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INVERSE PROBLEM AND CALIBRATION OF PARAMETERS

PART 1:
An example of inverse problem:
Quantification of the uncertainties of the physical models of the CATHARE code with the CIRCÉ method

1. Introduction
2. Rapid description of CIRCÉ
3. Examples of CIRCÉ studies
4. Introduction to the algorithm used by CIRCÉ
5. Methodology for a proper use of CIRCÉ
6. Conclusion

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CATHARE and CIRCÉ in few words

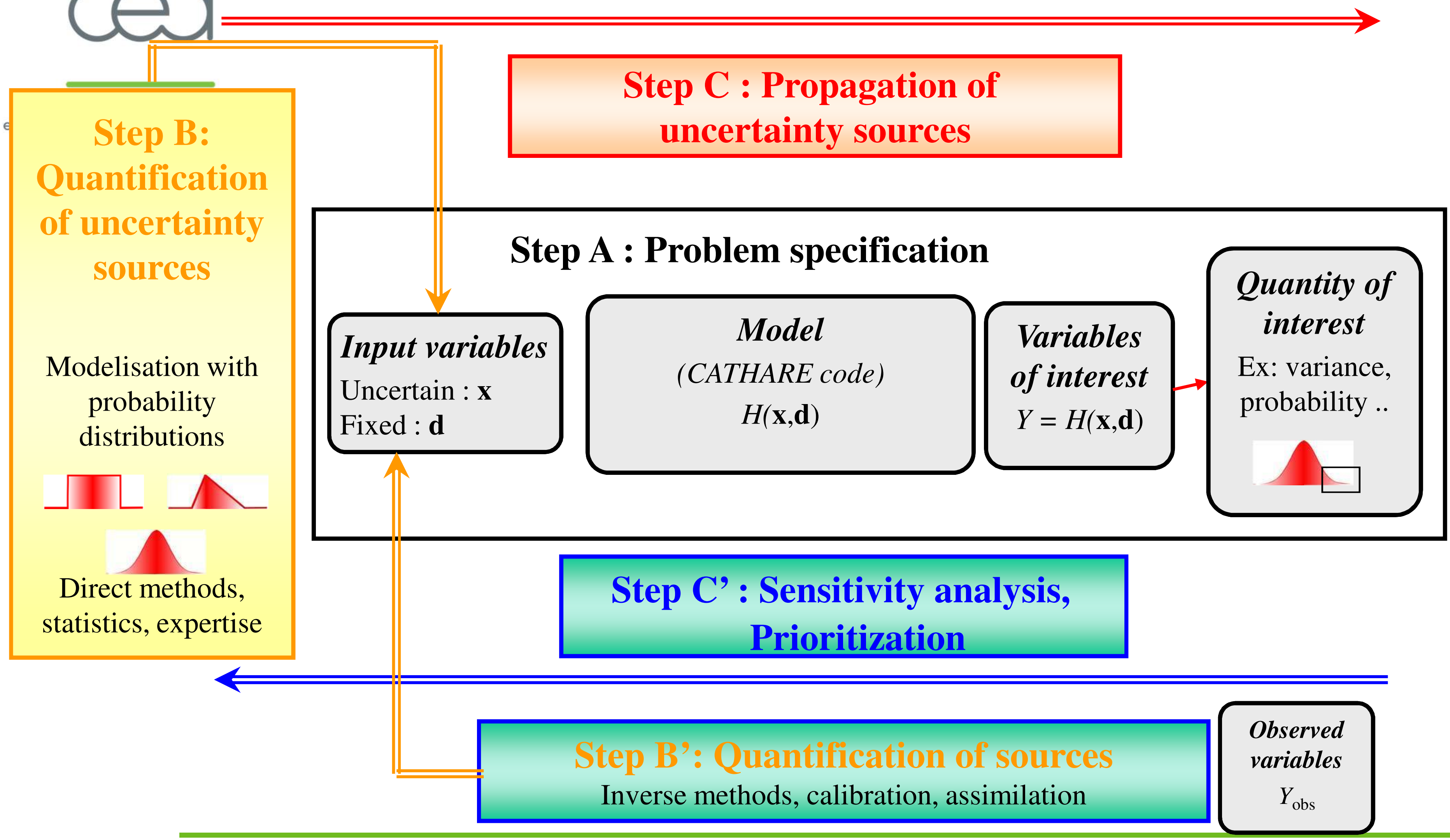
CATHARE:

- French thermohydraulics code modeling the behaviour of nuclear power plants, especially for accidental transients (ex: break in the primary circuit).
- But, for its validation, CATHARE can also model simple experiments devoted to the study of some few physical phenomena.
- Developed by CEA and funded by AREVA-CEA-EDF-IRSN.
- Man-power: roughly 20 men×years per year since 1978.

CIRCÉ:

- CIRCÉ is aimed at quantifying the uncertainties of the non-measurable physical models of CATHARE.
- Developed by CEA. More than 15 studies corresponding to roughly a 15 men×year manpower.
- Can be applied to any code.
- But needs the calculation of first order derivatives.
- For CATHARE, this calculation is performed by ASM (Adjoint Sensitivity Method) or finite differences with some precautions (ex: choice of the increment).

CIRCÉ in the general framework of uncertainty and sensitivity analyses: **step B'**



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Features of uncertainty analysis for CATHARE

The variables of interest (outputs):

- Quantities important for safety:
  Ex: Maximum cladding temperatures

The quantities of interest:

- Most general case: The output must not exceed a certain value, for example 1204°C for the maximum cladding temperature .
  ⇒ Estimation of high percentiles (ex: 95%) for the outputs.

The input variables (parameters):

- Boundary and initial conditions. Ex: initial power, containment pressure;
- Material properties. Ex: fuel thermal conductivity;
- **Physical models**. Ex: heat transfer coefficients;
- Numerical schemes;
- User's effect, etc.

A special attention is paid to the quantification of the uncertainty of the physical models because:

- They are often highly influential;
- Estimating their uncertainty is difficult because they are generally not measurable.

Non-observed data and observed data

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Goal of CIRCÉ:

Quantification of the uncertainty of non measurable physical models.

Examples of physical models:

- Friction coefficients, friction between liquid and vapour phases, transfer heat coefficients describing condensation or vaporization, etc.
- More precisely, in the most usual case, one multiplicative dimensionless parameter X is associated to each physical model PM, the nominal value of X being equal to 1:

$$PM = X \times PM_{nominal}$$

The X parameters are the <u>non-observed data</u> (one per physical model).

Rather simple (analytical) experiments exist, each of them being devoted to the study of few physical models (cf. slide 2).

Examples of measured data in these experiments:

- Fluid or wall temperatures, pressures, flow rates, proportion of vapour in a given section (void fractions), etc.

They are the <u>observed data, also called responses</u> and are denoted as Y.

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Let us consider an analytical experiment. In this experiment let us denote as:

- X_i the non-observed data. They are the dimensionless multiplicative parameters of the influential physical models (nominal value = 1). Typically 2 or 3 physical models.
- α_i: the parameters considered by CIRCÉ and related to X_i by :

$$X_i = 1 + \alpha_i \text{ or } X_i = exp(\alpha_i)$$

(nominal value of $\alpha_i = 0$, cf. slide 18 for more explanations about both changes of variables)

- Y_j the observed data (or responses). They are the measured quantities of the experiment and are also denoted more precisely as Y_j^{meas}.Typically several tens of responses (more precisely: several tens of realizations of one or two kinds of responses).
- Y_j^{code} the corresponding code results.

Input data

$Y_j^{meas} - Y_j^{code}$

$\frac{\partial Y_j^{code}}{\partial \alpha_i}$ (δY_j^{meas})

→ CIRCÉ →

Output

For each α_i parameter, calculation of
- its mean value: m_i (also called bias)
- its standard deviation: σ_i

Using m_i and σ_i, calculation, for example, of the 95% variation interval for the X_i parameters.

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With respect to the notations of inverse problems

- Y are the n observed data. n is equal to several tens.
- X are the q non-observed data. q is equal for example to 2 or 3.
- d are the control variables, i.e. the experimental conditions of the different tests of the considered experiment. They are known.
- H is the code (also called model ≠ physical models): CATHARE in our case.
- U are the experimental uncertainties of the observed data, denoted in the former slide as δY_j^{meas} . Only their covariance matrix is known and denoted as R.

$$Y_j = H(X_{j,1}, \ldots, X_{j,q}, d_j) + U_j$$

In the case of CIRCÉ:

- The observed data are scalar.
- H is the code and not a meta-model. Consequently, U_j represents only the experimental uncertainties of the observed data, i.e. $Y_j - Y_j^{real}$ and not the model error.
- H is supposed to be perfect. Consequently, if the exact values of X: $X_{j,1}, \ldots X_{j,q}$ were known for each observed data Y_j, $H(X_{j,1}, \ldots, X_{j,q}, d_j)$ would be Y_j^{real} , the real value of Y_j.
- The code values of X are equal to 1. Therefore: $H(X_{j,1} = 1, \ldots, X_{j,q} = 1, d_j) = Y_j^{code}$

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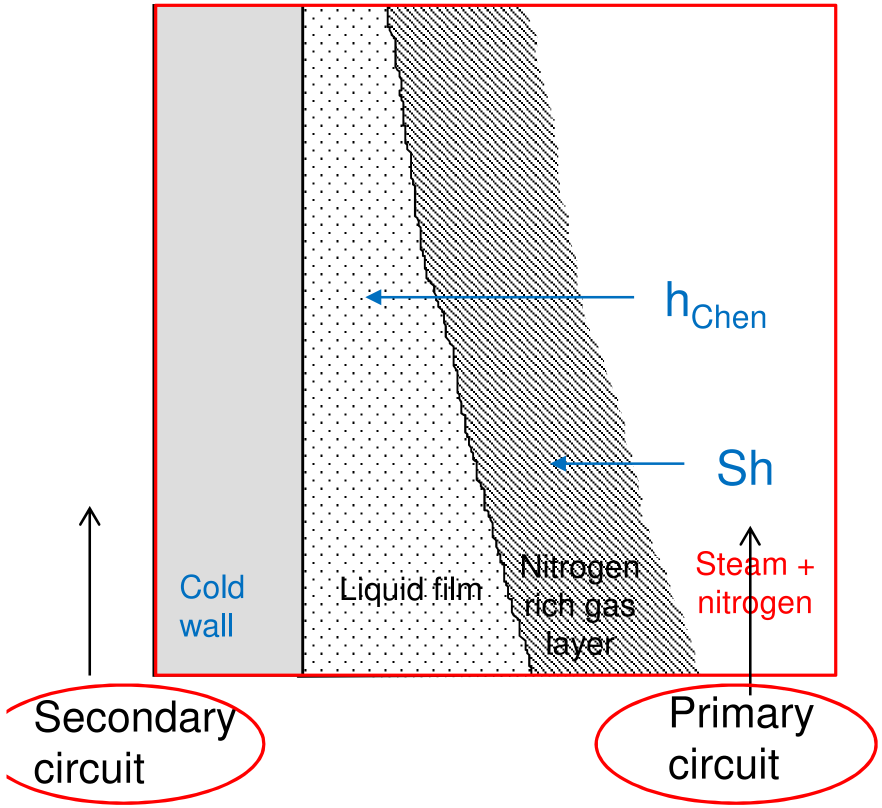
Heat transfers between primary and secondary circuits of a nuclear power plant: Condensation of the mixing “hot steam – nitrogen” in front of a cold wall



- Two phenomena:
  - The heat transfer through the liquid film described by the “Chen” heat transfer coefficient h_{Chen};
  - The steam mass diffusion through the gas layer, rich in nitrogen, described by the Sherwood number Sh.

⇒ Two parameters for CIRCÉ:

- α_1 associated with h_{Chen}.
- α_2 associated with Sh.

- The analytical experiment: COTURNE
- The observed data: Temperature measurements. 164 responses (82 different tests, 2 measures per test).

	Results for α_i CIRCÉ parameters			Results for X_i, the multiplicative dimensionless parameters			
Physical model	CIRCÉ parameter	Mean value	Standard deviation	Change of variable	Type of law	Bias	95% interval of variation
h_{Chen}	α_1	-0.05	0.35	$X_1 = 1 + \alpha_1$	Normal	0.95 = 1-0.05	[0.25 ; 1.65]
Sh number	α_2	-0.15	0.29	$X_2 = \exp(\alpha_2)$	Log-normal	0.86 = exp(-0.15)	[0.48 ; 1.53]

Final results for the X_i non-observed data.

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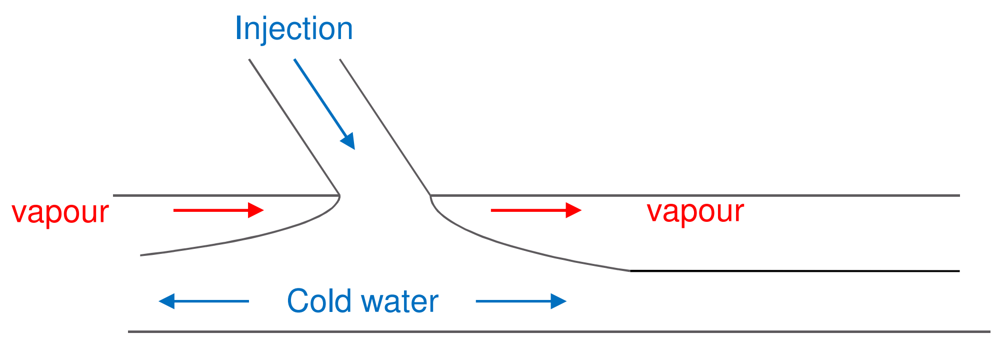
Injection of cold water in the primary circuit in case of accident:
Condensation of the warm vapour in contact of the injected water



The condensation of the vapour warms up the cold water in the bottom of the pipe.

- Two phenomena due to two types of condensation:
  - Just below the jet: Condensation with turbulences
  - Far from the jet: Stratified flow

  $\Rightarrow$ 2 CIRCÉ parameters: α_1 and α_2
- The analytical experiment: COSI, 59 tests.
- The observed data: water temperatures and total condensation flow rates (118 responses).

Results: for X_1 and X_2, multiplicative parameters associated with both modes of condensation: 95% variation intervals and type of law (log-normal). The results are not authorized to be published.

- Algorithm used by CIRCÉ: the E-M algorithm, well known in statistics and based on:
  - The principle of maximum likelihood.
  - Bayes' theorem on conditional probabilities.

- Two main hypotheses:

  - Linear dependence between the code responses and the α_i parameters

    Since derivatives $\frac{\partial Y_j^{code}}{\partial \alpha_i}$ are used by CIRCÉ.

    CATHARE: These derivatives are calculated by ASM or by finite differences.

  - Normality of the α_i parameters considered by CIRCÉ :

    Consequence: the X_i multiplicative parameters obey a normal or a log-normal law, depending on the retained change of variable:

    $$X_i = 1 + \alpha_i \quad \text{or} \quad X_i = exp(\alpha_i)$$

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The linearity hypothesis

For each response Y_j, one writes:

$$Y_j^{meas} - Y_j^{code} = \underbrace{\left(Y_j^{meas} - Y_j^{real}\right) + \left(Y_j^{real} - Y_j^{code}\right)}_{\text{Sum of 2 independent random variables}}$$

First random variable = $\left(Y_j^{meas} - Y_j^{real}\right) = U_j$: experimental uncertainty of Y_j^{meas}

Obeys a normal law $N(0, R)$, R being known

Second random variable = $$Y_j^{real} - Y_j^{code} = \sum_{i=1}^{q} \frac{\partial Y_j^{code}}{\partial \alpha_i}\left(\alpha_{j,i} - \alpha_i^{nominal}\right)$$

First order development with respect to the q α_i parameters, with:

$\alpha_{j,i}$: unknown value to be given to i^th parameter so that:

$$Y_j^{code}\left(\alpha_{j,1}, \dots, \alpha_{j,q}\right) = Y_j^{real}$$

$\alpha_{j,i}$ is different for each Y_j observed data

$\alpha_i^{nominal}$: nominal value of the i^th parameter, generally equal to 0.

4. Introduction to the algorithm used by CIRCÉ

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The normality hypothesis

$$\underbrace{Y_j^{meas} - Y_j^{code}}_{\text{known}} = U_j + \sum_{i=1}^{q} \frac{\partial Y_j^{code}}{\partial \alpha_i} (\alpha_{j,i} - \alpha_i^{nominal})$$

- $Y_j^{meas} - Y_j^{code}$: known
- U_j: Realization of $N(0,R)$, R known
- $\frac{\partial Y_j^{code}}{\partial \alpha_i}$: known
- $\alpha_i^{nominal}$: known (=0)
- $\alpha_{j,i}$:
  - Unknown if q > 1 or if $U_j \neq 0$
  - Several solutions if q > 1

- Unknown ⇒ The $\alpha_{j,i}$ are known only via their statistical features: m_i and σ_i
- Several solutions:

⇒ A criterion of choice among the different solutions is needed.

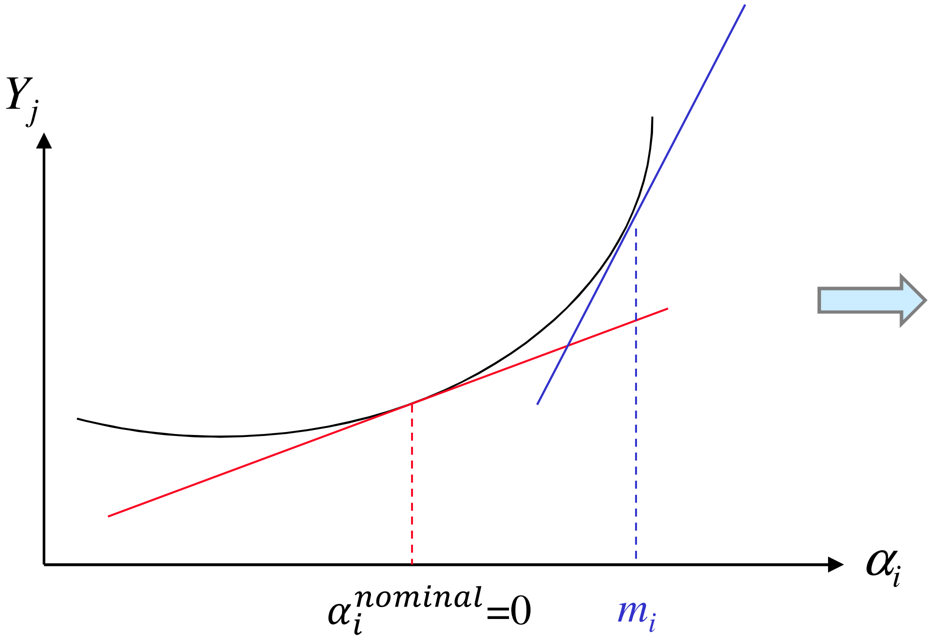
⇒ This criterion is the **maximum of likelihood**.

This criterion obliges to make an hypothesis on the form of the law followed by the α_i parameters: that is the normal law.

A necessary improvement of CIRCÉ: iterative CIRCÉ

Recall: CIRCÉ makes an hypothesis of linearity around the nominal value of the $\alpha_i = 0$, since it uses $\frac{\partial Y_j^{code}(\alpha_i=0)}{\partial \alpha_i}$.

If the biases are high in absolute value, one can have the following situation:



The derivatives must be considered at $\alpha_i = m_i$ instead of $\alpha_i = \alpha_i^{nominal}$

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To this end, CIRCÉ is used with an iterative way, by considering:

Y_j^{code} and $\frac{\partial Y_j^{code}}{\partial \alpha_i}$

At the point $\vec{\alpha} = \vec{m}_1$ (vectorial notation for the biases found with nominal CIRCÉ for the q unknown parameters α_i) instead of $\vec{\alpha} = \vec{\alpha}^{nominal}$

A new value of the bias vector is found: $\delta\vec{m}_1$ which is used to increment the first estimation $\vec{m}_1$.

The process is performed until the bias increments are close to 0 and the standard deviations are stabilized.
3-4 iterations are generally sufficient.

Final bias = sum of the biases = $\vec{m}_1 + \delta\vec{m}_1 + \delta\vec{m}_2 + \ldots$
Final standard deviations = those found at convergence

CIRCÉ is a statistical tool which must not be used as a black box.

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In addition CIRCÉ relies on two hypotheses: linearity and normality (cf. slide 11) which must be checked.

Consequence: Some precautions must be taken when using CIRCÉ.

✓ Before using CIRCÉ:

Check the **relevance** of the used analytical experiment with respect to the reactor transient for which uncertainty analysis is planned.

In the case of the 1st example (slide 8): heat transfers between primary and secondary circuits:

Experimental database COTURNE

- Pressure: [2; 70] bars
- Gas temperatures: [100 ; 400] °C
- Thermal flux: [0.1 ; 6] W/cm^2,
- Vapour flow rate: up to 4 g/s
- Etc.

Reactor transient :

- Pressure:
- Gas temperatures:
- Thermal flux:
- Vapour flow rate:
- Etc.

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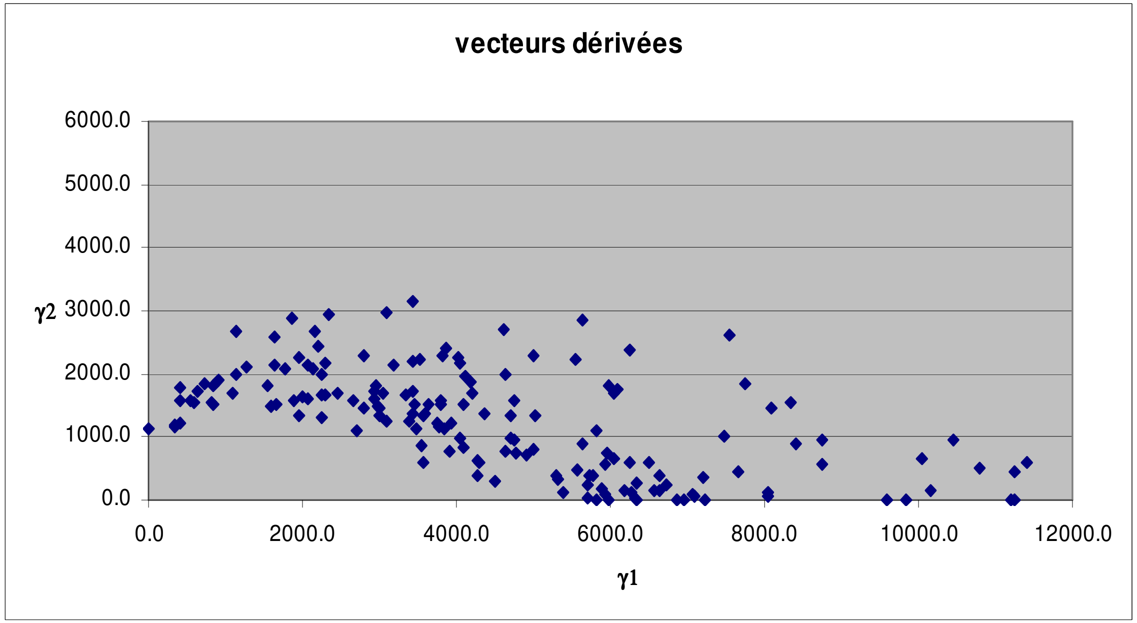
✓ Before using CIRCÉ (cont'd):

Check that the problem is **identifiable**:
In CIRCÉ algorithm, a matrix cannot be inverted for some configurations of the derivative vectors, especially if they are collinear.
⇒ Check the distribution of these vectors:

In the case of the 1st example (two physical models):
The points $\left(\frac{\partial Y_j^{code}}{\partial \alpha_1}, \frac{\partial Y_j^{code}}{\partial \alpha_2}\right)$ are distributed as follows:



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✓ Checking the hypothesis of linearity

Thanks to the iterative use of CIRCÉ (slides 14 and 15), the hypothesis is made in the final range of variation of each α_i parameter: $[m_i\text{-}2\sigma_i \,;\, m_i\text{+}2\sigma_i]$.

Each α_i parameter is varied inside its range of variation.

For each Y_j response , the dependence Y_j^{code} with respect to α_i is observed for both formulations:

$$X_i = 1 + \alpha_i \quad \text{or} \quad X_i = exp(\alpha_i)$$

Considering all the Y_j responses, the formulation for which the linear dependence is the best verified is retained.

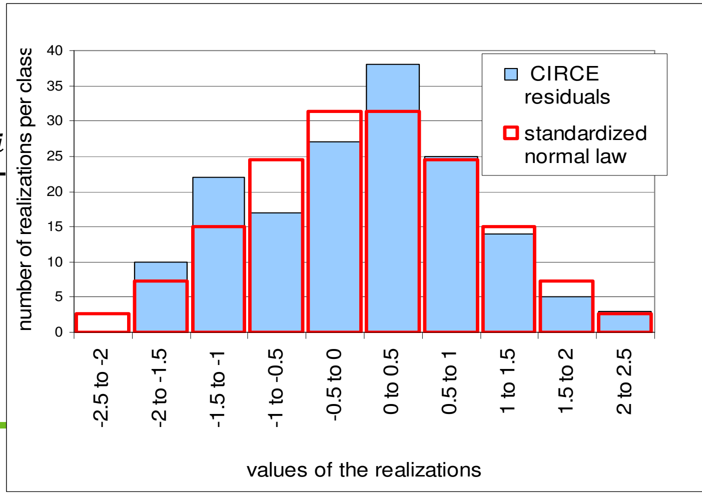
✓ Checking the hypothesis of normality

Not possible with the individual realizations of α_i, because CIRCÉ does not calculate them.

But if each α_i obeys a normal law,

the residuals: $$r_j = \frac{Y_j^{meas} - Y_j^{code} - \sum_{i=1}^{q} \frac{\partial Y_j^{code}}{\partial \alpha_i} m_i}{\sum_{i=1}^{q} \left(\frac{\partial Y_j^{code}}{\partial \alpha_i}\right)^2 \sigma_i^2 + R}$$

obey a standardized normal law.



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✓ Final check: The envelop calculations

- **An uncertainty analysis is performed for the used experiment :**
  - Outputs: the Y_j responses considered by CIRCÉ.
  - Inputs: The X_i parameters with their statistical features deduced from CIRCE results.
  - Number of calculations: e.g. 100.

- The 100 values found for each response are sorted by increasing order:

$$Y_j(1) < Y_j(2) < \cdots < Y_j(100)$$

  - $Y_j(3)$: estimation of the 2.5% percentile of Y_j
  - $Y_j(98)$: estimation of the 97.5% percentile of Y_j

- If, in the ideal case,:
  - One had a very high number of responses,
  - Very numerous calculations of the experiment were performed, in order to have precise estimations of both percentiles,
  - One would check that 95% of the measured responses are included between estimations of the 2.5% and 97.5% percentiles.

- Practically, one will only check that this property is verified for ***roughly*** 95% of the responses.

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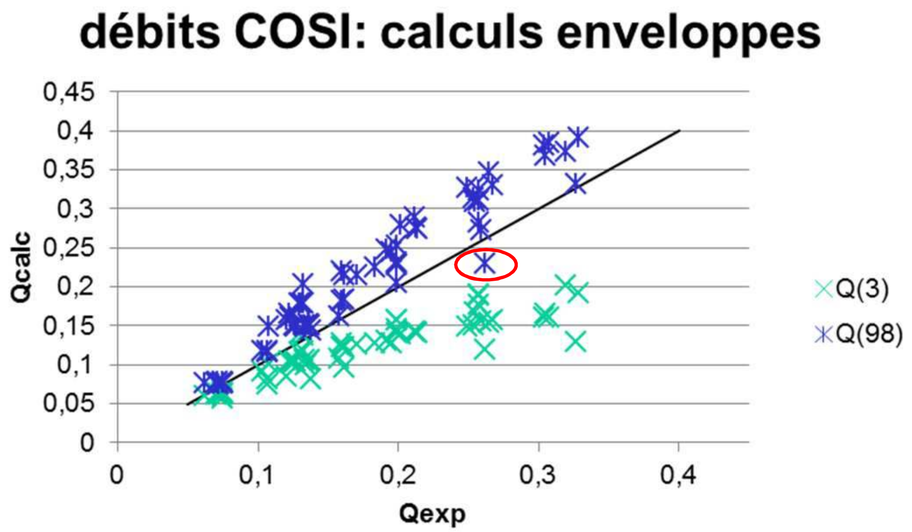
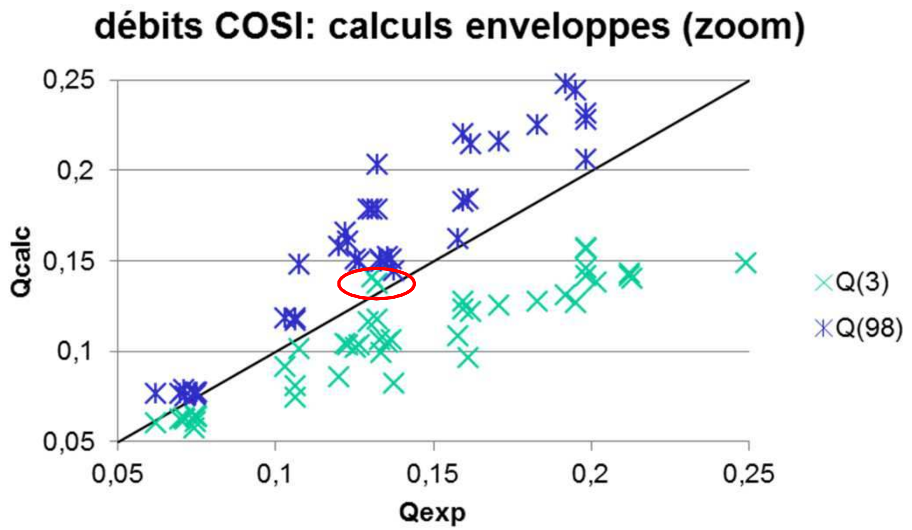
Example of results: injection of cold water (example 2, slide 10):

Two kinds of responses: 59 flow rates and 59 liquid temperatures.

For the 59 flow rates:

- 2 flow rates such as: $Q_{meas} < Q(3)$
- 1 flow rate such as: $Q_{meas} > Q(98)$





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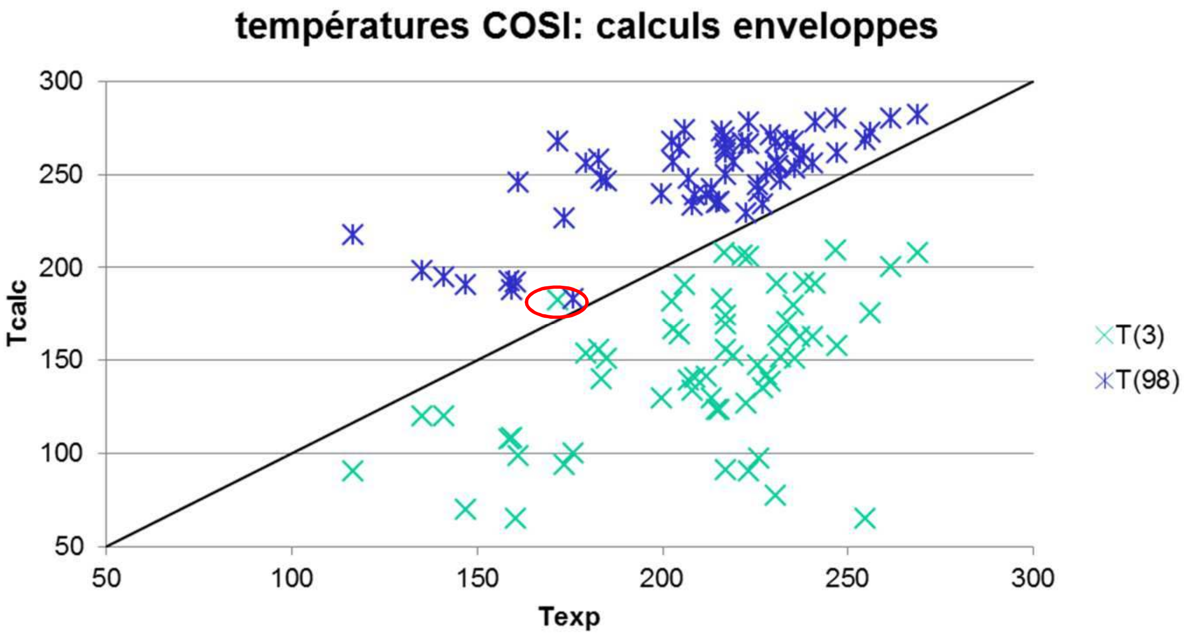


For the 59 liquid temperatures:

- 1 temperature such as $T_{meas} < T(3)$
- 0 temperature such as $T_{meas} > T(98)$

Both kinds of responses (flow rates and temperatures) together:

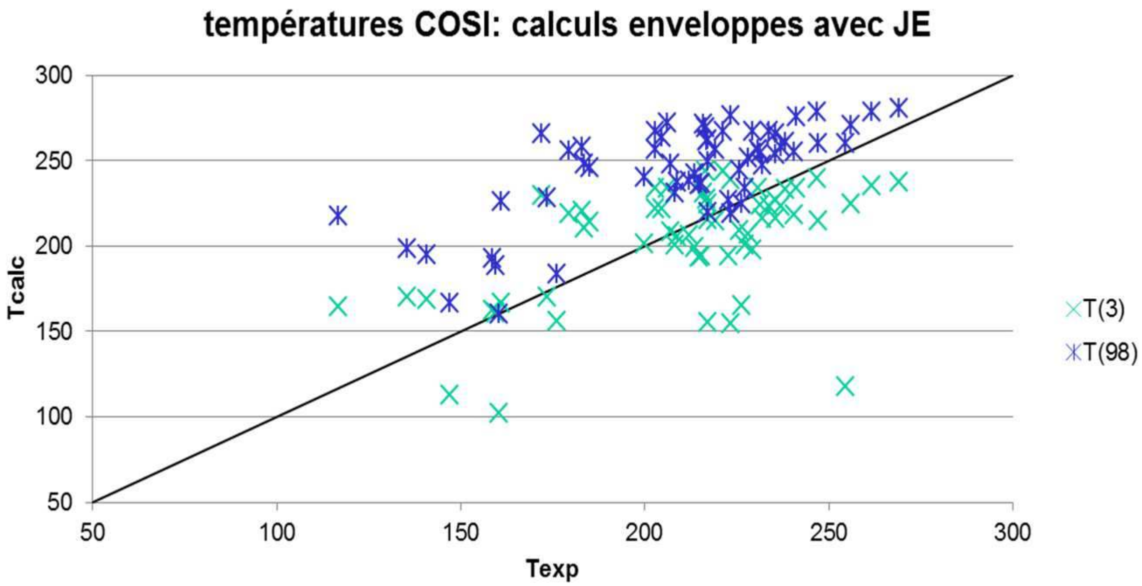
- 3 responses such as $Y_{meas} < Y(3)$ instead of $118 \times 0.025 = 2.95$. Perfect.
- Only 1 response such as $Y_{meas} > Y(98)$. A little bit too low.

Globally, the envelop calculations are considered as satisfactory.

Having correct envelop calculations is not so obvious.

For example, a first estimation by expert judgment was given for the uncertainty of both considered condensation terms (the physical models).

Results of the envelop calculations with this estimation, for the temperatures:



Among the 59 considered temperatures, 24 are such as: $T_{meas} < T(3)$!

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1. CIRCÉ estimates the uncertainty of non-measurable physical models, which are the X_i non-observed data, thanks to the Y_j observed data: the responses.

   ⇨ CIRCÉ is a method of inverse quantification of uncertainties.

2. More precisely, CIRCÉ uses:
   - The measured data of simple experiments where the considered physical models are influential.
   - The corresponding code results.
   - The derivatives of the code results with respect to dimensionless parameters α_i related to the physical models.

   CIRCÉ can be applied to any code, if these derivatives are available. For their calculation, using finite differences is possible, with some precautions.

   - CIRCÉ calculates the mean value and the standard deviation of the intermediate α_i parameters, from which variation intervals of the X_i multiplicative dimensionless parameters of the physical models can be deduced.

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3. CIRCÉ is based on a very classical algorithm - the EM algorithm - using:
   - Bayes' theorem;
   - Maximum of likelihood.

Two main hypotheses are made in this algorithm:

- Linearity of the calculated responses with respect to the α_i parameters;
- Normality of the α_i parameters ($\Rightarrow$ normality or log-normality for the final X_i multiplicative parameters of the physical models).

Thank to iterative CIRCÉ, the hypothesis of linearity is made only in the final range of variation of each α_i parameter: $[m_i-2\sigma_i\ ;\ m_i+2\sigma_i]$.

4. CIRCÉ must not be used as a black box:

⇒ Development of a methodology for a proper use of CIRCÉ

- Are the conditions of the simple considered experiment similar to those of the studied reactor transient?
- Check that the problem is identifiable (distribution of the derivatives);
- Checking the hypothesis of linearity. Generally well verified;
- Checking the hypothesis of normality;
- Performing envelop calculations.