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Development of Inferential Models for Fractionation Reformate Unit

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Abstract— **Industrial facilities show an increasing need for continuous measurement and monitoring a large number of process variables due to strict product quality requirements, environmental laws and for advanced process control application. On-line analyzers typically suffer from long measurement delays not desirable in continuous control. Suitable alternative are soft sensors and inferential control.**

In this paper the development of soft sensor models for the estimation of light reformate benzene content is carried out. Linear dynamical autoregressive model with external inputs (ARX), autoregressive moving average model with exogenous inputs (ARMAX) and Box-Jenkins (BJ) models are developed. For the regression vector optimization usually performed by trial and error, Genetic Algorithm (GA) and Simulated Annealing (SA) methods have been applied.

The results indicate that the GA and SA as global optimization methods are suitable for the regressor order estimation of linear dynamical models with multiple inputs. Based on developed soft sensors, it is possible to apply advanced process control schemes.

Keywords—soft sensors; system identification; genetic algorithm; simulated annealing; fractionation reformate unit

I. INTRODUCTION

In refineries, chemical and petrochemical plants it is necessary to continuously monitor the product properties as they may greatly influence to the final product quality. Companies are required to respect environmental laws with strict product specifications and pollutant emissions.

Those product properties are mainly measured by on-line analyzers which are often under maintenance and can have a long processing time (e.g. gas chromatographs). This can cause a significant measurement delay which reduces the efficiency of dedicated process control logic. On the other hand, laboratory analyses are infrequent and time-consuming. This problem can be solved with the application of soft sensors and inferential control logic. The soft sensing technique utilizes continuously measured process variables to predict the product quality variable applying certain modelling approaches, such as first principle modeling, statistical modeling, artificial intelligence modeling, etc. Soft sensors can work in parallel with real sensors (analyzers) keeping control loops to work fast and properly and to guarantee product specification without undertaking conservative production policies [1], [2].

Different model structures can be used to model real plant problems. In the case of industrial processes, due to their complexity, the development of first principles models can be very complex and time-consuming resulting with a large number of unknown parameters. However, large amounts of stored measured data suggest the application of empirical models. Jiao, Li, Shen and Sun [3] solved large-time delay problem with predictive control method based on the extended Kalman filter model which estimates the coal outlet mass flow of the coal mill. Ansari and Bawardi [4] developed various inferential models for the refinery product qualities, such as light naphtha 95% point, diesel flash point of hydrocracker fractionators and reformate octane numbers. Tham, Montague, Morris and Lant [5] presented two adaptive estimators for inferring process outputs for a feedback control that are subject to large measurement delays.

Typical industrial soft sensor applications have parametric polynomial structures like linear autoregressive models with external inputs (FIR, ARX, OE and BJ) or autoregressive moving average model with exogenous inputs and their nonlinear versions.

Zhang, Tao and Gao [6] proposed usage of an improved genetic algorithm for the optimization of ARX Takagi-Sugeno fuzzy model. The model accuracy is compared with a BJ gas furnace model showing good results. Muddu and Patwardhan [7] developed adaptive model predictive control scheme based on ARX model which was validated by experimental studies on a heater-mixer setup. Muddu, Narang and Patwardhan [8] developed ARX model for novel model predictive control scheme. The efficacy of algorithm was demonstrated by simulation studies on a staged distillation column and by experimental evaluations on a laboratory scale packed bed distillation column.

The procedure of soft sensor design includes: selection of historical data from the plant database, data pre-processing (outlier detection, data filtering, removing drifts, etc.), model structure and regressor selection, model estimation and model validation [9]. Here, the emphasis is given to regressor selection, as choosing the optimal model structure can be crucial for soft sensor performance [10].

To develop dynamical polynomial models, the model order i.e. the number of coefficients for each polynomial of model structure and time delays, must be predefined. Akaike's information criterion [11], [12] and the minimum description length criterion [13] are some of the classical methods for linear polynomial model order selection. For nonlinear polynomial model order determination Lipschitz method [14] is mostly used. Due to application complexity of existing model order selection methods the common used method is trial-and-error or the approximation is based on the plant operator's experience. This paper proposes using genetic and SA algorithms for model order estimation.

In Chen, Worden, Peng and Leungc [15] ARX and NARX model coefficients and time delays were optimized using GA on the simulated dynamic system.

Typical soft sensor application areas, as shown in Fortuna, Rizzo, Sinatra and Xibilia [15], are the measuring equipment replacement, monitoring and process control as well as fault-detection and diagnostics.

Primary application of the soft sensors developed in this case study is its incorporation into closed-loop control, with the aim to achieve more stable control leading to better and more stable product quality. In this work ARX, ARMAX and BJ models were considered.

II. Theory - Soft sensor model structures and optimization algorithms

In a large number of industrial processes nonlinearity is slightly expressed and time variability is slow enough, so it is possible to use linear and time-invariant process models [16]. One of the commonly used linear dynamic process models which contains noise model is the ARX model:

$$\hat{y}(k) = \left[1 - \mathrm{A}(q)\right] y(k) + \sum_{i=1}^{nu} \mathrm{B}_i(q) u_i(k - \mathrm{nk}_i) \qquad (1)$$

where $\mathrm{A}(q) = \mathrm{I} + \mathrm{A}_1 q^{-1} + \mathrm{A}_2 q^{-2} + ... + \mathrm{A}_{na} q^{-na}$ is the polynomial matrix by q^{-1} of dimensions $\mathrm{n}(y)\times\mathrm{n}(y)$.

$\mathrm{B}_i(q) = \mathrm{B}_{i,1} + \mathrm{B}_{i,2} q^{-1} + \mathrm{B}_{i,3} q^{-2} + ... + \mathrm{B}_{i,nbi} q^{-nb_i+1}$ is the polynomial matrix by q^{-1} of dimensions $n(y)\times n(u)$. na is the number of past process output samples. *nb* is the number of past process input samples and *nk* is the time delay for the *i*-th input expressed with the number of samples.

Autoregressive Moving Average with exogenous inputs model *(*ARMAX) extends the ARX structure by providing more flexibility for modeling noise using the moving average of a white noise. ARMAX model predictor in developed form is the following:

$$\hat{y}(k) = \left[1 - \mathrm{A}(q)\right] y(k) + \sum_{i=1}^{nu} \mathrm{B}_i(q) u_i(k - \mathrm{nk}_i) + \mathrm{C}(q) e(k) \qquad (2)$$

where $\mathrm{C}(q) = \mathrm{I} + \mathrm{C}_1 q^{-1} + \mathrm{C}_2 q^{-2} + ... + \mathrm{C}_{nc} q^{-nc}$ is the polynomial matrix by q^{-1} of dimensions $\mathrm{n}(y)\times\mathrm{n}(e)$. nc is the number of past white noise samples and $e(k)$ is the prediction error.

ARMAX model is used when disturbances have a significant impact on the model output.

Box-Jenkins (BJ) model provides independent parameterization for the dynamics and the noise using rational polynomial functions. Predictor of BJ model:

$$\hat{y}(k) = \sum_{i=1}^{nu} \mathrm{B}_i(q) u_i(k - \mathrm{nk}_i) + \left[\ \mathrm{I} - \mathrm{F}(q)\ \right] \hat{y}_s(k) + \\ + \left[\ \mathrm{C}(q) - \mathrm{I}\ \right] e(k) + \left[\ \mathrm{I} - \mathrm{D}(q)\ \right] e_s(k) \qquad (3)$$

where $\mathrm{F}(q) = \mathrm{I} + \mathrm{F}_1 q^{-1} + \mathrm{F}_2 q^{-2} + ... + \mathrm{F}_{nf} q^{-nf}$ and

$\mathrm{D}(q) = \mathrm{I} + \mathrm{D}_1 q^{-1} + \mathrm{D}_2 q^{-2} + ... + \mathrm{D}_{nd} q^{-nd}$ is the polynomial matrix by q^{-1} of dimensions $n(y)\times n(e_s)$. $e_s(k)$ is the past simulated prediction error. $\hat{y}_s(k)$ is the simulated process output (or output of OE model), i.e. process output without disturbance model. *nf* is the number of past model output samples and *nd* is the number of past simulated prediction error samples.

BJ model is usually used when the noise does not enter at the input, but is primary a process disturbance [17].

After choosing an appropriate model structure, model orders are estimated by GA and SA optimization techniques.

The process of evolution in GA begins from an initial chromosomes population consisted of randomly generated individuals (initial solutions). In each algorithm's iteration, the fitness function of each individual is evaluated. Further on, multiple individuals are stochastically selected from the current population according to their fitness function and afterword's recombined and mutated (modified). The new created population is then used in the next generation of the algorithm. The algorithm evolves toward better solutions and usually stops when a maximum number of iterations have been produced or a satisfactory objective function level has been reached [18].

SA algorithm has taken inspiration from annealing in metallurgy where it involves heating and controlled cooling of a material to increase the size of its crystals and reduce their defects. The state of some physical system at some temperature can be expressed with the value of the objective function which needs to be minimized. The goal is to bring the system to a state with the minimum possible energy using Boltzmann probability. In each algorithm's iteration, new nearby state as a random displacement from the current states of the system is generated. If the new state has a lower energy than the current, the transition is accepted. As long as the temperature is reduced the chance of accepting worse solutions is smaller. After a certain decreasing point, the

temperature is raised again in order to restart the search and move out from the local minimum [19].

III. PROCESS DESCRIPTION

Fractionation reformate plant raw material is a mixture of catalytic reformed naphtha and benzene fractions. The flowrate is controlled by FC-001 and temperature by TC-001 as shown on Fig 1. Since the boiling points of the benzene fraction, light and heavy reformate naphtha are very close, one part of the benzene will be separated as top and the rest as bottom column product. Light reformate flows to the reflux drum V-1 where it is separated as top column product. Top column temperature TC-002 is controlled in cascade with the pumparound flowrate FC-002. Column pressure is controlled by the control valve at the outlet top column stream. Bottom column temperature TC-018 is controlled with the furnace H-1 inlet fuel gas flowrate FC-009.

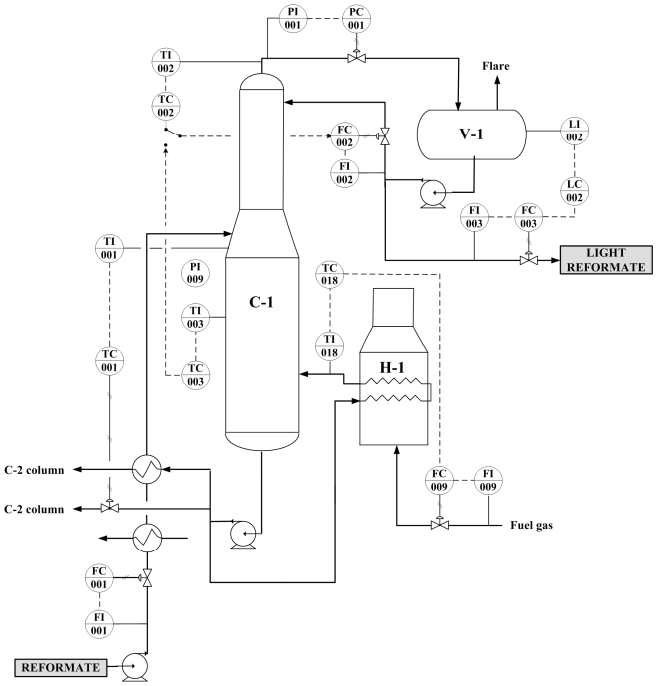

Fig. 1. Fractionation light reformate plan

Desired top product composition is determined by column top temperature. Inlet column temperature, flowrate and bottom column temperature can influence column temperature profile as well as the product composition.

For estimation of benzene content in light reformate following five variables have been chosen as input variables: column inlet stream temperature, TC-001; column bottom temperature, TC-018; column temperature, TC-003; column pressure, PI-009 and pumparound flowrate, FC-002.

IV. SOFT SENSOR MODEL DEVELOPMENT

Process data from the plant database was collected in the continuous period of three weeks. According to the process dynamics sampling interval was set to five minutes. Data was preprocessed including missing data and outlier detection and replacement, data detrending and filtering.

The benzene content (model output) determined by on-line analyzer is available every twenty minutes. Additional output data is interpolated using cubic spline. The data set for the model estimation includes 4500 samples and 1500 independent samples for the model validation.

The soft sensor models are developed in *System Identification Toolbox* and *Global Optimization Toolbox* in MATLAB.

A. Optimizing model parameters by genetic algorithm and simulated annealing

Adjustable model order parameters and their ranges are chosen based on the process engineers experience as well as rational model structure complexity, as shown in Table I.

TABLE I. MODEL ORDERS OF ARX, ARMAX AND BJ MODEL

Parameter	Minimum value	Maximum value
na	1	8
nb	1	8
nk	0	15
nc	1	8
nf	1	5
nd	1	5

TABLE II. GA AND SA OPTIMIZATION PARAMETERS

GA: Population size	50
GA: Number of generation	60
GA: Function evaluation	3000
GA: Selection	Stochastic uniform
GA: Crossover	Scattered
GA: Mutation	Uniform
GA: Mutation probability rate	0.1
GA: Fitness scaling	Rank
GA: Number of elite individuals	1
GA: Crossover fraction	0.7
SA: Acceptance function	acceptancesa
SA: Annealing function	annealingboltz
SA: Initial temperature	300
SA: Function evaluation	3000
SA: Reannealing interval	100
SA: Temperature function	temperatureexp
SA: Termination function tolerance	$1e^{-5}$

The numbers of configurable parameters is 11, 12 and 17 for ARX, ARMAX and BJ model, respectively.

Based on the preliminary tests and rational calculation time GA and SA parameters are selected and used for model order evaluation as presented in Table II. The search spaces for the models are as follows: ARX ($8^1*8^5*16^5$ = $2.1990\cdot10^{12}$), ARMAX ($8^1*8^5*16^5*8^1 = 1.7592\cdot10^{13}$) and BJ ($8^5*16^5*5^5*8^1*5^1 = 4.2948\cdot10^{15}$).

B. *Model Evaluation Criteria*

Developed models are evaluated based on the following evaluation criteria: FIT criterion, final prediction error (FPE) and root mean square error (RMS). The FIT is calculated according to the following expression:

$$\mathrm{FIT} = \left(1 - \frac{\sqrt{\sum_{i=1}^{n}\left(\hat{y}_i - y_i\right)^2}}{\sqrt{\sum_{i=1}^{n}\left(y_i - y_m\right)^2}}\right)\cdot 100 \qquad (4)$$

where y is the measured output, $\hat{y}$ is the predicted output, and y_m is the mean of y. FPE is defined as follows:

$$\mathrm{FPE} = V\,(1 + 2d / n) \qquad (5)$$

where V represents the loss function, d is the number of estimated parameters, and n is the number of values in the estimation data set. The V is calculated as follows:

$$V = \det\left(\frac{1}{n}\sum_{1}^{n}\varepsilon\left(t,\theta_n\right)\left(\varepsilon\left(t,\theta_n\right)\right)^T\right) \qquad (6)$$

where θ_n represents the estimated parameters and ε is output error [20]. The FPE criterion is a compromise between model accuracy and model complexity in terms of the number of estimated parameters [21].

Preliminary research based on the non-preprocessed data showed that FIT and FPE are not correlated, but both are frequently used criteria for model evaluation. Therefore, they are integrated in the multi-criteria objective function using the weighted sum method [22]:

$$y_{of} = (100 - \mathrm{FIT}) + 1000*\mathrm{FPE} + 100*\mathrm{RMS} \qquad (7)$$

V. Results and Discussion

Applying GA and SA algorithm *na*, *nb*, *nk*, *nc* and *nd* were estimated by minimizing the objective function given by eq. (7). The polynomial coefficients of $B_i(q)$ and $F(q)$ were estimated using the MATLAB *System Identification Toolbox*.

A. *ARX model results*

ARX model evaluation criteria obtained by five runs using GA and SA for model order estimation are shown in Table III.

TABLE III. ARX MODEL EVALUATION CRITERIA

Run	***1***	***2***	***3***	***4***	***5***
GA FIT	86.470	87.111	86.541	86.766	86.559
GA FPE	$7.63\cdot10^{-6}$	$7.71\cdot10^{-6}$	$7.70\cdot10^{-6}$	$7.79\cdot10^{-6}$	$7.64\cdot10^{-6}$
GA RMS	0.033	0.032	0.033	0.032	0.033
GA fitness function, y_{of}	16.855	**16.056**	16.767	16.486	16.743
SA FIT	82.733	83.358	85.481	82.901	83.617
SA FPE	$7.91\cdot10^{-6}$	$3.04\cdot10^{-6}$	$7.53\cdot10^{-6}$	$7.99\cdot10^{-6}$	$7.67\cdot10^{-6}$
SA RMS	0.042	0.041	0.036	0.042	0.040
SA fitness function, y_{of}	21.508	20.725	18.086	21.299	20.407

For defined function evaluation number GA in all runs gives better and less diverse results in comparison with SA, as is shown in Table III

According to the lowest fitness function the model order parameters from the 2nd run of GA are considered as the best. Obtained model order parameters are: na = [2]; nb = [8 1 4 7 5]; nk = [0 5 5 6 11].

Fig. 2 and Fig. 3 show the comparison between predicted and measured output for the validation data set. One can notice very good matching between the model and measured data for both of the ARX models.

ARX model residual distribution obtained by GA algorithm shows that 87.6 % of all residuals lie in the range of ±0.05 vol. %. The same distribution for SA algorithm shows 78 % of all residuals lie in the same range.

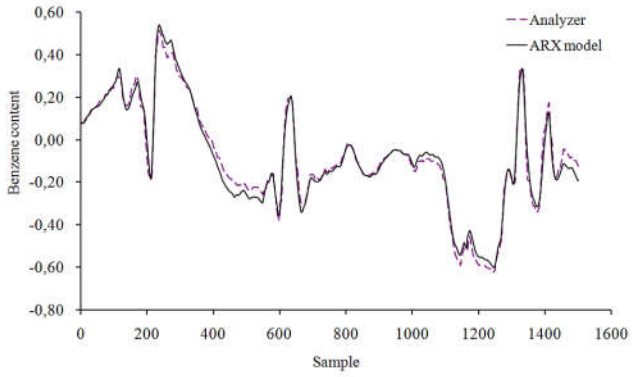

Fig. 2. Comparison between measured data and ARX model using GA algorithm.

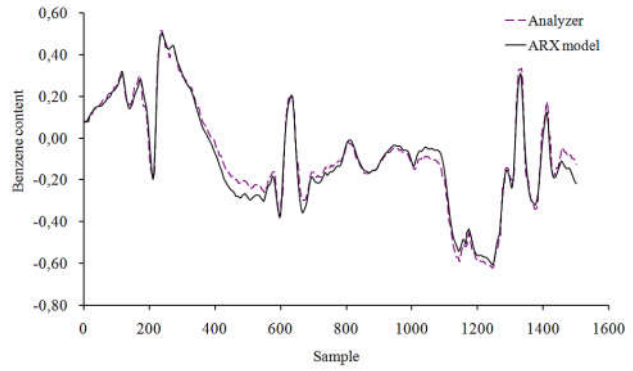

Fig. 3. Comparison between measured data and ARX model using SA algorithm.

B. *ARMAX model results*

ARMAX model evaluation criteria for the validation data set using GA and SA are shown in Table IV.

TABLE IV. ARMAX MODEL EVALUATION CRITERIA

Run	***1***	***2***	***3***	***4***	***5***
GA FIT	85.344	86.143	85.708	85.578	85.971
GA FPE	$1.98\cdot10^{-6}$	$1.95\cdot10^{-6}$	$1.92\cdot10^{-6}$	$2.02\cdot10^{-6}$	$2.03\cdot10^{-6}$
GA RMS	0.036	0.034	0.035	0.035	0.034
GA fitness function, y_{of}	18.252	**17.257**	17.798	17.960	17.471
SA FIT	84.631	83.286	82.998	79.074	84.871
SA FPE	$1.89\cdot10^{-6}$	$1.87\cdot10^{-6}$	$1.92\cdot10^{-6}$	$1.73\cdot10^{-6}$	$1.88\cdot10^{-6}$
SA RMS	0.038	0.041	0.042	0.051	0.037
SA fitness function, y_{of}	19.138	20.813	21.172	26.058	**18.840**

GA results of ARMAX model are more consistent in all runs compared with corresponding SA results. Comparing the results of ARMAX and ARX models using the SA it can be seen that ARMAX results show more variability. ARMAX model parameters for GA in 2nd run are: na = [2]; nb = [7 3 4 4 4]; nc = [6]; nk = [3 5 4 5 11]. It can be noticed that the ARMAX model has somewhat smaller model order compared to the ARX model with the similar model evaluation criteria values.

From Fig. 4 and Fig. 5 and statistical evaluation criteria from Table IV it can be seen that the ARMAX model follows very well process data. For the ARMAX model obtained by GA algorithm, 88.3 % of all residuals lie in the range of ±0.05 vol. % while with SA algorithm 62 % of all residuals lie in the same range.

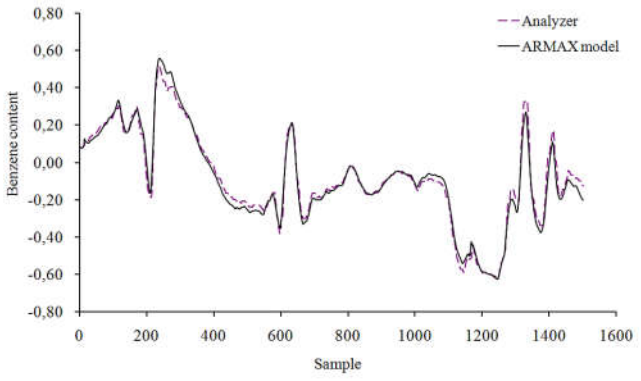

Fig. 4. Comparison between measured and ARMAX model using GA algorithm.

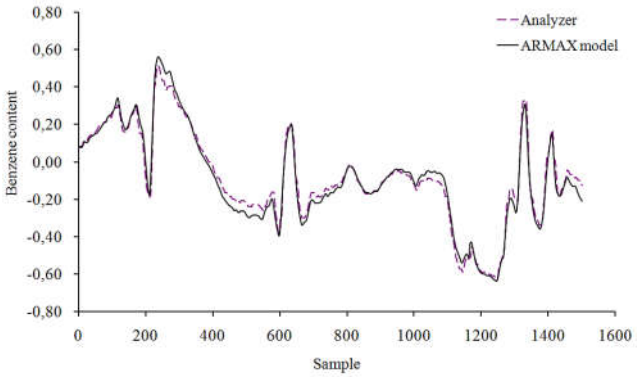

Fig. 5. Comparison between measured and ARMAX model using SA algorithm.

C. *BJ Model results*

Due to the real plant process complexity and frequent occurrence of the process disturbances BJ model is developed. BJ evaluation criteria are presented in Table V.

TABLE V. BJ MODEL EVALUATION CRITERIA

Run	***1***	***2***	***3***	***4***	***5***
GA FIT	89.199	88.890	88.920	88.809	89.453
GA FPE	$1.08\cdot10^{-5}$	$2.10\cdot10^{-5}$	$5.26\cdot10^{-5}$	$1.05\cdot10^{-5}$	$1.85\cdot10^{-5}$
GA RMS	0.027	0.027	0.027	0.027	0.026
GA fitness function, y_{of}	13.460	13.854	13.849	13.945	**13.151**
SA FIT	88.948	89.408	88.602	89.009	85.510
SA FPE	$2.39\cdot10^{-5}$	$7.89\cdot10^{-5}$	$4.98\cdot10^{-5}$	$8.70\cdot10^{-5}$	$6.73\cdot10^{-4}$
SA RMS	0.027	0.026	0.028	0.027	0.036
SA fitness function, y_{of}	13.785	**13.268**	14.243	13.772	18.715

For the best BJ model order parameters are: *nb* = [2 1 2 3 1]; *nc* = 4; nd = 4; *nf* = [2 1 2 3 1]; *nk* = [14 2 12 8 9].

Fig. 6 and 7 display the comparison between BJ model data and the measured data. As can be seen from Table VII and Fig. 6 BJ model shows the best performances among the developed models since it included disturbance dynamics. BJ residual distribution achieved by GA, shows that 93.5 % of all residuals lie in the range of ±0.05 vol.% while the model obtained by SA shows that 74.3 % of all residuals lie in the same range.

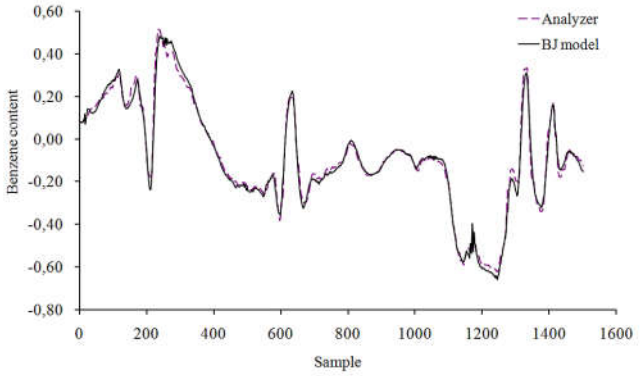

Fig. 6. Comparison between measured and BJ model output data using GA algorithm.

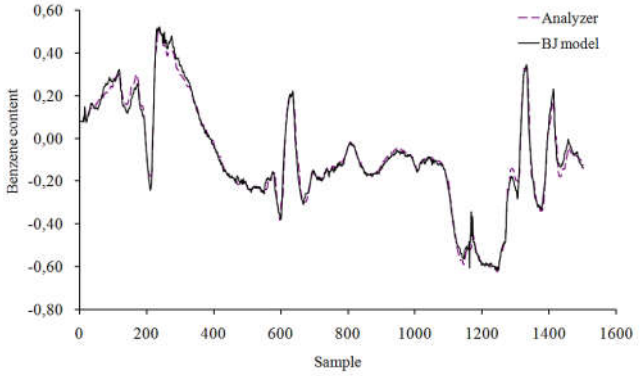

Fig. 7. Comparison between measured and BJ model using SA algorithm.

VI. Conclusion

Our results show that all developed models should be suitable for application in advanced process control strategy. In addition, the focus of this investigation was on application of GA and SA model order optimization which speeds up and facilitates soft sensor development procedure. For smaller search spaces (ARX and ARMAX model) and larger search spaces (BJ model) GA approach gives better estimation of input-output polynomial models in comparison with SA approach. The best overall model performance is achieved by BJ model.

Keeping in mind that the optimal model for industrial implementation is the simplest one with relatively small prediction error, ARX model is good choice for on-site implementation in advanced process control schemes.

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