Extended Kalman Filter and Markov Chain Monte Carlo Methods for Uncertainty Estimation. Application to X-Ray Fluorescence Machine Calibration and Metal Testing

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Abstract: This paper is concerned with a method for uncertainty evaluation of steel sample content using X-Ray Fluorescence method. The considered method of analysis is a comparative technique based on the X-Ray Fluorescence; the calibration step assumes the adequate chemical composition of metallic analyzed sample.
It is proposed in this work a new combined approach using the Kalman Filter and Markov Chain Monte Carlo (MCMC) for uncertainty estimation of steel content analysis. The Kalman filter algorithm is extended to the model identification of the chemical analysis process using the main factors affecting the analysis results; in this case the estimated states are reduced to the model parameters. The MCMC is a stochastic method that computes the statistical properties of the considered states such as the probability distribution function (PDF) according to the initial state and the target distribution using Monte Carlo simulation algorithm. Conventional approach is based on the linear correlation, the uncertainty budget is established for steel Mn(wt%), Cr(wt%), Ni(wt%) and Mo(wt%) content respectively. A comparative study between the conventional procedure and the proposed method is given. This kind of approaches is applied for constructing an accurate computing procedure of uncertainty measurement.

Keywords: Kalman filter, Markov Chain Monte Carlo, X-Ray fluorescence calibration and testing, steel content measurement, uncertainty measurement.

1 Introduction

Chemical analysis of material is a basic and an important activity needed along the production and quality control process. From raw material until the final product, quality control and testing need a continuous evaluation for decision making. In the field of the material sciences and engineering, many characteristics must be monitored to obtain product free or acceptable defects. Characterization of such material can be made in static laboratory or in online measurement using the adequate instrument and equipment. The measurement instrument and equipment must be calibrated with an uncertainty which is recommended by the inspection procedure and the manufacturing process capability.
The uncertainty measurement during the testing and calibration is a fundamental and an important operation particularly in the laboratory. The measurement capability is defined by the measurement uncertainties which are affected by the following factors:

- Method: Typically standardized and non standardized method,
- Means: The equipment performance i.e. Calibration Measurement Capability (CMC) of different instrument and equipment,
- Man: The mean such as competence of the human resources,
- Ambient: The environment conditions and parameters,
- Material: The consumed of the used material.

The uncertainties budget can be expressed as a complex relationship between these factors and the concerned parameter i.e. the measured parameters to be considered. The uncertainty quantity is a value of the standard

deviation; it is defined as a sum of the quadratic components [1, 2].

The measurand can be described by a soft sensor or by an analytical model obtained by the required methods and the techniques of modeling and identification. The estimation of the model output parameter based on the inferential model can be obtained using the first principle, known as mechanistic modeling, or by using grey or black box identification methods. Because the systems are complex such as the steel carbon - sulfur content analysis – based on non standardized method i.e. the infrared combustion method, in this situation, complex phenomena and interactions take place, it is strongly recommended to use a combined approach using an estimation of uncertainties of type A and type B [3, 4].

In the case of the non analytical model i.e. statistical approach, Monte Carlo simulation is strongly recommended; the model is perturbed by the corresponding Probability Distribution Function (PDF) at the target input.

The steel carbon - sulfur content analysis is a complex system defined by multivariate interactions between different factors such as the ambient conditions, metal preparation, contamination risk, and the equipment state and operator must be processed to obtain accurate results.

There are some existed methods which can be extended to evaluate the uncertainty, from which we cite:

- Conventional statistical approaches and its allied methods such as multivariate identification [1, 2,3,4,5,6,7,8,9,10].
- Multivariate Statistical Process control, data driven and data mining [11, 12, 13, 14, 15].

For our application, there are few related works in the field of the uncertainty evaluation of the steel analysis using X-Ray fluorescence machine calibration and testing. Modeling and simulation using stochastic approach is an important tool in uncertainty evaluation where PDF of each variable is simulate to generate random samples from the corresponding distribution.

In this paper, a new idea based on the combined use of Extended Kalman Filter (EKF) and Markov Chain Monte Carlo (MCMC) is introduced to uncertainty evaluation with a specific application to steel carbon - sulfur content measurement. This approach consists of the following steps:

The first step is a modeling and identification of the dynamic behavior of the measurement process i.e. a mathematical description of the state of the combustion chamber. An EKF algorithm is used to model the dynamical changes of the measurement process parameters; an adaptive way is applied to minimize the modeling error defined by the difference between the reference and the computed model output.

The second step is a validation and an evaluation of the model in basis of the generated error using the Sum Squared Error (SSE) i.e. uncertainties. The above cited reference output is given by the value of the calibrated reference material. The standard deviation of the error is adopted as uncertainty.

The third step is an online model estimation combined to the random changes of the measurement process conditions using stochastic methods, the uncertainties are then evaluated according to the model changes.

The main motivations to use such approach are:

- The measurement process is an unsteady state multivariable system,
- The measurement principle present non-linear and unsteady state reactions, and hence a combined form is needed.

The application of the sensitivity method based on the Guide of Uncertainty Measurement (GUM) is relatively limited for such measurement process.

An accurate and precise measurement is needed.

This paper is organized as follows. In section 2, the proposed method based on the EKF is developed: A computing scheme is implemented and tested. Section 3 gives a description of measurement process of carbon and sulfur using combustion method. Simulation results are also presented and commented using the GUM and EKF-MCMC methods for uncertainties evaluation. A comparative study based on the uncertainties values is also provided at the end of the paper.

2 Extend Kalman Particle Filter Based on Markov Chain Monte Carlo

The conventional Kalman filter algorithm is generally applied for a state estimation using noisy measurement, we extend this approach to the model parameter estimation (θ_t) defined by the following system:

$$\theta_t = f(\theta_{t-1}, u_{t-1}) + w_t \quad (1)$$

$$y_t = h(\theta_t, u_{t-1}) + v_t \quad (2)$$

where $\theta_t \in \Re^n$ is the state of the system, $y_t \in \Re^m$ the measurement output, ut the system input, wt the state noise, v_t the measurement noise, Q_t the system noise covariance matrix, R_t the measurement covariance matrix, f the system dynamic function and h the measurement function.

2.1.Conventional Kalman Filter

The conventional Kalman filter algorithm is implemented as follows:

Initialization

$$\theta_{(1)} = f(\theta_{(0)}, u_{(0)}) + w_{(1)}$$

Define ut, wt, Qt, Rt,

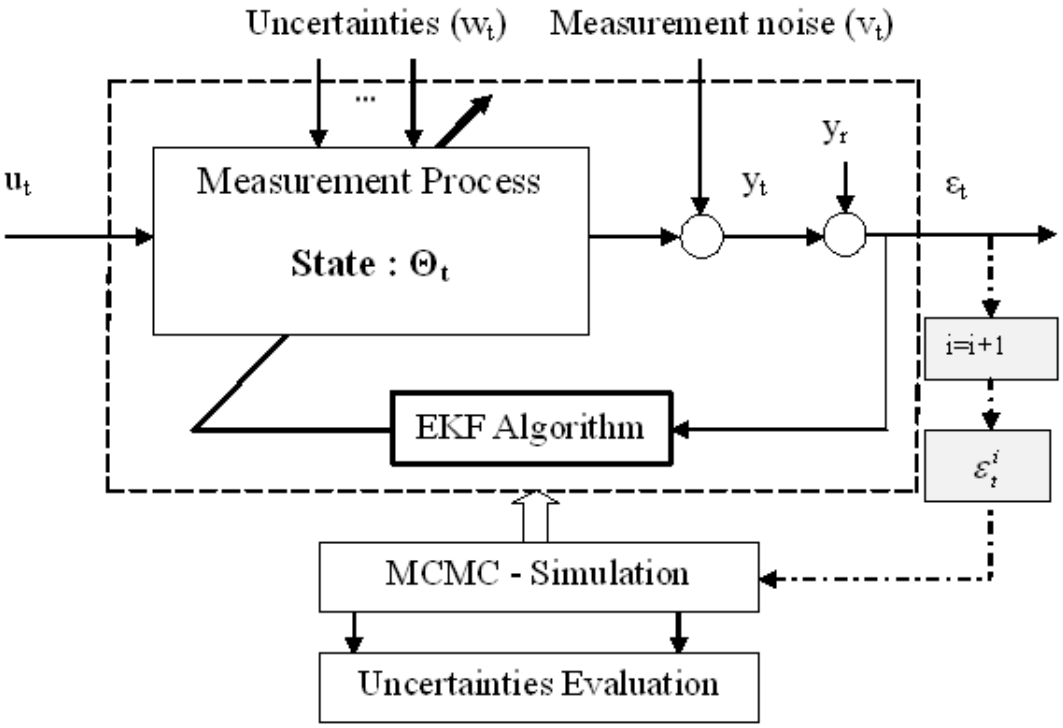

Fig.1 Combined use of EKF and MCMC

Computing loop

For t = 0 :t_{Max}

$$\theta_t = f(\theta_{t-1}, u_{t-1}) + w_t \quad (3)$$

$$F_t = (\frac{\partial f}{\partial \theta}) \quad (4)$$

$$H_t = (\frac{\partial h}{\partial \theta}) \quad (5)$$

$$P_t = F_t P_{t-1} F_t^T + Q_{t-1} \quad (6)$$

$$S_t = H_t P_t H_t^T + R_{t-1} \quad (7)$$

$$K_t = P_t H_t^T S_t^{-1} \quad (8)$$

$$\theta_t = \theta_{t-1} + K_t[y_t - h(\theta_{t-1}, u_{t-1})] \quad (9)$$

$$y_t = h(\theta_t, u_{t-1}) + v_t \quad (10)$$

End,

2.2.Extended Kalman Filter

Extend Kalman Filter can be easily extended to generate a proposal distribution, which can integrate the observed information, the principle is based on the model perturbation using the adequate distribution function of inputs, this principle can be summarized by the following scheme,Fig.1. The EKF scheme is combined with MCMC to give an integrated system for sensitivity analysis. EKF algorithm generates the optimal state (θ_t) associated with its corresponding PDF are used as a basic tool to the MCMC method, Monte Carlo simulation is used to compute the final PDF and its statistical properties [19], uncertainties are then evaluated. The corresponding algorithm is implemented as follows: For each iteration (i), the state the initial state (θ_0^i) is generated from the prior PDF.

Computing Loops

For i=1:N,

For t=t_{Max}, Compute the new state using the EKF algorithm,

$$\theta_t^i = f(\theta_{t-1}^i, u_{t-1}) + w_t^i \quad (11)$$

$$F_t = (\frac{\partial f}{\partial \theta}) \quad (12)$$

$$H_t = (\frac{\partial h}{\partial \theta}) \quad (13)$$

$$P_t^i = F_t P_{t-1}^i F_t^T + Q_{t-1} \quad (14)$$

$$S_t^i = H_t P_t^i H_t^T + R_{t-1} \quad (15)$$

$$K_t^i = P_t^i H_t^T (S_t^i)^{-1} \quad (16)$$

$$\theta_t^i = \theta_{t-1}^i + K_t^i[y_t^i - h(\theta_{t-1}^i, u_{t-1})] \quad (17)$$

$$\varepsilon_t^i = y_t^i - h(\theta_{t-1}^i, u_{t-1}) - v_t^i \quad (18)$$

end

end

3 Measurement and Analysis of the Content of Metallic Material

3.1.Principle

The principle of measurement is given by the following scheme,Fig. 2.

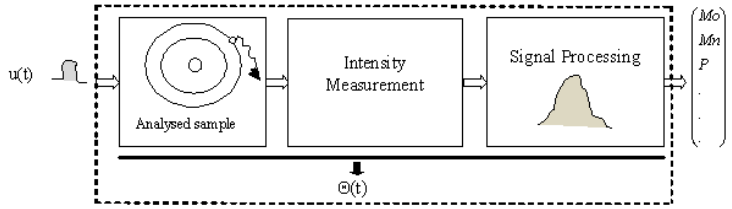

Fig.2 Principle of metallic sample analysis using X-ray fluorescence

In X-Ray Fluorescence (XRF) uncertainty evaluation of metal analysis is of the great importance particularly in the case of laboratory accreditation. In this work, we present a statistical method based on the repeatability and reproducibility analysis using certified reference material. The main factors influencing the metal analysis results are identified and quantified; this approach assumes a conformity assessment to the accreditation standard ISO /CEI 17025.

A real evaluation of uncertainty is obtained by developing and application of statistical methods extended to GUM and other references. The computed uncertainty is useful for product quality and conformity declaration according to the used standard.

XRF spectrometry is one of the most widely used and versatile analytical technique. An XRF spectrometer normally uses primary radiation from an X-ray tube to excite secondary X-ray emission from a sample. The radiation emerging from the sample includes the characteristic X-ray peaks of major and trace elements present in the sample. Dispersion of these secondary X-ray into a spectrum, usually by X-ray diffraction, allows identification of these elements present in the sample.

The height of each characteristic X-ray peaks relates to the concentration of the corresponding element in the sample, allowing quantitative analysis of the sample for most elements. The solid samples are analyzed in the form of pressed powder pellets.

The spectrum analysis can be done in two ways:

- Dispersive wave analysis (WD-XRF, Wavelength Dispersive X-ray fluorescence spectrometry) length;
- Energy dispersive analysis (ED-XRF, Energy Dispersive X-ray fluorescence spectrometry).

When a specimen is excited by irradiation by a beam of sufficiently short-wavelength X-radiation, the specimen emits characteristic fluorescence lines. The energy emitted by the excited element has a wavelength characteristic of that element and intensity proportional to the number of excited atoms. The scattered fluorescence is collimated by the entrance slit of the goniometry and directed onto the plane surface of the analyzing crystal. The line radiations, reflected according to the Bragg condition($n\lambda = 2d \sin\theta$), pass through an exit slit to the detector where the energy of the X-ray quanta is converted into electrical impulses or counts

The relationship between different standard i.e. reference value and the measured data can be expressed by a correlation function.

$$y = f(x) + \varepsilon \quad (19)$$

Where y is the reference value i.e. the value given by the certified reference material and x is the measured value given by the machine in the normal operating conditions (repetitive and reproducible conditions).

3.2.Modeling of the Measurement Process

The above developed method, Fig. 1, using the EKF algorithm is applied to model the measurement process of analyzed sample using the XRF, the measurement process is considered as a system characterized by the followings deviations parameters:

- The control input affecting the ambient conditions such the room temperature that affects the measurement cell behavior,
- The state vector parameters θ_t characterizing the cells properties,
- The measurement values affected by different noises such as the deviation of the electronic components as non linearity,
- Metal preparation.

Before each analysis, the measurement system must be calibrated using a reference certified material, it has been used nine standard with different certified values given by Table. 1.

The reference output of the model (y_t) defined in Fig. 1 is equal to the Certified Reference Material (CRM) values with a normal distribution.

To model the measurement process, an experiment plan has been used with a time series of 27 tests points obtained by an analysis repeatability of 03 one of each reference standard (see, Table. 1).

The following model has been considered to model the relationship between the reference certified value and the result of the analysis (predicted value).

$$\theta_t = \theta_{t-1} + w_t \quad (20)$$

$$y_t = C\theta_t + v_t \quad (21)$$

with: $\theta_t \in \Re^{2\times 1}$: the model parameters to be estimate, $\theta_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$,

$u_t \in \Re^{1\times 1}$ is equal to the input power of X-ray excitation which is constant, $w_t \in \Re^{2\times 1}$ normally distributed with a standard deviation taken from the calibration certificate of energy stability.

$C=[y_{t-1},1]$ is the measurement process data as a linear, this is a linear relationship. $v_t \in \Re^{2\times 1}$ is the measurement noise, normally distributed with a standard deviation taken from the reference certified material.

The EKF-MCMC developed in the section 2 is applied to predict the measurement output given by the XRF, and then the corresponding uncertainty is quantified. The measurement is considered as Markovian process, the repeatability of measurement assumes the convergence the measurand to its best estimated value.

The followings figures explain the uncertainties evaluation in two steps:

- Research of the correlation model (Fig.3a, Fig.4a and Fig.5a),
- Use of the EKF-MCMC algorithm to evaluate the uncertainty of the measurement repeated process in basis of the correlation model (Fig.3b, Fig.4b and Fig.5b).

Table1: Standard Reference data

Standard reference		Mo (wt%)	Cu(wt%)	Ni(wt%)	Mn(wt%)	Cr(wt%)	V(wt%)	Si(wt%)	P(wt%)
401/2	Certified value	0,495	0,101	0,019	1,197	0,138	0,496	0,602	0,027
	Uncertainty	0,011	0,003	0,002	0,010	0,005	0,009	0,011	0,001
402/2	Certified values	0,140	0,302	0,808	0,228	0,652	0,194	0,111	0,016
	Uncertainty	0,008	0,006	0,008	0,005	0,014	0,008	0,006	0,001
403/2	Certified values	0,088	0,221	0,223	1,677	0,463	0,341	0,209	0,055
	Uncertainty	0,004	0,004	0,004	0,014	0,012	0,008	0,005	0,002
404/2	Certified values	0,307	0,427	0,393	0,532	0,774	0,107	1,121	0,048
	Uncertainty	0,008	0,010	0,007	0,009	0,012	0,005	0,010	0,001
405/2	Certified values	0,025	0,022	0,102	0,903	0,206	0,411	0,947	0,010
	Uncertainty	0,003	0,002	0,004	0,008	0,006	0,010	0,014	0,001
406/2	Certified values	0,980	0,289	1,620	0,447	2,001	0,010	0,342	0,010
	Uncertainty	0,020	0,009	0,030	0,008	0,008	0,002	0,004	0,001
407/2	Certified values	0,830	0,397	0,527	0,195	3,030	0,190	0,660	0,038
	Uncertainty	0,020	0,008	0,011	0,006	0,020	0,010	0,020	0,001
408/2	Certified values	0,098	0,694	4,130	0,557	0,111	0,067	0,237	0,056
	Uncertainty	0,007	0,006	0,040	0,005	0,004	0,004	0,005	0,001
409/2	Certified values	0,599	0,205	3,020	0,559	1,318	0,008	1,180	0,014
	Uncertainty	0,007	0,004	0,030	0,009	0,010	0,002	0,010	0,001

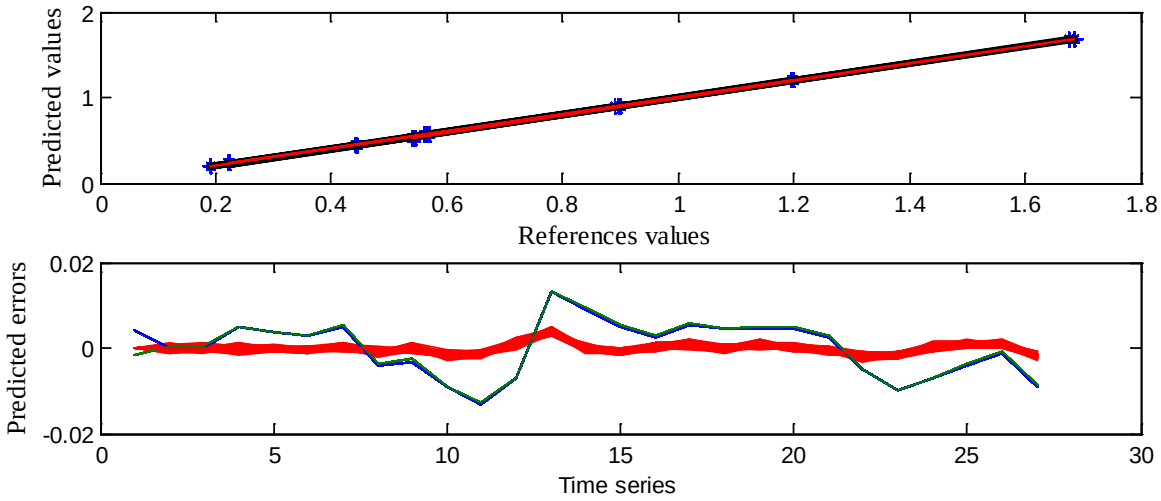

Fig.3 Modeling of the measurement process of Mn (wt%)

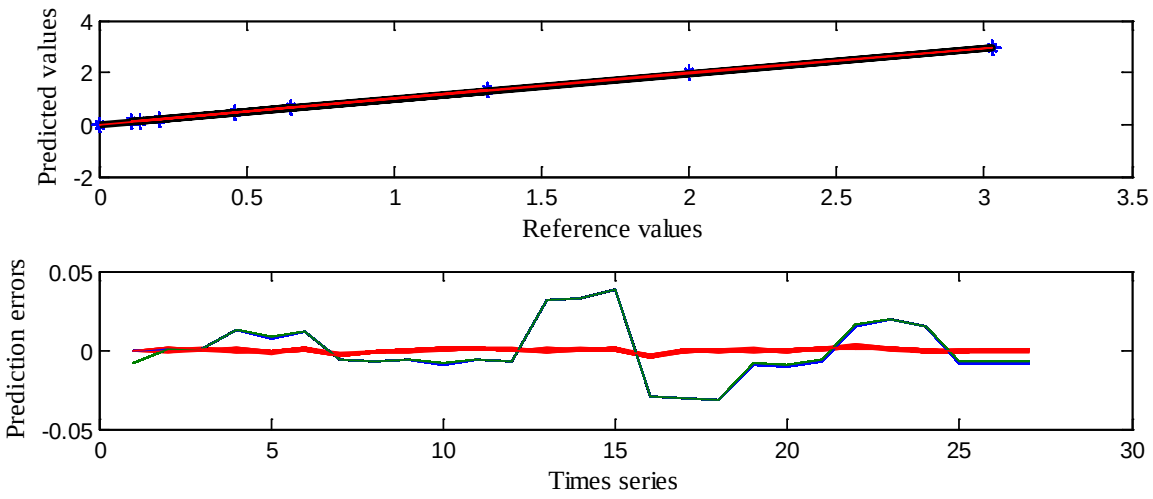

Fig.4 Modeling of the measurement process of Cr (wt%)

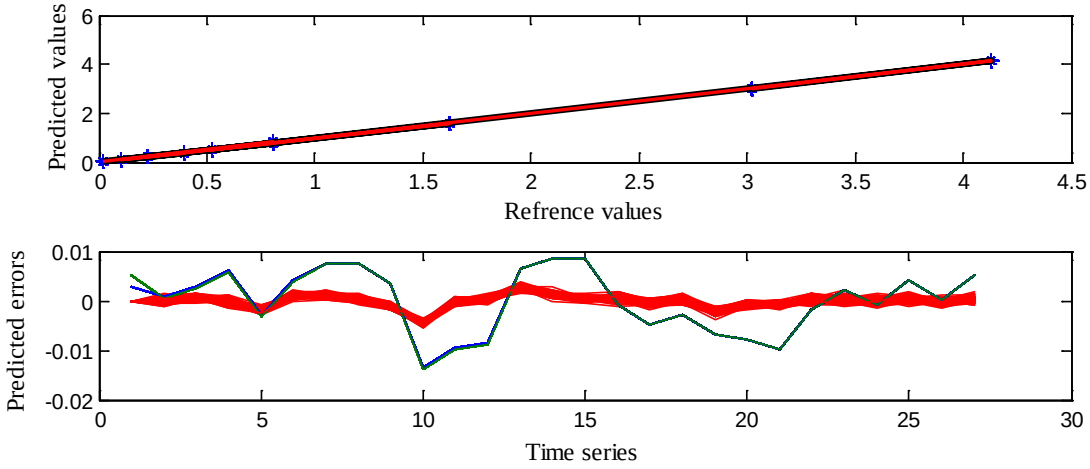

Fig.5 Modeling of the measurement process of Ni (wt%)

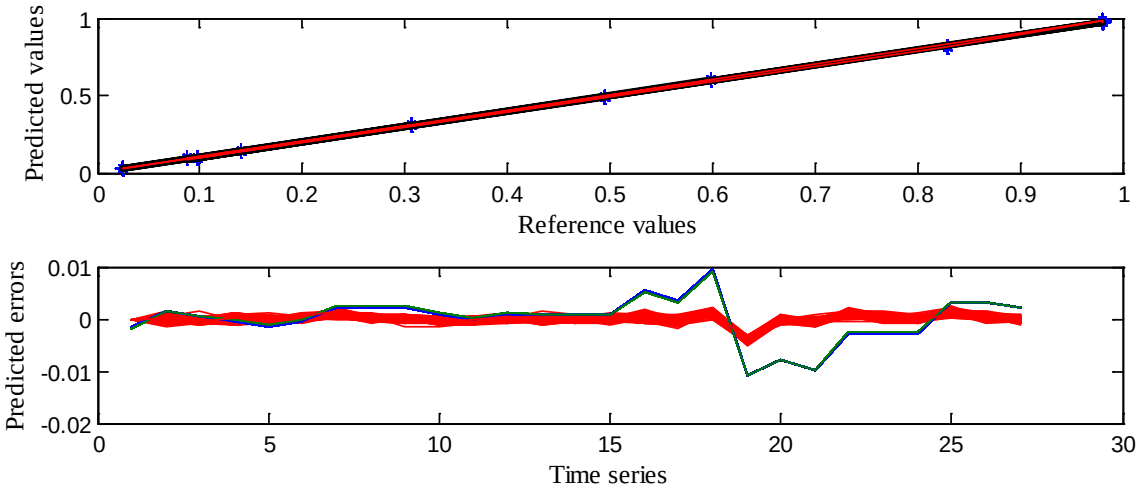

Fig.6 Modeling of the measurement process of Mo (wt%)

3.3.Uncertainties Evaluation

As presented below, the uncertainties are evaluated using two methods, the first approach is based on the linear model using a simple correlation method and the second is based on the EKF–MCMC. The global uncertainty budget is composed from three components: certified uncertainty of the reference material, random uncertainty of the measurement process and the bias uncertainty from the certified value.

$$u(\Delta y) = \sqrt{u_{STD}^2 + u_{RND}^2 + u_{BIAS}^2} \qquad (22)$$

The random components are generated by the measurement process, all random changes such as material imprecision of calibration, ambient etc. This component is estimated using EKF-MCMC by the standard deviation of generated random sequence by Monte Carlo simulation red curves of Fig.3b, Fig.4b and Fig.5b. The random component for the linear case is also estimated by the same manner as EKF-MCMC see blue – green curves of Fig.3b, Fig.4b and Fig.5b.

The bias is estimated as follows:

$$u_{BIAS} = (Certified\ value - \bar{y}_t)/\sqrt{3} \qquad (23)$$

where $\bar{y}_t$ is the mean value of the generated sequence using EKF-MCMC algorithm.

The difference between the certified value and the mean value is divided by $\sqrt{3}$ because the bias has a rectangular distribution.

The uncertainty of the reference material i.e. u_{STD} is given by the calibration certificate of the reference material.

The uncertainty budget is shown in Table. 2 and Table.3 respectively for the linear model and EKF-MCMC models.

Two methods have been used to evaluate the uncertainties: simple approach using linear correlation and a prediction using EKF-MCMC. As shown in Table. 3, the uncertainty budget of EKF-MCMC is more accurate than the linear correlation, the uncertainty of the standard is equivalent to the two methods, it is defined in the calibration certificate of the CRM.

Tables.2and 3 show the uncertainties budget respectively for the linear correlation and EKF-MCMC methods using a time series of 27 points of measured data.

As shown in these results, the global uncertainty budget for all analyzed components [Mn(wt%) Cr(wt%) Ni(wt%) Mo(wt%)] using EKF-MCMC is less than that obtained using the linear correlation.

4 Conclusion

A new method based on EKF-MCMC stochastic method was designed and implemented to the uncertainty estimation of measurement process of metallic analysis using X-Ray Fluorescence. The modeling and estimation procedure was carried on real world data using calibration and measurement samples tests. The obtained results show that the stochastic method based on the EKF-MCMC gives more precise uncertainty compared to the linear correlation. The main findings are:

A computing procedure using EKF-MCMC is developed and applied to the uncertainty evaluation,

A prediction model is obtained and tested, a bias is detected and more accurate uncertainty is obtained,

A comparative study between the conventional linear correlation model and the new EKF-MCMC is made using uncertainty budget.

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