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Prediction of thermal and mass loss behavior of mineral mixture using inferential stochastic modeling and thermal analysis measurement data

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ABSTRACT

Characterization methods of material are widely used in different steps of quality control in material sciences and engineering. Such methods are relatively complex according to the considered case. This paper is concerned by a characterization method for mineral material analysis using thermal analysis i.e. Differential Scanning Calorimetric. The thermal analysis is a physical method based on the heating; the sample is heated using a ramped set point of the input temperature, according to its properties, the sample gives a thermal response qualified by endothermic and exothermic reactions: Such responses are fundamental for phase's identification.

In mineral industry, different material mixture is used in different stage of manufacturing process; the thermal behavior prediction of mixture between two or more materials is very interesting. The thermal mixture behavior is predicted in basis of individual thermal behavior of each input element and the mixture ratio.

A mathematical modeling based on artificial neural network is designed to have a soft sensor for predicting the thermal and mass behavior of the mixture, validation using measurement and prediction uncertainties is also considered.

Using such approach, the prediction of the mineral mixture characteristics is given by an implementation of the obtained model using the individual behavior and the mixture proportion of the inputs elements.

1. Introduction

Quality control and evaluation of material is a basic and important activity needed along the production and testing processes. From raw material until the final product, quality control and evaluation need a continuous monitoring for decision making. In the field of mineral and material engineering, the final product is generally obtained by a mixture of different inputs materials, many characteristics must be known to decide about the quality level of a product. We are interested in this particular work to the thermal and mass analysis. Thermal and mass analysis of material is defined as a technique where the change of sample property is bound to an imposed temperature variation. In case of a temperature change is imposed over time, we distinguish, for example, thermo gravimetric analysis (TGA) and differential scanning calorimetry (DSC), thermo gravimetric analysis (TGA) is also obtained by a measurement technique of change in sample of mass under a temperature and controlled atmosphere. The loss and/or a gain of the weight as a function of time or temperature are of great importance for the phenomenon and reactions analysis.

At different temperatures, chemical reactions can get gaseous species or oxides resulting from mass variation. This change in mass is analyzed dependently of temperature [1–6].

The principle of thermal analysis is given by Fig. 1.

The input sample with its initial mass and temperature (m, T) is heated: The change of mass and temperature are observed and recorded during the characterization process. At the end of the characterization process, the following data are obtained:

- A global mass loss (Δm),
- A temperature change (ΔT) and a computed enthalpy variation (Δh).

The input and the output of testing process are considered as the input and output of the mathematical model.

In this work, particular importance is given to the prediction of parameters normally given by the thermal analyzer; these param-

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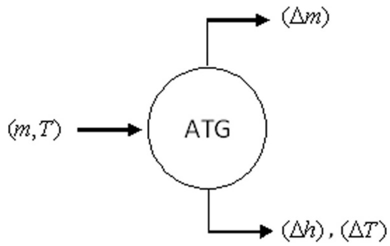

Fig. 1. Principle of thermal analysis.

eters will be predicted by the considered mathematical model based on different mass proportions of mixtures and their relative property. Individual heat signature of inputs: in our case calamine oxide and pigment characteristics are taken into account.

Model validation is performed by the experimental data obtained by thermal analysis equipment, valid both model will use to predict the thermal behavior of mixture, mainly the loss of mass and energy (enthalpy).

2. Proposed modeling and identification scheme

New idea based on the combined use of ANN model and MTCS is introduced to predict the main characteristic i.e. model output according to random changes of model inputs. This approach consists of the following steps: The proposed method based on the modeling and identification methods is presented. A computing scheme is developed and implemented. Then a description of measurement analysis will constitute the validation made by the residual evaluation. Simulation results are also presented and commented using MTCS methods for uncertainties evaluation. A comparative study based on the computed uncertainties values is also provided at the end of the paper.

2.1. Combined use of inferential model and Monte Carlo Simulation

As shown on Fig. 2, the inferential model is combined to Monte Carlo simulation method for uncertainty estimation and related computing procedure is implemented [7–10].

The evaluation method given by the above Fig. 2 is implemented as follows:

Step1: Acquisition of a new set of inputs/outputs (X^t, y_t) different of that used in the learning step (Section 2.2),

For i = 1 to N,

a): Perturbation of the input by adding a random value $[\Delta X^t]_i$ at each iteration (i), the input becomes $[X^t \pm \Delta X^t]_i$,
b): Compute the model output $\hat{y}_t$ using the artificial neural network model obtained in the Section 2.2,
c): Compute the modeling error $\varepsilon^t = y_t - \hat{y}_t$,
d): Affect $\varepsilon^t \rightarrow E_i^t$ at each iteration (i), E_i^t is a large random error.

End

Step 2: Statistical evaluation of the random matrix E_i^t: Analysis of the random distribution P_i,

Step 3: Estimation of the global uncertainties from P_i and E_i^t. i.e. use the standard deviation,

Step 4: End.

2.2. Artificial neural network model identification

Advanced process, quality control and monitoring require accurate process models. The development of analytical models from the relevant physical and chemical knowledge, especially for complex systems with phase changes, can be too costly or even technically impossible. For such models, based mainly on the data production, operational data should be capitalized. Many systems and processes are characterized by a non-linear dynamic behavior. Then, they need non-linear models. Indeed, Artificial Neural Networks (ANN) have been shown to be able to approximate continuous non-linearity's and have been applied in modeling of non-linear and complex. In practice, many non-linear processes are approximated by reduced order and possibly linear models and which are clearly related to the underlying process characteristics. The model identification principle using ANN is given by Fig. 3. A model structure is chosen, the input and the output variables are defined, the modeling residual or error is computed and used as a tool to adapt the model parameters w_{ij}^t by means of the computing procedure which generally includes a recursive form, more details about this method can bed founded in different documents [11–17].

The model output is defined by:

$$y_t = f(x, w_{ij}^t) \tag{1}$$

f is a model structure, x is the model input and w_{ij}^t are the ANN weights. They are estimated by the corresponding algorithm that minimizes the modeling error as shown in Fig. 6. The recursive form is given by the following equation.

$$w_{ij}^t = w_{ij}^{t-1} + \alpha \frac{\partial f}{w_{ij}} \varepsilon(t) \tag{2}$$

With α a constant $(0 < \alpha < 1)$.

Many published works have been developed in modeling and identification field using artificial neural networks [13–19], the computing procedure is described by the following steps:

Step 1: Initialize the network weights $w_{ij}^0 = [-0.5 \text{ to } +0.5]$
Step 2: Acquisition of inputs/outputs (x^t, y_t)
Step 3: Compute the model output $\hat{y}_t$

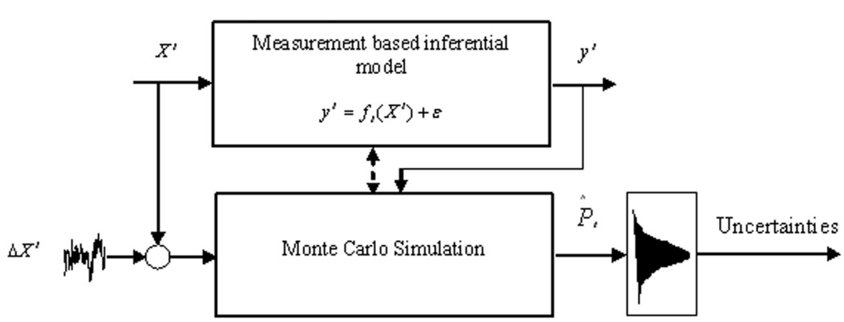

Fig. 2. Principle of modeling using inferential model and Monte Carlo Simulation.