Construction the Statistics Distributions for Characterizing the Transfer Factors of Metals from Soil to Plant (TFsp) Using Bayesian Method

Pratnya Paramitha Oktaviana[1] and Marie-Pierre Etienne[2]

Abstract—Plants have the faculty of levy the metals in the soil. The consumption of this plants can represent in some situations a health risk to be assessed. The transfer of contaminants from soil to food crops is a major route connecting the soil contamination to human exposure. The Transfer Factors Soil-Plant (TF$_{sp}$) (the ratio between the concentration of contaminants in plants and the concentration of contaminants in the soil) is a value commonly used in the assessment of exposure and health risks. This research use the BAPPET database (database contents the informations of elements metal traces plants and vegetables). The goal of this research is for define the variable that influent the variability of TF$_{sp}$ and for characterizing their effects from their posteriors distributions using bayesian methods, Metropolis-Hastings. There are 3 metals (Cd, As and Pb), 4 plant types (leaf, fruit, root and tuber) and 2 analysis (using 4 plant types and 3 plant types, without tuber) with 4 models of analysis of varians (ANOVA, using normal and lognormal distribution for likelihood) that used in this research. The results of analysis for 4 plant types is chosing the model II with lognormal distribution for likelihood (y$_i$ ~ LN(μ$_i$, σ$_i^2$)) for the best model and for 3 plant types is chosing the model IV with lognormal distribution for likelihood (y$_i$ ~ LN(μ$_i$, σ^2), μ$_i$ = μ + α$_i$ + B$_j$ + δ$_k$, B$_j$ ~ N(0, σ$_B^2$)) for the best model. The contains of metal Cd, As and Pb in leaf has the highest risk for the health because that has the biggest posterior mean of TF$_{sp}$

Keywords— BAPPET Database, Metropolis-Hastings, Plant Types, ANOVA, Health Risk, Posterior Distribution.

I. INTRODUCTION

The plant foods consumed by humans not only come from agriculture but also the cultivation of plants in gardens and gathering. Plants have the ability to remove metals in the soil, consumption of vegetables can represent in some situations a health risk to be assessed. The transfer of contaminants from soil to food crops is a major route connecting the soil contamination to human exposure. The transfer factors of metals from soil to plant (TFsp) (ratio between the concentration of contaminants in plants and the concentration of contaminants in the soil) is a value commonly used in the assessment of exposure and health risks. Especially in studies of exposure modeling, it is recognized as one of the key parameters. BAPPET database (database contents Elements metal traces Plants Vegetables) which contains many experimental data of contaminated vegetable plants by trace metals, and therefore information on the TFsp parameter is used. This data is analyzed with the Bayesian approach.

The aim of the research is to define the variables responsible for the variability of TFsp and characterize their effects through posterior distribution. In these analyzes, the three metals (Cd, As and Pb), four plant types (leaf vegetable, fruit vegetable, root vegetable and tuber vegetable) and two methods of extracting the amount of metals in soil (extraction total and semi-total) are used.

II. METHOD

Bayesian method that explained in this chapter is used in the analysis for this research. The step of analysis will be explained after the theory of Bayesian.

Hierarchical Bayesian models are really a combination of two things: i) written in hierarchical form which model is ii) estimated using Bayesian methods. A hierarchical model is one that is written in a modular way, or in terms of sub-models. The sub-models are combined to form a hierarchical model, Bayes' theorem is used to integrate the pieces together and realize all the uncertainty that is present. The MCMC (Monte Carlo Markov Chain) are numerical methods to describe the posterior distributions and work especially well with hierarchical models, and it is the engine that has fueled the development and application of Bayes' theorem [1].

A. Bayes Formula

In the sequel, the notation [.] Is used for a probability of whether they are of a probability density function or a discrete distribution. In a Bayesian framework the estimation of a model is defined by updating the prior distribution of the parameters $[\theta]$ due to the training data contained in it, through the Bayes formula [9].

$$[\theta|y] = \frac{[y|\theta].[\theta]}{[y]} = \frac{[y|\theta].[\theta]}{\int [y|\theta].[\theta] d\theta} \qquad (1)$$

with $[\theta|y]$ is posterior density of θ.

B. Markov Chaine and MCMC Metropolis-Hastings Method

This section begins with a brief review of Markov chains that define the MCMC method of Metropolis-Hastings algorithm.

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1) Markov Chain Theory

Let $\theta = \{\theta_n\,; n \geq 0\}$ is a sequence of dependent random variables, θ is a Markov chain if

$$[\theta_{n+1}|\theta_0, \theta_1, \ldots, \theta_n] = [\theta_{n+1}|\theta_n] \tag{2}$$

for all $n \geq 0$. That is to say that the probability distribution of θ_{n+1} given past variables depends only on θ_n. This conditional probability distribution is called transition kernel K is K (θ_n, θ_{n+1}) [11].

Most of Markov chains encountered in Monte Carlo Markov Chain (MCMC) methods have a property of very high stability to ensure convergence to a stationary probability distribution, that verifies Markov Chain is irreducible, aperiodic and recurrent.. There is a probability distribution f such that if $\theta_n \sim$ f, then $\theta_{n+1} \sim$ f.

2) Metropolis-Hastings Algorithm

The Metropolis-Hastings algorithm associated with the objective (target) density f and conditional density g produces a Markov chain $\{\theta_n\}$ are defined by Robert and Casella [11] as follows:

a. Given θ_n, generates the candidate $Y_n \sim g(y|\theta_n)$, which is randomly distributed

b. take

$$\theta_{n+1} = \begin{cases} Y_n \text{ with probability } \rho(\theta_n, Y_n) \\ \theta_n \text{ with probability } 1 - \rho(\theta_n, Y_n) \end{cases} \text{ where}$$

$$\rho(\theta, y) = Min\left[\frac{f(y)g(\theta|y)}{f(\theta)g(y|\theta)}, 1\right] \tag{3}$$

Distribution g is called the candidate probability distribution and $\rho(\theta,y)$ is called the probability of acceptance of Metropolis-Hastings.

This algorithm is the basis of the operation of OpenBUGS software that was used to carry out the inferences of the models considered.

3) The Method of Gelman-Rubin Convergence Diagnostics in MCMC

To calculate the Gelman-Rubin statistic, as modified by Brooks and Gelman [2], the basic idea is to generate multiple chains from dispersed initial values, and assess convergence by comparing the extra variability and international channels. The researcher denote the number of strings generated by M and the length of each chain 2T. We take as a measure of the variability of the posterior width of the 100 (1 - α)% credible interval for the parameter of interest (in OpenBUGS, α = 0.2). According to the final iterations of T, calculate empirical credible interval for each channel, then the average width intervals through chains of M and denote by W. Finally, calculate the width B of the empirical credibility interval based on all samples MT grouped together. The ratio

$$R = \frac{B}{W} \tag{4}$$

pooling to medium widths range must be greater than 1 if the starting values are dispersed on properly, it will also tend to 1 as convergence is approached, so we can assume convergence for practical reasons if R <1.05, for example.

4) Deviance Information Criterion

In Bayesian analysis, Deviance Information Criterion (DIC) summarizes the model fit in posterior expectation of deviance, $\overline{D}$, and the complexity of a model by the actual number of parameters, p_D [3]. Models that receive the most support from the data are those that have the lowest values of the DIC. The definition of DIC is

$$DIC = \overline{D} + p_D \tag{5}$$

where:

$$D(\theta) = -2 \log p(y|\theta) \tag{6}$$

$$\overline{D} = \mathrm{E}_{\theta|y}[D(\theta)] \tag{7}$$

$$p_D = \overline{D} - D(\overline{\theta}) \tag{8}$$

The process has six steps. Stages of data analysis that are used to achieve the desired objectives are as follows:

1. Calculate the factors of soil-plant transfer (TF_{sp})
2. Identify outliers:
a. Transform the original data to TFsp natural logarithm (Ln) of TFsp function. To overcome the complexity issues related to asymmetric information in the process of outlier detection , transformation functions and algorithms exist that can help to increase the symmetry of the distribution [4]. Symmetrical data is important in most methods for detecting outliers because they were designed around the management of data following a normal distribution. Two commonly used functions are the functions log and square root because they have advantageous properties compared to the variance.
b. Calculate $\overline{X} \pm 2SD$ of transformed data. (SD = Standard Deviation)
   This is the method of standard deviation, if the transformed data are less than or greater than are therefore these data are outliers [12]. Study again the data identified as outliers, if there is sufficient reason to doubt the value of the data (usually in the case of a framework for testing other very different experiences based) on deletes this data. If there is no objective reason to remove it from the guard.
3. Several models will be considered, modeled through a random variability of plant species considered within its group (leaf vegetable , fruit vegetable , root vegetable and tuber vegetable) effect. Since the potato tuber is only representative group was removed when the group considered this model. It is therefore
   The analysis of four types of plant
   For this analysis, all data TFsp metals (Cd , As, Pb) is used for all types of plant (leaf vegetable , fruit vegetable , root vegetable and tuber vegetable). Model I and II are used for this analysis.
   The analysis of three types of plant (without tuber)
   For this analysis, data TFsp metals (Cd , As, Pb) is used for three types of plant (leaf vegetable , fruit vegetable , root vegetable) , without tuber vegetable. All models (I, II , III and IV) was used for this analysis.
4. The estimation is conducted under OpenBUGS.
   We need to file that contained both models, data and boots. For the (likelihood) probability data (TFsp), normal and log normal distribution is used.
5. The outputs of the software are then analyzed in R (R Script). It is the Bayesian analyzes (the MCMC , Metropolis -Hastings algorithm , 3 chains) by using the R software package BRUGS .

6. Choose the best model that has the smallest value of DIC (Deviance Information Criterion).

Depending on the model chosen (best model), we can assess which variables responsible for the variability of TFsp and also we can characterize their effects on each type of plant according to the posterior distribution.

Detail of the model compared is presented in Table 1.

III. RESULT AND DISCUSSION

This chapter discusses analysis of TF_{sp} metals Cadmium (Cd), arsenic (As) and lead (Pb) using the Bayesian method. The variability of TF_{sp} of each metal type of plant (leaf vegetable [1], fruit vegetable [2], root vegetable [3] and tuber vegetable [4]) and characterize their effects according to the results the posterior distribution analysis can be known. 4 models are used for this analysis, the model I and II for analysis four types of plant, while all models (I to IV) for analysis of three types of plant (without tuber vegetable).

A. Application to Metal Cadmium (Cd)

In this section, we will apply the method described above to analyze the factors of soil-plant transfer (TF_{sp}) metal cadmium (Cd). The number of data used to analyze four types of plant is 820; 330 data TF_{sp} in leaf vegetables, 163 data TF_{sp} in fruit vegetable, 198 data TF_{sp} in root vegetable and 129 data TF_{sp} in tuber vegetable; and then, for three types of plant analysis, 691 data are used (without tuber vegetable).

1) The Outputs of the Metropolis-*Hastings* MCMC Method

Before the discussion the MCMC output, the first is to show the descriptive analysis TFsp metal Cd Descriptive statistics TFsp metal Cd plant types is shown in the box plots in Figure 1. Figure 1. shows that the value of TFsp metal Cd in leaf vegetables is greater than other types of plant (vegetable, fruit, vegetable and vegetable root tuber). There is still data that are not included in interval (based on the boxes in Figure 5.1), while it was already removing outliers, but it cannot deleted because there not strong evidence. Values can TFsp great for concentration Metal Trace Elements (ETM) in the plant is large, it depends on the context.

a. Analysis 4 Plant Types

Table 2 present values of DIC for model I and II analysis four types of plant using likelihood normal and log normal.

According to the DIC value in Table 2, the model II that uses the likelihood of y_i is log normal distribution ($y_i \sim LN(\mu_i, \sigma_i^2)$) as the best model because it has the smallest DIC value (828.4) is chosen.

Figure 2 shows the posterior densities (the red line and also the histogram) of parameters μ_i and σ_i^2 (i = 1, 2, 3, 4) TFsp metal Cd Musample1 is the sample parameter μ_1 and all are sigmasample4 is similar to the sample parameter σ_4^2. The green line shows the prior density.

Summary subsequently shown in Table 3 were calculated. The effects of each type of plant that is encapsulated by each parameter μ_i (*mu[i]*) for i = 1, 2, 3, 4, value of TFsp metal Cd can be evaluated by the statistics in this table. The average value for Cd metal TFsp kind leaf vegetable is a posteriori should be equal to 0.095 (*mu[1]*) compared with others that are negative

(for 2167 fruit vegetable (*mu[2]*) ; 1107 for root vegetable (*mu[3]*) and 2436 for tuber vegetable (*mu[4]*)).

The conclusion is the first type of plant (leaf vegetable) has a higher value TFsp Cd metal effect and the fourth type of plant (vegetable tuber) has a lower value TFsp metal Cd in effect the results of this model. The posterior variance (sigma[i]) that this uncertainty in the parameter *mu[1]* is 1187; 2192 for parameter *mu[2]* ;1041 for parameter *mu[3]* and 1101 for parameter *mu[4]*.

b. Analysis 3 Plant Types

Table 4 shows the value of DIC for each model of analysis three plant types. According to the results in this table, the model IVb using log normal distribution as the likelihood of yi is chosen. It has the smallest DIC value (909.8). Then the best model for analysis of three types of plant is the model with the likelihood IV b log normal ($y_i \sim LN(\mu_i, \sigma^2)$ where $\mu_i = \mu + \alpha_i + B_j + \delta_k$, $B_j \sim N(0, \sigma_B^2)$).

B. The Results for The Others Metal

1) Metal Arsenic (As)

The comparasion of value of DIC for model I and II analysis four types of plant is shown in the following Table 5. The model II with likelihood log normal is chosen (DIC = -473.3).

Table 6 presents the comparison of the value of DIC for the analysis of three types of plant models. According to the results in Table 6, the value of DIC is smaller in all likelihood is the model with log normal distribution. The difference between these values is not very large. So we must consider what model you choose. According to the results previously Cd metal analysis, Model IV is chosen b log normal. We will most definitely consider this model. Then, because the smallest DIC is the log normal model IV and the difference with the DIC model IV b is only 0.6, the model is still IV b chooses with the likelihood of yi is log normal distribution (DIC = -453.1) as the best model for this analysis.

2) Metal Plomb (Pb)

The value of DIC analysis of four types of plant using model I and II is presented in Table 7. Model II is chosen with the probability distribution of yi is log normal again as the best model (DIC = -4047). Model IV b with probability yi is log normal distribution (DIC = -2954) is chosen as the best model (with the same consideration of metal analysis As before, because the difference is small) in Table 8.

IV. CONCLUSION

Based on the results and discussion that has been done in the previous chapter, we can conclude that:

1. For analysis of four types of plant for TFsp (metal Cd, As and Pb), the best model is selected Model II with the lognormal probability distribution ($y_i \sim LN(\mu_i, \sigma_i^2)$). Variable responsible for the variability of TF_{sp} metals is only the type of plant.

   a. The mean posterior (μ_i) and varians posterior (σ_i^2) of TF_{sp} metal Cd :
   $\mu_1 = 0.095$; $\sigma_1^2 = 1.187$ (leaf)
   $\mu_2 = -2.167$; $\sigma_2^2 = 2.192$ fruit)
   $\mu_3 = -1.107$; $\sigma_3^2 = 1.041$ (root)
   $\mu_4 = -2.436$; $\sigma_4^2 = 1.101$ (tuber)

   b. The mean posterior (μ_i) and varians posterior (σ_i^2) of TF_{sp} metal As :

$\mu_1 = -3.606$; $\sigma_1^2 = 2.248$ (leaf)
$\mu_2 = -4.881$; $\sigma_2^2 = 5.411$ fruit)
$\mu_3 = -5.307$; $\sigma_3^2 = 1.426$ (root)
$\mu_4 = -4.877$; $\sigma_4^2 = 2.378$ (tuber)

c. The mean posterior (μ_i) and varians posterior (σ_i^2) of TF$_{sp}$ metal Pb :
$\mu_1 = -3.784$; $\sigma_1^2 = 2.769$ (leaf)
$\mu_2 = -5.286$; $\sigma_2^2 = 4.066$ (fruit)
$\mu_3 = -4.639$; $\sigma_3^2 = 2.359$ (root)
$\mu_4 = -6.396$; $\sigma_4^2 = 4.157$ (tuber)

2. For analysis of three types of plant (without vegetable tuber) for TFsp (metal Cd, As and Pb), the best model is selected model IVb with lognormal probability distribution ($y_i \sim LN(\mu_i, \sigma^2)$, $\mu_i = \mu + \alpha_i + B_j + \delta_k$, $B_j \sim N(0, \sigma_B^2)$). The variables responsible for the variability of TFsp metal Cd are the type of plant species plant type and also fashion metal extractions.

3. TF$_{sp}$ metals is only the type of plant.

a. The mean posterior (μ_i) and varians posterior (σ^2) of TF$_{sp}$ metal Cd :
$\mu_1 = -0.444$ (leaf)
$\mu_2 = -1.496$ (fruit)
$\mu_3 = -0.992$ (root)
$\sigma^2 = 1.016$

b. The mean posterior (μ_i) and varians posterior (σ^2) of TF$_{sp}$ metal As :
$\mu_1 = -3.942$ (leaf)
$\mu_2 = -5.070$ fruit)
$\mu_3 = -5.782$ (root)
$\sigma^2 = 1.617$

c. The mean posterior (μ_i) and varians posterior (σ^2) of TF$_{sp}$ metal Pb :
$\mu_1 = -3.731$ (leaf)
$\mu_2 = -5.317$ (fruit)
$\mu_3 = -4.333$ (root)
$\sigma^2 = 2.862$

4. The metal content of Cd, As and Pb in leafy vegetable is more health risk because it has posterior mean of transfer factors soil-plant (TFsp) which is larger than other types of plant. The effect of metals TFsp leafy vegetable is most at risk for health and then root vegetable, vegetable, fruit and vegetable tuber last.

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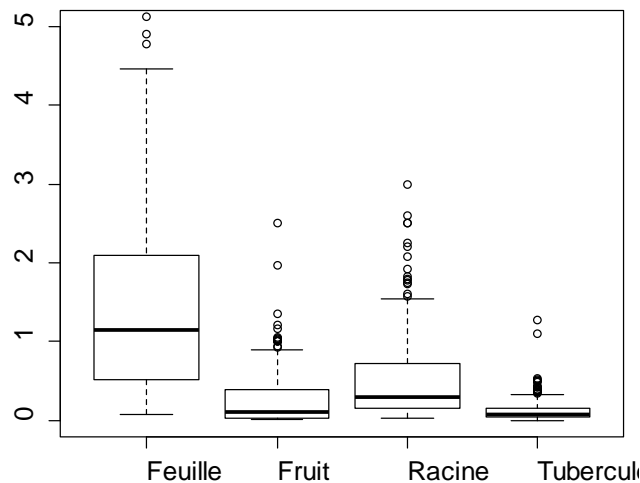[13]. Spiegelhalter, D. (2006). Some DIC Slides. MRC Biostatistics Unit, Cambridge. IceBUGS: Finland.

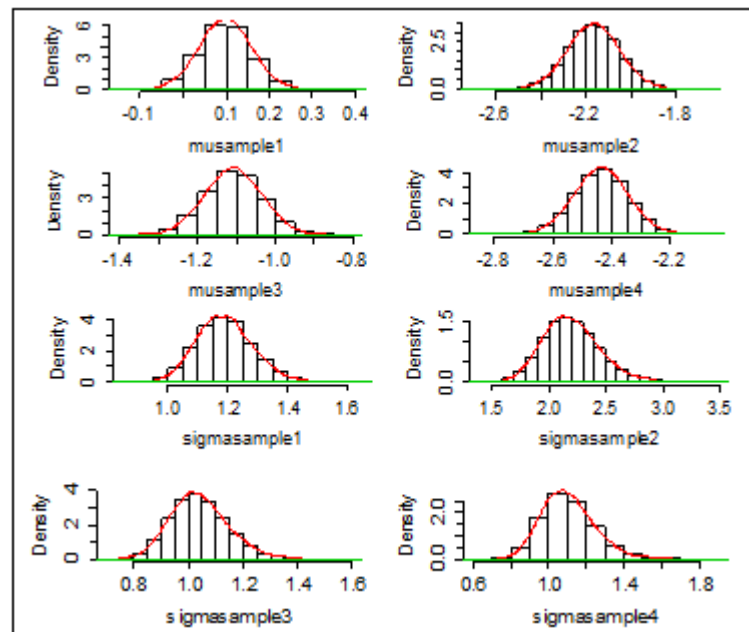Figure 1. The Boxplot of TFsp Metal Cd for Each Plant Types

Figure 2. The Graph of Parameters Density for μi and σi2 (i = 1, 2, 3, 4) Model II TFsp Metal Cd (Likelihood Log Normale)

TABLE 1.
EXPLANATION OF MODEL ANALYSIS OF VARIANCE (ANOVA)

Model	Explanation
I $Y_{ij} = \mu_i + E_{ij}$ $E_{ij} \sim N(0, \sigma^2)$	$Y_{ij} =$ the j-th TF$_{sp}$ on the i-th type of plant $\mu_i =$ the effect due to i-th level of type of plant $E_{ij} =$ the random error present in the j-th TF$_{sp}$ on the i-th type of plant
II $Y_{ij} = \mu_i + E_{ij}$ $E_{ij} \sim N(0, \sigma_i^2)$	$(i = 1, 2, 3, 4)$ for analysis 4 plant types (1 = leaf, 2 = fruit, 3 = root, 4 = tuber) $(i = 1, 2, 3)$ for analysis 3 plant types (without tuber) $(j = 1, 2, …, n$ observations)
III a) $Y_{ijk} = \mu + \alpha_i + B_j + E_{ijk}$ $E_{ijk} \sim N(0, \sigma^2)$ $B_j \sim N(0, \sigma_i^2)$	$\mu =$ the overall mean response $\alpha_i =$ the effect due to i-th level of type of plant (fixed) $B_j =$ the effect due to j-th level of species (random)
b) $Y_{ijk} = \mu + \alpha_i + B_j + E_{ijk}$ $E_{ijk} \sim N(0, \sigma^2)$ $B_j \sim N(0, \sigma_B^2)$	$(i = 1, 2, 3)$ $(j = 1, 2, …, n$ species) $(k = 1, 2, …, n$ observations)
IV a) $Y_{ijkl} = \mu + \alpha_i + B_j + \delta_k + E_{ijkl}$ $E_{ijk} \sim N(0, \sigma^2)$ $B_j \sim N(0, \sigma_i^2)$	$\mu =$ the overall mean response $\alpha_i =$ the effect due to i-th level of type of plant (fixed) $B_j =$ the effect due to j-th level of species (random)
b) $Y_{ijkl} = \mu + \alpha_i + B_j + \delta_k + E_{ijkl}$ $E_{ijk} \sim N(0, \sigma^2)$ $B_j \sim N(0, \sigma_B^2)$	$\delta_k =$ the effect due to k-th level of extraction (fixed) $(i = 1, 2, 3)$; $(j = 1, 2, …, n$ species) $(k = 1, 2$; 1 = extraction total, 2 = extraction semi-total) $(l = 1, 2, …, n$ observations)

TABLE 2.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 4 PLANT TYPES TO TF$_{SP}$ METAL CD

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	2983
	Distribution Log Normale	856.4
II	Distribution Normale	1927
	Distribution Log Normale	828.4

TABLE 3.
POSTERIOS SUMMARY FOR PARAMETERS μ_1 AND Σ_i^2 (I = 1, 2, 3, 4) OF ANOVA MODEL II TF$_{SP}$ METAL CD (LIKELIHOOD LOG NORMAL)

node	mean	SD	MC error	val 2.5pc	médian	val 97.5pc	start	sample
mu[1]	0.0947	0.0580	0.0010	-0.0205	0.0953	0.2073	5001	30000
mu[2]	-2.1670	0.1146	0.0023	-2.3850	-2.1660	-1.9420	5001	30000
mu[3]	-1.1070	0.0755	0.0014	-1.2620	-1.1060	-0.9642	5001	30000
mu[4]	-2.4360	0.0923	0.0015	-2.6170	-2.4360	-2.2570	5001	30000
sigma[1]	1.1870	0.0932	0.0017	1.0150	1.1860	1.3790	5001	30000
sigma[2]	2.1920	0.2357	0.0045	1.7760	2.1760	2.7080	5001	30000
sigma[3]	1.0410	0.1052	0.0020	0.8559	1.0320	1.2680	5001	30000
sigma[4]	1.1010	0.1402	0.0027	0.8698	1.0900	1.4040	5001	30000

TABLE 4.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 3 PLANT TYPES TO TF$_{SP}$ METAL CD

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	2630
	Distribution Log Normale	1104
II	Distribution Normale	1992
	Distribution Log Normale	1077
III a	Distribution Normale	2605
	Distribution Log Normale	929.2
III b	Distribution Normale	2605
	Distribution Log Normale	928
IV a	Distribution Normale	2585
	Distribution Log Normale	911,6
IV b	Distribution Normale	2586
	Distribution Log Normale	909.8

TABLE 5.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 4 PLANT TYPES TO TF$_{SP}$ METAL AS

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	-309
	Distribution Log Normale	-471.7
II	Distribution Normale	-326.4
	Distribution Log Normale	-473.3

TABLE 6.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 3 PLANT TYPES TO TF$_{SP}$ METAL AS

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	-282.8
	Distribution Log Normale	-433.8
II	Distribution Normale	-309
	Distribution Log Normale	-437.3
III a	Distribution Normale	-294.5
	Distribution Log Normale	-442.1
III b	Distribution Normale	-295.5
	Distribution Log Normale	-440.2
IV a	Distribution Normale	-295.5
	Distribution Log Normale	-453.7
IV b	Distribution Normale	-295.5
	Distribution Log Normale	-453.1

TABLE 7.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 4 PLANT TYPES TO TF$_{SP}$ METAL PB

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	-507.9
	Distribution Log Normale	-4033
II	Distribution Normale	-1499
	Distribution Log Normale	-4047

TABLE 8.
THE VALUE OF DIC FOR EACH MODEL OF ANALYSIS 3 PLANT TYPES TO TF$_{SP}$ METAL PB

Modèle	La Vraisemblance de y_i	DIC
I	Distribution Normale	-302.4
	Distribution Log Normale	-2947
II	Distribution Normale	-768.2
	Distribution Log Normale	-2956
III a	Distribution Normale	-297.2
	Distribution Log Normale	-2955
III b	Distribution Normale	-301
	Distribution Log Normale	-2955
IV a	Distribution Normale	-296.9
	Distribution Log Normale	-2954
IV b	Distribution Normale	-300.7
	Distribution Log Normale	-2954