# Sensor Monitoring of the Concentrations of Different Gases Present in Synthesis of Ammonia Based On Multi-Scale Entropy and Multivariate Statistics

S. Aouabdi, M. Taibi

***Abstract*—**This paper presents powerful techniques for the development of a new monitoring method based on multi-scale entropy (MSE) in order to characterize the behaviour of the concentrations of different gases present in the synthesis of Ammonia and soft-sensor based on Principal Component Analysis (PCA).

***Keywords*—**Ammonia synthesis, concentrations of different gases, soft sensor, multi-scale entropy, multivariate statistics.

## I. Introduction

THE monitoring of chemical processes and the diagnosis of faults in these processes is an important aspects of process systems engineering because they are integral to the successful execution of planned operations and to improving process productivity and safety. Recently designed industrial process plants, numerous variables are measured in various operating units, and these variables are recorded at many time points [1].

In the absence of an appropriate method for processing such data, only limited information can be extracted and consequently plant operators have only a poor understanding of the process. This lack of understanding leads to unstable operation. However, if properly processed, the abundance of process-data recorded in modern plants can provide an insight into potential faults and malfunctions, enabling plant operators to understand the status of the process and therefore to take appropriate actions when abnormalities are detected [2]. This can be done by checking if particular measurable or estimated variables are within a certain tolerance of the normal value [3].

The interaction of different variables of ammonia synthesis process constitutes a dynamic chemical system. The chemical mechanisms taking place in ammonia synthesis process appears that the Ammonia process is multivariable and strongly nonlinear [4]. Ammonia is physically complex and proves difficult to both operate and control because of operational constraints and process variable interactions [5].

Fault diagnosis is crucial for the high-performance operation of complex systems to meet stringent requirements on system availability and safety in the event of component failures [6].

Model-based diagnosis relies on information redundancy concepts. Its principle is generally based on consistency checking between an observed behaviour of the process and the mathematical representation of the process [7]. This mathematical representation may take the forms of analytical redundancy which is an explicit input-output relationship, but in many situations it may be difficult to obtain due to complexity of the process and high process dimensionality.

Principal component analysis (PCA) is data-driven method which needs little priori knowledge in the problem-solving process; therefore PCA is well applicable to the complex problems with a large number of data [8]. The key idea of PCA model is to reduce the number of variables by building their linear combinations, PCA has been widely applied in multivariate statistical process monitoring due to its capability to extract information in multivariate environments [9].

In this paper, we propose a method to monitor sensors of the concentrations of different gases present in synthesis of ammonia based on multi-scale entropy (MSE) and construct a PCA model that can sufficiently provide relevant information on the process variables and stability of reactor operation. The stability of reactor operation can be characterized by its response to change in a regime parameter. Many researchers have addressed the use of principal component analysis (PCA) modeling in the monitoring and fault detection of process sensors [10]-[12].

## II. Methodology and Tools

As shown in Fig. 1, the variables are highly correlated, meaning that they vary together. This redundancy in the measurements allows us the interest of the inspection of the different gases based on Multi-scale entropy and PCA approach in order to analyse the nonlinarity existing in these variables. MSE refers to the calculation of entropies across a sequence of scales, which takes into account not only the dynamic nonlinearity but also the interaction and coupling effects between ammonia processes, thus providing much more information regarding Ammonia processes condition.

The data was collected from the fertilization plant (Fertial Spa-Annaba). The process documentation was provided by KBR [13].

The research follows these steps:

- $CH_4$ S (101B), CO S (HTS), CO S(LTS), CO2( 106D) and $H_2$(105D) were recorded from Ammonia process.

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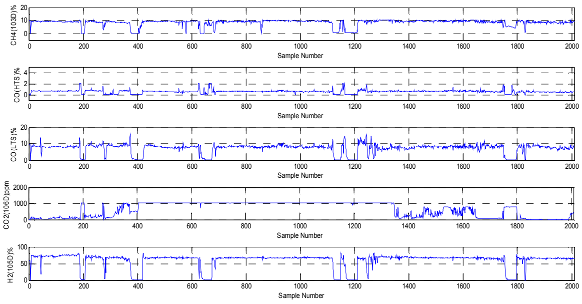


Fig. 1 Data points

- Application of The multi-scale entropy MSE algorithm latter is based on the application of SampEn for different scales of the same process instead of traditionally used regularity measure ApEn statistics [14], [15].

SampEn measures the regularity in serial data. It provides a likelihood measure that two sequences of $m$ consecutive data points within given tolerance $r$ remain similar when one consecutive pointsare included. SampEn increases as $r$ decrease, because the criterion for sequence matching becomes more stringent. Therefore, the determination of these two parameters is of importance. In the MSE analysis, a coarse-grained time series isfirst constructed from the original time series $\{x_1, \ldots, x_i, \ldots, x_N\}$. One constructed consecutive coarse-grained time series$\{y^{(\tau)}\}$ with scale factor $\tau(\tau = 1,2, \ldots N)$, according to:

$$y_j^{(\tau)} = 1/\tau \sum_{i=(j-1)\tau+1}^{j\tau} x_i \quad (1)$$

where$\tau$ represents the scale factor and $1 \leq j \leq N/\tau$

- Five statistics over the MSE are calculated (mean $(m_i)$, Std$(s_i)$, geo mean $(gm_i)$ max and min $(mx_i)$).
- PCA model and evaluation of squared prediction error (SPE) by taking the square difference between the observed values and predicted values from the normal condition or reference model [16], [17]:

$$SPE = \sum_{i=1}^{k} (x_{ij} - \bar{x}_{ij})^2 \quad (2)$$

where$x_{ij}$ and $\bar{x}_{ij}$ are measured and predicted values, respectively by the PCA model. Initially, a model was developed from a normal condition data set using k principal components and this data set was decomposed as:

$$X = TP^T \quad (3)$$

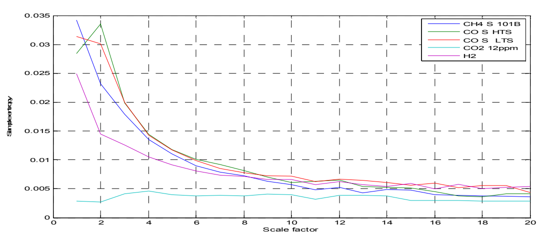


Fig. 2 MSE over 20 scales of the corresponding signals shown in Fig. 1

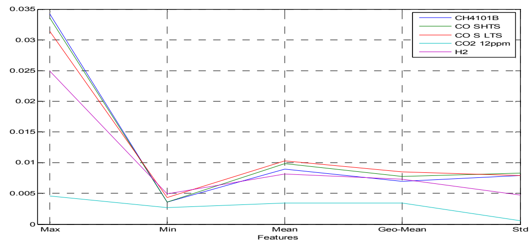


Fig. 3 Five statistics over MSE of the signals shown in Fig. 2, depicted in Fig. 2

The multi-scale entropy is used to inspect different gases present in synthesis of ammonia, MSEs across 20 scales are calculated to form a feature set containing rich condition-indicating information of the evolution of the concentrations of different gases present in synthesis. And five parameters are extracted from the original feature set, which are maximum value, minimum value, arithmetic mean value, geometric mean value and standard deviation value.

Fig. 2 gives the MSE over 20 scales corresponding to the signals shown in Fig. 1. From Fig. 3, we can see that the MSE of different gases varies together and hasn't the largest entropy values over most scales in comparison with each other, which means that the concentration of different gases present in synthesis of ammonia stabilizes through the same operating point in different gases present in synthesis of ammonia.

In order to estimate the concentrations of different gases present in synthesis of ammonia, a soft sensor model based on PCA approach is proposed shown in Figs. 5 and 6.

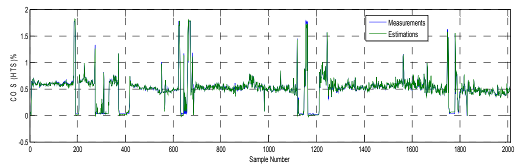


Fig. 5 Measurements and estimations of the CO S (HTS)

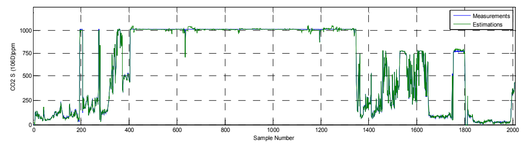


Fig. 6 Measurements and estimations of the $CO_2$ (106 D)

TABLE I
CONTROL OF PROCESS PARAMETERS

| Measure | Interval value |
|---|---|
| $CH_4$ S (101D) | (101B) <11% |
| CO S(HTS) | (HTS) <6 % |
| CO S(LTS) | (LTS) <0.5% |
| $CO_2$ S (106D) | (106D) <12PPM |
| $H_2$(105D) | 55%-70% |

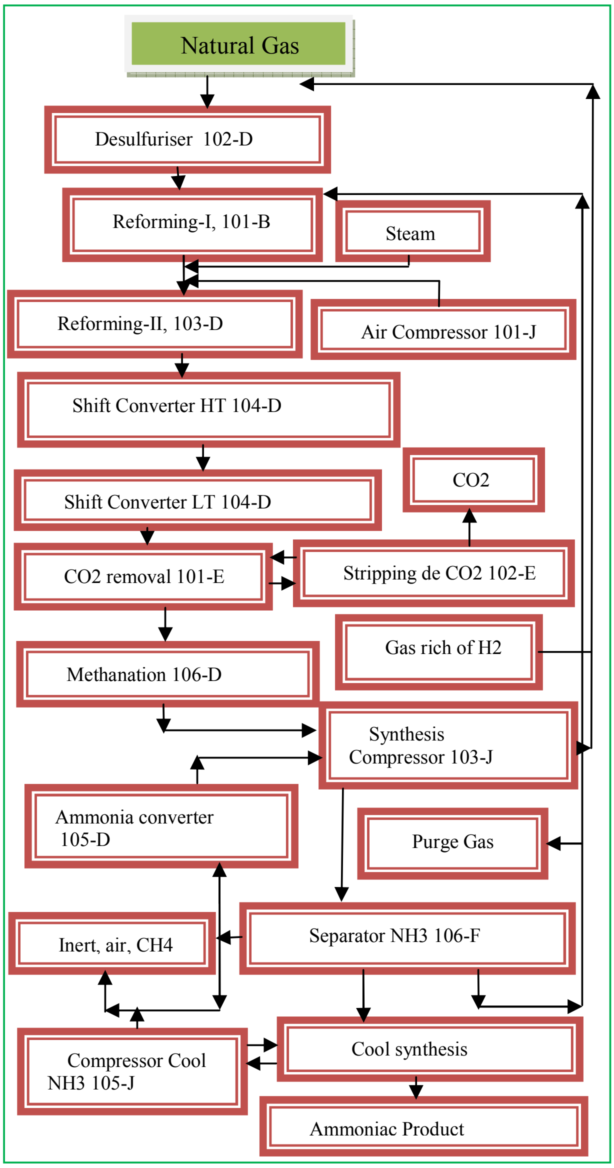


Fig. 7 Flow diagram of the ammonia synthesis process

In order to understand these interactions, depicted in flow diagram Fig. 7, let us for example see the effect of operator actions to adjust or control the : ration in the synthesis loop (the desulfurized gas in mixed with the medium pressure steam in a steam/natural gas= 1/3. as indicates Fig. 8).

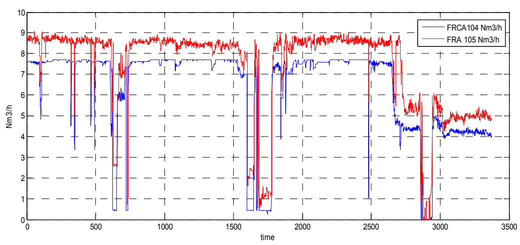


Fig. 8 Measurement (vapor /natural gas)

## III. Conclusion

Real time monitoring and control of product quality variables play an essential role in the chemical process due to the required high and well defined purity specifications and improvements in the controllability of these variables. An important aspect of the safe operation of chemical process is the rapid detection of faults, process upsets, or other special events and the location and removal of the factors causing such events. However, hundreds of variables may be monitored in a single operating unit, and these variables may be recorded hundreds or thousands of times per day. In the absence of appropriate processing method, only limited information can be extracted from these data. Hence, a tool is required that can project the high-dimensional process space into a low-dimensional space amenable to direct visualization, and that can also identify key variables and important features of the data. The need to analyze high-dimensional and correlated process data has led to the development of many monitoring schemes based on principal component analysis (PCA) as modeling technique that transforms a set of correlated variables into a smaller set of new variables that are uncorrelated and retain most of the original information. .The multi-scale entropy is used to inspect different gases present in synthesis of ammonia.

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