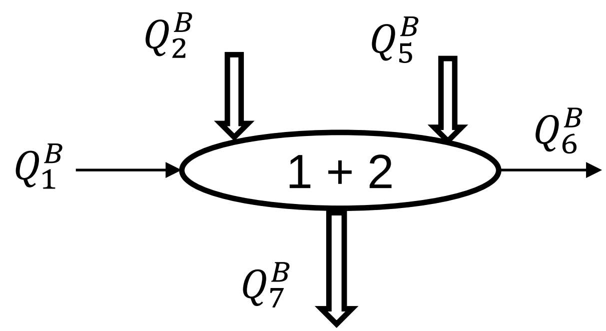


Directed arcs = mass flow

graph node = unit

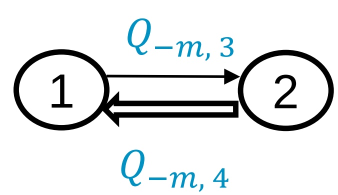
Redundant data ?

Two nodes are merged if they are linked by at least one unmeasured flow.



Observable data ?

All measured flow are erased from the graph.
Search for cycle of unmeasured flow :
no observability.



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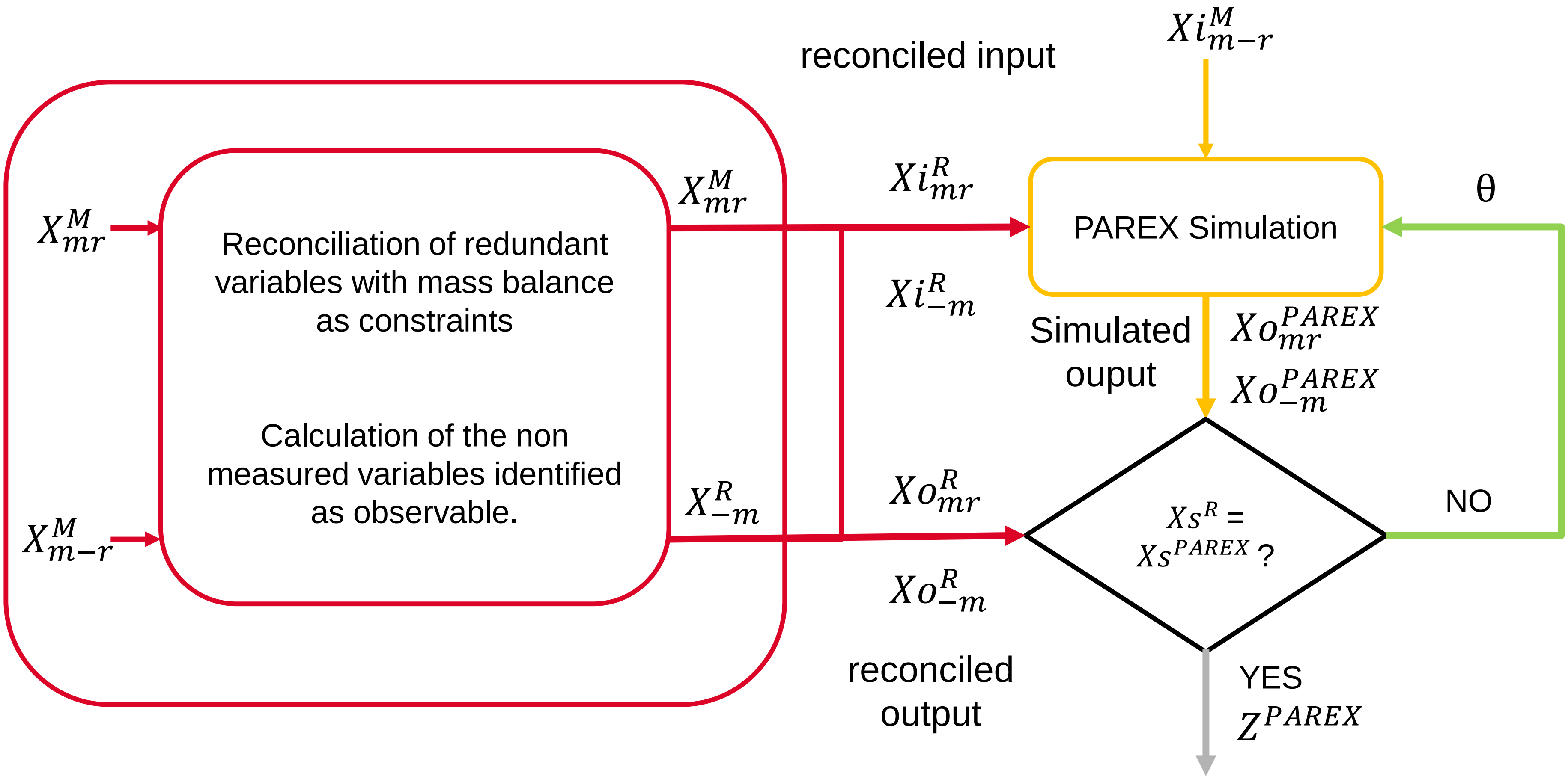
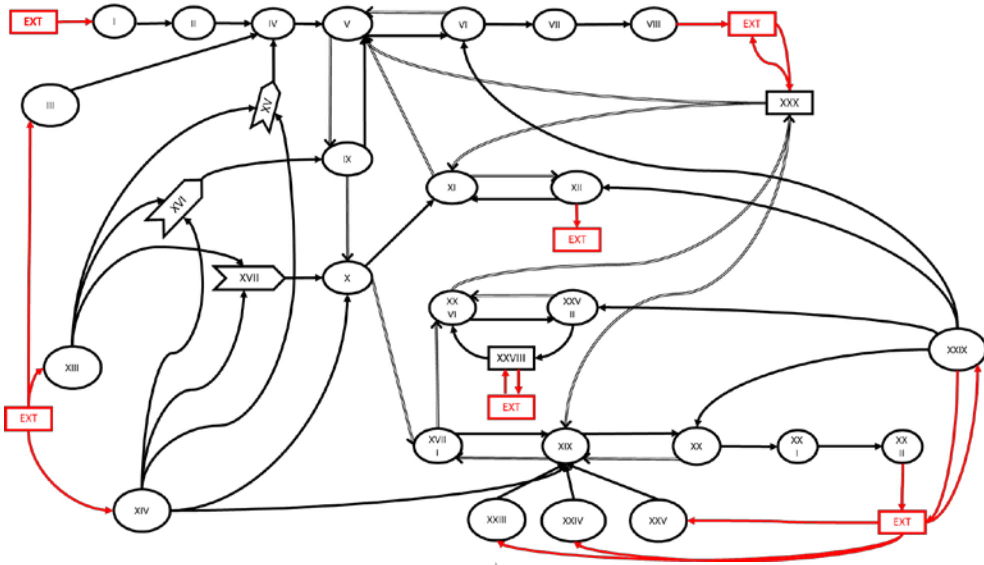
Data reconciliation and state estimation

Step 1 : Data reconciliation

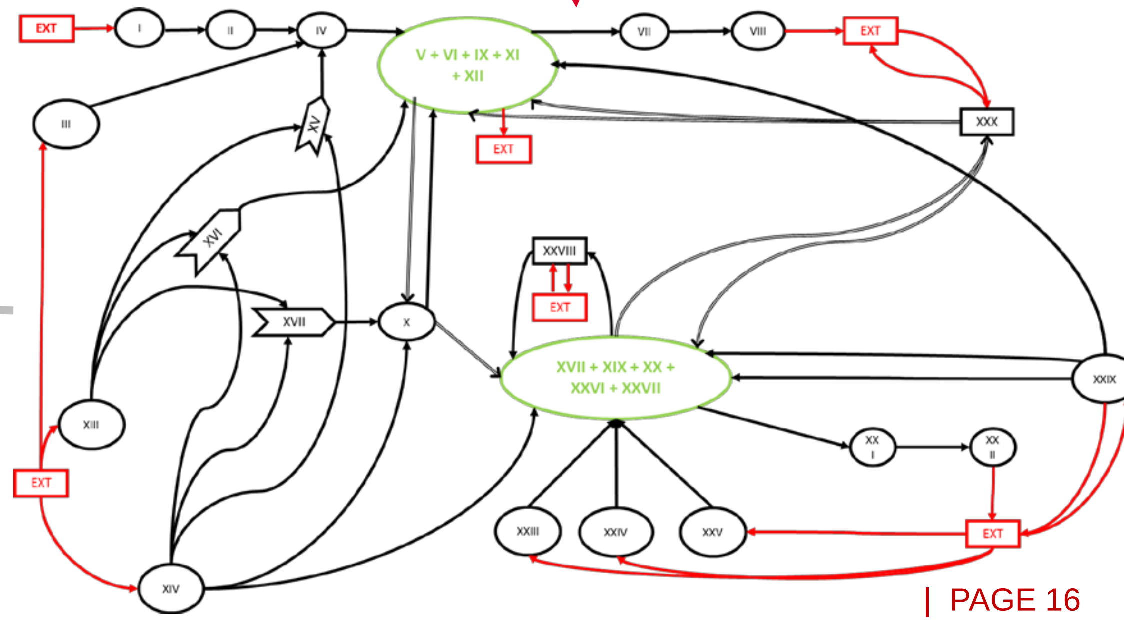
Step 2 : state estimation
(for a qualified code)



Data reconciliation and state estimation
Application example



- **Step 1**: data reconciliation on redundant measures, data calculation for observable physical quantities.



- Step 2: the PAREX code allows to estimate the process state (T, P, concentration, flowrate…).

CONCLUSION

Conclusion

- Data reconciliation allow us to:
  - to optimally exploit **all information available** on site to calculate the most probable values of observable physical quantities (measured or not measured), taking into account the **measurement uncertainties**;
  - to give **consistent information** (in respect of mass balances etc.) as input data to a model;
  - to estimate model parameters by comparison between simulated and reconciled output data (**model validation)**;
  - to support captor positioning, gross error detection …
- A qualified model is a powerful tool to:
  - understand physical and chemical phenomena at stake (first-principles model);
  - represent the process behaviour to simulate scenarii;
  - design and sizing of processes.

➢ The objective is to combine data reconciliation and a qualified model, to create an online tool to monitor and control chemical processes.

Conclusion

- A practical application for CEA and Areva: the **PUREX process**, liquid-liquid extraction units in order to reprocess nuclear spent fuel. Such a tool would reinforce the safety of the plant (crucial in a nuclear facility) and allow an efficient process operation management (reduced operation margins).

- Studies already applied data reconciliation in mineral processing industries 30 years ago. Still in research. Reconciliation of measurement data with only mass conservation as constraints can be very useful : **no model uncertainty will disrupt the results** [2].

- A question: **is data reconciliation frequently and/or efficiently applied to industrial mineral processes ?**

[2] Methods for automatic control, observation, and optimizatoin in mineral processing plants, Daniel Hodouin, Journal of Process Control 21 (2011) 211-225.

Thank you for your attention

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ANNEXES

Data reconciliation – some tools examples

STEP	TOOLS
Data classification	- Graph theory - Matrix pivot
Data reconciliation	- Least square method - Filter (Bayésien ou Kalman) - Estimator with a non quadratique fonction to minimize (ex : fair function pas de grosses erreurs à enlever)
Gross error detection	- PCA (for corolated data – calculation time can be high) - Global test (to know if there is at least 1 gross error) - - Measurement test (MT)

Some integrated software for industries:

VALI

RECON

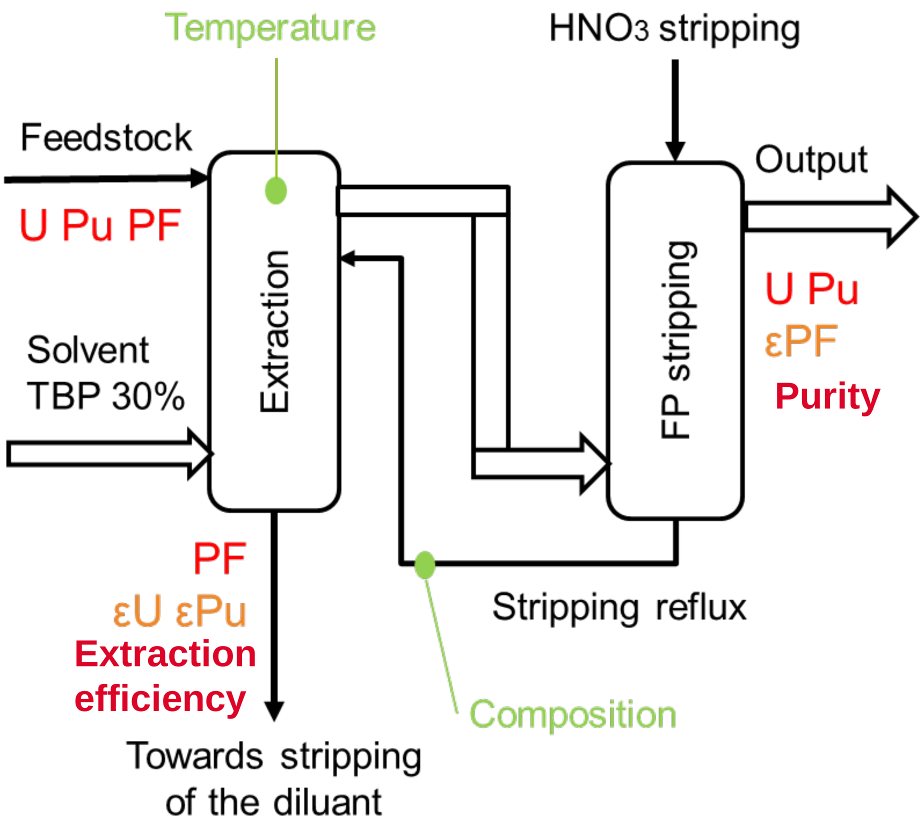
DatRec

Bilco

The PUREX process

$$UO_2^{2+} + 2\,NO_3^- + 2\,\overline{TBP} \rightleftharpoons \left(\overline{UO_2(NO_3)_2, 2\,TBP}\right)$$

Extraction mechanism of uranium by TBP.



Simplified scheme of extraction and stripping operation in the PUREX process [3]

- Products specific features :

High purity demanded,
High extraction efficiency (> 99,9%),

=> Accurate control of the uranium and plutonium loading ratio in TBP

- Control thanks to a dynamic simulator PAREX through the monitoring of state indicators such as:

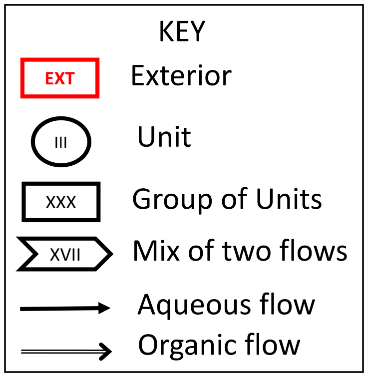
Temperature profile in the extraction column,

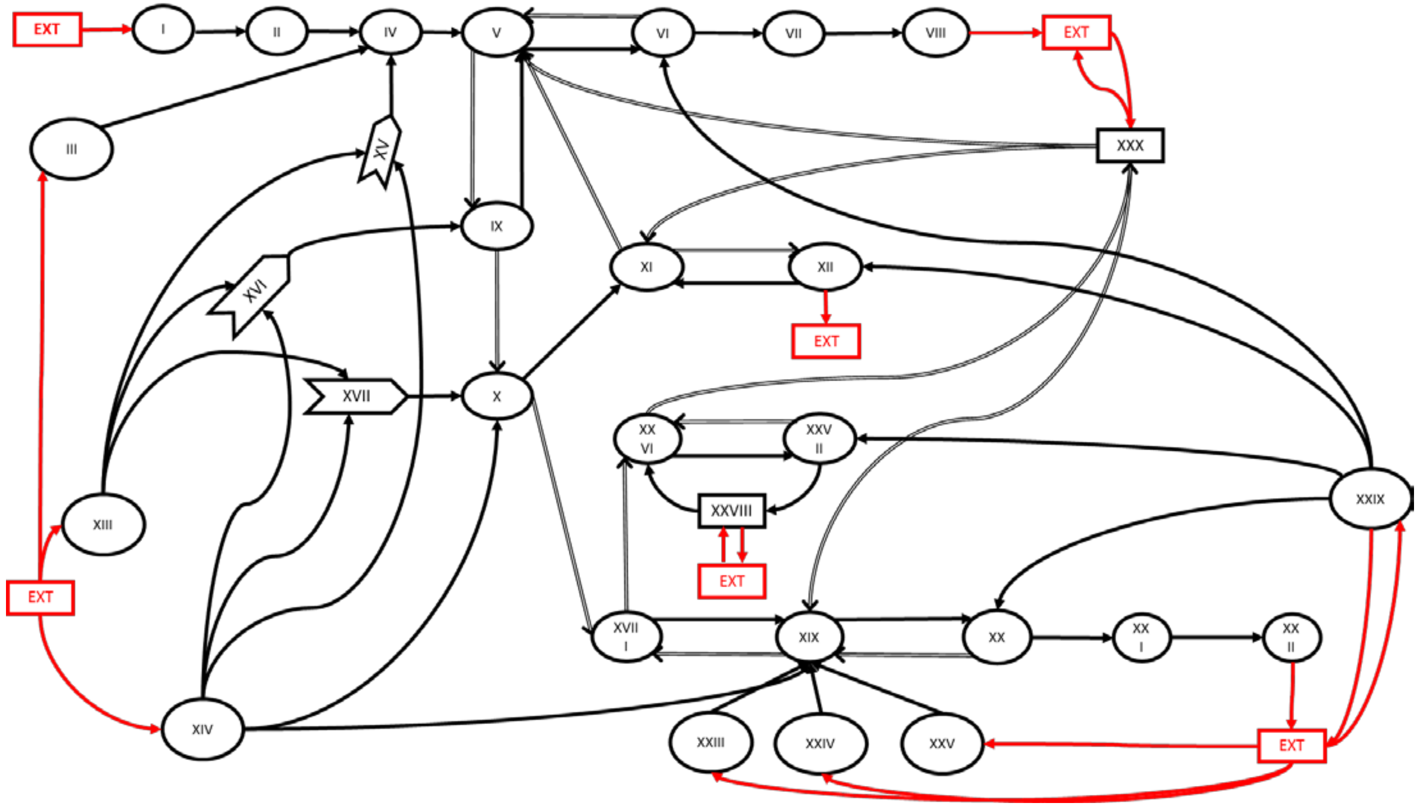
Composition of the stripping reflux.

[3] Treatment and recycling of spent nuclear fuel, B. Dinh, P. Baron and J. Duhamet, monograph of CEA Nuclear Energy Division, the PUREX process separation and purification operations pp 55-70, CEA Saclay et Groupe Moniteur, Paris, 2018

Graph theory

- Initial graph :





- Raising questions allows to :
  - represent the quantity of information available;
  - decide which type of data reconciliation can be done (mass and/or energy balances);
  - discuss potential bias.

Data reconciliation – Mathematical formulation

➢ Mathematical formulation and solution

- For **direct measures**, in the **absence of gross error**, the measurement error ε is the gap between measured values X_m and true values X^* :

$$X_m = X^* + \varepsilon$$

- The measurement error is supposed to follow a normal law centered in 0 :

$$\varepsilon = N(0, R)$$

With R the covariance matrix.

- The true values X^* and the parameters (non-measures physical parameters) θ* have to respect the set of contraints h :

$$h(X^*, \theta^*) = 0$$

➢ Mathematical formulation and solution

- The maximum likelihood estimation problem is equivalent to minimizing the function:

$$\varphi = \frac{1}{2} * \left\| X - \hat{X} \right\|^2_{R^{-1}}$$

$$\text{with : } M\,\hat{X} = 0$$

M is the incidence matrix or constraint matrix
$\hat{X}$ best estimator of measured variables

- Global mass balances constraints are linear. Analytical solution (with Lagrange multipliers method) :

$$\hat{X} = (I - V\,M^t\,(MVM^t)^{-1}\,M)\,X_m$$

- Nonlinear constraints : linearization of the constraints or minimisation algorithm.

Différentes techniques d'évaluation de paramètres inconnus

Utilisation de lois physiques (identification des paramètres en utilisation les données expérimentales).

Modèles de connaissance pure (approche mécanistique ou déductive)

Modèles phénoménologiques

PAREX

Filtres de Kalman

Modèles hybrides

Modèles empirique (modèles boîte noire, comportementaux, approche inductive)

Corrélation empirique définie à partir de données expérimentales.