Available online at www.sciencedirect.com

ScienceDirect

Procedia Chemistry 9 (2014) 226 – 234

Procedia Chemistry

International Conference and Workshop on Chemical Engineering UNPAR 2013, ICCE UNPAR 2013

State of the Art in the Development of Adaptive Soft Sensors based on Just-In-Time Models

Agus Saptoro*

Department of Chemical Engineering, National Institute of Technology (ITENAS), Jl. PHH. Mustofa No. 23, Bandung 40124, Indonesia

Abstract

Data-driven soft sensors have gained popularity due to availability of the recorded historical plant data. The success stories of the implementations of soft sensors, however, involved some practical difficulties. Even if a good soft sensor is successfully developed, its predictive performance will gradually deteriorate after a certain time due to changes in the state of plants and process characteristics, such as catalyst deactivation and sensor and process drifts due to equipment ageing, fouling, clogging and wear, changes of raw materials and so on. To get soft sensor automatically updated, different kinds of methods have been introduced, such as Kalman filter, moving window average, recursive and ensemble methods. However, these methods have some drawbacks which motivate the development and implementation of just-in-time (JIT) model based adaptive soft sensor. This paper aims to report the current status of adaptive soft sensors based on just-in-time modelling approach. Critical review and discussion on the original and modified algorithms of the JIT modelling approach are presented. Proposed topics for future research and development are also outlined to provide a road map on the developing improved and more practical adaptive soft sensors based on JIT models.

Peer-review under responsibility of the Organizing Committee of ICCE UNPAR 2013

Keywords: Soft sensor; adaptive, just-in-time model; state of the art.

*Corresponding author. Current address: Department of Chemical and Petroleum Engineering, Curtin University Sarawak Campus, CDT 250, Miri 98009, Sarawak, Malaysia.
Tel.: +60 85 443939 Ext. 2202; fax: +60 85 443837
E-mail address: agus.saptoro@curtin.edu.my

Peer-review under responsibility of the Organizing Committee of ICCE UNPAR 2013
doi:10.1016/j.proche.2014.05.027

Nomenclature

C	Covariance Matrix
CoJIT	Correlation based JIT where the Hotelling's T^2 and Q statistics derived from PCA
d	Eucledian distance
JIT	Just-In-Time
MJIT	Mahalanobis distance based JIT
md	Mahalanobis distance
PCA	Principal Component Analysis
S	Scaling Matrix
S	Similarity factor
SVDD	Support Vector Data Description
λ	Parameter in correlation based similarity factor
γ	Parameter in distance and angle measures based similarity factor

1. Background

Operational excellence of processing plants has become, more than ever, important for achieving economic and environmental targets in the process industry. Overall, operational excellence is a continuous pursuit for improving the processes and qualities of their associated products. As such, it leads to higher cost efficiency, better plant capacity exploitation and loss reduction as well as achieving compliance with environmental and safety legislations. These can be achieved by operating the processes in their optimal states. Due to these reasons, different industries in different areas are seeking reliable tools to monitor and control increasingly complicated processes from food processing, pharmaceutical industries, and steel-making and semiconductor processes to chemical refineries and nuclear plants. Such tools employ inferential sensing technology which utilizes easy-to-measure process variables to estimate unmeasured or hard-to-measure variables. Soft sensors have proved themselves to be a valuable alternative to their hardware counterparts. This is due to their ability to measure and predict important process variables that are difficult to measure using hardware sensors where these difficulties might be associated with cost, long time delays and reliability [1 - 2].

Inferential sensors, having other common terms of soft sensors or virtual on-line analyzers, may be developed using one of these approaches: physical model based soft sensor (model-driven soft sensor) or historical data based soft sensor (data-driven soft sensor). Building soft sensors using model-driven approach is difficult since accurate fundamental models need to be developed. These fundamental models are often unavailable due to the lack of complete physicochemical knowledge of the process. Thus, an alternative approach is to use data-driven methods to build models from process data measured in industrial processes. Consequently, data driven soft sensors have the potentials to be a new generation of operational excellence at a relatively low cost because they can be developed from already available historical database of plant operations [3]. Moreover, soft sensors may be used to extract and exploit hidden or latent information available in the plant operational database to better understand the process and to early detect the process faults.

The success stories of implementation of soft sensors, however, involved some practical difficulties. Even if a good soft sensor is successfully developed, its predictive performance will gradually deteriorate after a certain time due to changes in the state of plants and process characteristics, such as catalyst deactivation and sensor and process drifts due to equipment ageing, fouling, clogging and wear, changes of raw materials and so on [2, 4 – 5]. When a good soft sensor has been developed, the maintenance is also very important to keep its estimation performance. This is consistent with the survey to the engineers where majority of them indicated that the main problem of the soft sensor applications is the deterioration of the accuracy due to changes in the process [6]. This survey result confirms that the maintenance of the soft sensor is the major issue concerning soft sensor. Therefore, from practical point of view, to cope with process changes and maintain its good performance, a soft sensor should be updated regularly as the process characteristics change.

To get soft sensor automatically updated, different kind of methods have been introduced, such as Kalman filter [7 – 8], moving window techniques [9], recursive methods [5 - 6, 9 - 16] and ensemble approach. The Kalman Filter based technique shows particularly stable performance and is simple to implement in the computer, however, this online adaptation method normally suffers from over-fitting to a particular operation range, which causes deterioration of the predictive capability [7]. Moving window requires to store all data within the window and this can be problematic for large window and memory limited applications. This method has also difficulties in setting appropriate window and step sizes. Meanwhile, although recursive methods are capable of adapting the soft sensor model to a new operation condition recursively, they cannot cope with the abrupt changes of the process [5, 6, 10, 13 – 16]. Moreover, when the process is operated within a narrow range for a certain period of time, the recursive methods will adapt the model excessively because they perform blind-updating [5, 16]. Another drawback of the recursive approaches is that there is a time delay when the recursive methods update the soft sensor to a new process operating condition which may cause the malfunctioning of the updated soft sensor in the new operation region until a sufficient period of time [5]. Ensemble learning approach suffers from its modelling complexities [9]. Adaptive neural network and neuro-fuzzy models have also been proposed, however, network structure and model parameters may need to be updated and changed simultaneously. These simultaneous updates are not only time-consuming, but they will also interrupt the plant operation. In this regard, to alleviate the aforementioned problems, just-in-time (JIT) modeling was developed as an attractive solution for building adaptive soft sensor.

JIT modeling has been proposed to cope with process nonlinearity [5, 17 - 18] and changes in process characteristics [35] and also to overcome drawbacks in recursive techniques [13 – 16]. JIT modeling is inspired by the ideas from database technology and local modeling and in the literature it is also known as instance-based learning, locally weighted model, lazy learning or model-on-demand [19]. In the JIT modeling approach, there is an assumption that all available observations are stored in the historical database and the models are built dynamically upon query. Different from traditional methods which are global modeling in nature, a JIT model is a local model developed from historical dataset around a query data sample when estimated value of this point is required. While the global model is constructed offline, the JIT model is built online [5, 19]. For this reason, JIT model can trace the current state of the process well.

Despite the significant efforts of many researchers in the past in the development and improvement of JIT model, there are still several theoretical and practical challenges that have yet to be overcome, for example the way the relevant training data is selected and how to make this technology more practical for the industrial applications. This paper aims to report the current status of adaptive soft sensors based on just-in-time modelling approach. Critical review and discussion on the original and modified algorithms of the JIT modelling approach are presented. Future directions for the JIT model based soft sensor are also outlined to provide a road map on the developing improved and more practical adaptive soft sensors based on JIT models. After discussing the basic theory of JIT modelling approach in section 2, variants of JIT models are outlined in section 3. Some open issues and future steps of JIT model based adaptive soft sensor are discussed in section 4 which arrive at the proposed topics for future research and development.

2. Just-In-Time Modeling

Just-in-time modeling is inspired by the ideas from local modeling and database technology. In this approach, model building is postponed until an estimated output for a given query data is required. When new input and output are available, they are stored in a database. Models are built dynamically upon query using this stored data. These local models are constructed from samples located in a neighbor region around the query point, and predicted output for the query data is computed. After the predicted output is used for estimation, then the constructed local model is discarded [5, 14, 19]. Fig. 1 outlines and shows the differences between traditional modelling and JIT modelling approaches. Traditional models are typically trained in off-line mode and the database is discarded after the training phase is completed. On the other hand, JIT model gathers and store the data into the database and the modelling is not performed until prediction is required for the query point.

The key step in JIT modelling is the selection of relevant data set for model building. The selected data set from the database is neighboring data around the query data. The neighborhood is defined as any data having similarity with the query point. To evaluate this similarity, distance based measure, especially Eucledian distance is commonly used due to its simplicity [5, 19]. Assume that a database consisting of N process data $(y_i, \mathbf{x}_i)_{i=1\sim N}$, $y_i \in R$, $\mathbf{x}_i \in R^n$ is collected. Given a specific query data $\mathbf{x}_q \in R^n$, JIT model is used to predict the model output $\widehat{y_q} = f(\mathbf{x}_q)$ according to the known database $(y_i, \mathbf{x}_i)_{i=1\sim N}$. Assume that a database consisting of N process data $(y_i, \mathbf{x}_i)_{i=1\sim N}$, $y_i \in R$, $\mathbf{x}_i \in R^n$ is collected. Given a specific query data $\mathbf{x}_q \in R^n$, JIT model is used to predict the model output $\widehat{y_q} = f(\mathbf{x}_q)$ according to the known database $(y_i, \mathbf{x}_i)_{i=1\sim N}$. According to the Euclidean distance, the similarity factor (s_i) of $\mathbf{x}_q$ and each data in the database can be calculated as follows

$$s_i = \sqrt{e^{-d^2(x_q, x_i)}} \tag{1}$$

where $d^2(x_q, x_i)$ is the Eucledian distance between x_q and x_i.

After all s_i are computed, they are rearranged in the descending order. In the local model construction, only M relevant data samples $\{x_i, y_i\}_{i=1,2,\ldots,M}$ which correspond to the M largest similarity factors are chosen for model building. Thus, these samples serve as training data set for online local model development.

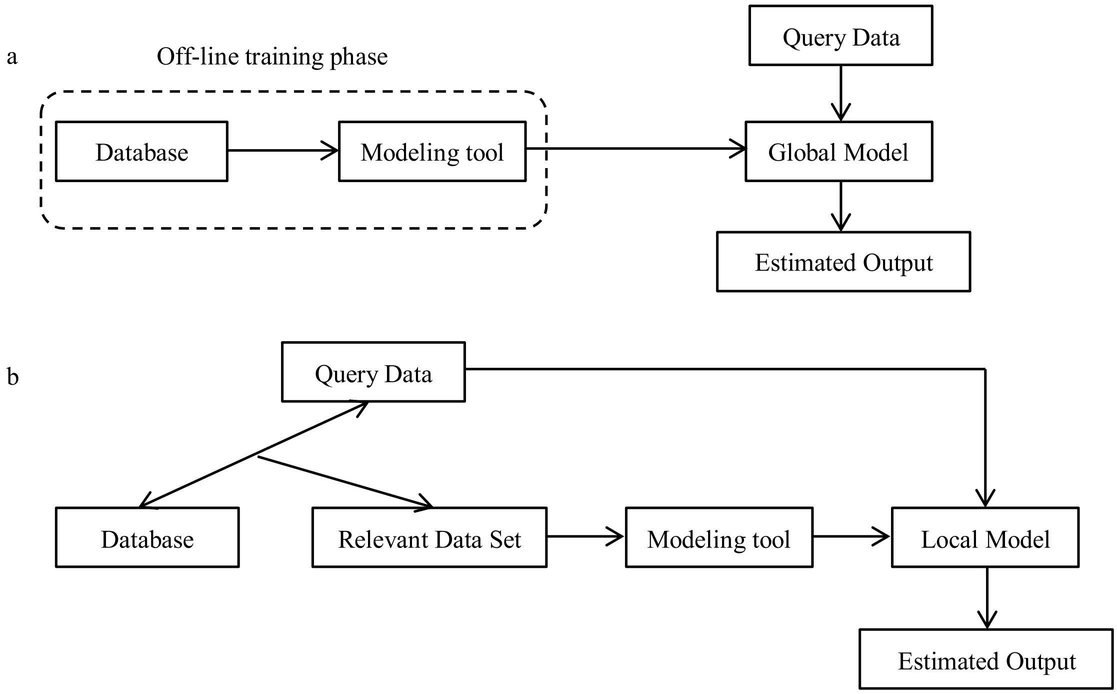

Fig. 1. (a) Traditional approach of data driven modeling; (b) JIT modeling approach.

3. Variants of Just-In-Time Modeling

In the last decade, research works on JIT models have been directed toward three areas: soft sensor applications, control applications and improvements in the selection of relevant data set through modifications of similarity factor. JIT models have been applied as soft sensors in various units and processes: blast furnace [20], methane steam reforming process [21], CSTR 10, 13 - 15, 19, 22 - 23), waste water plant [16], water heating process [24], fuel cell engine [25], polymerization reactor [19], rolling mill process [26], Tennessee Eastman process [5] and debutanizer column [5]. Meanwhile, Yang et al. [27] and Cheng et al. [23] had successfully incorporated JIT based soft sensors in the adaptive decentralized PID controller and robust PID controller, respectively. Kano et al. [28] had also proposed JIT based statistical process control for vinyl acetate monomer production plant. Overall, similarity factors used for JIT modeling can be categorized into three groups as indicated by Fig. 2.

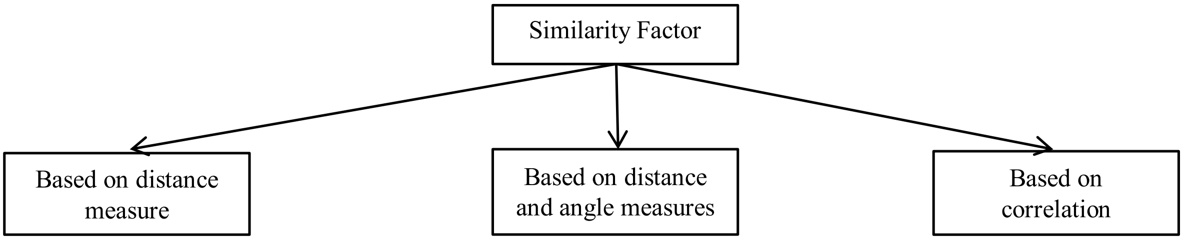

Fig. 2. Classifications of similarity factors used for JIT modeling.

3.1. Distance based similarity factor

There are few variants of distance based similarity factor: Eucledian distance based, weighted Eucledian distance based [20] and Mahalanobis distance based [21]. JIT modeling is carried out by selecting the relevant data set according to the similarity factor as defined in Eq. (1) and specified distance measure. However, each distance can be formulated as follows:

Eucledian distance [20]

$$d^2(x_q, x_i) = (x_q - x_i)^T (x_q - x_i) \tag{2}$$

Weighted Eucledian distance [20]

$$d^2(x_q, x_i) = (x_q - x_i)^T \boldsymbol{S}\, (x_q - x_i) \tag{3}$$

where **S** is scaling matrix.

Mahalanobis distance [21]

$$md^2(x_q, x_i) = (x_q - x_i)^T\, C^{-1}\, (x_q - x_i) \tag{4}$$

where C is covariance matrix between x_q and x_i.

3.2. Distance and angle based similarity factor

The basic idea of this approach is to use both distance and angular measures in calculating similarity factor [19, 22, 29]. Consequently, Eq. (1) is modified to accommodate the distance and angular relationships among x_q and x_i. The equation used to calculate the similarity factor (s_i) is then defined as

$$s_i = \gamma\sqrt{e^{-d^2(x_q,x_i)}} + (1-\gamma)\cos(\theta_i) \tag{5}$$

where $d^2(x_q, x_i)$ is the Eucledian distance between x_q and x_i, γ is a weight parameter and $\cos(\theta_i)$ is

$$\cos(\theta_i) = \frac{\Delta x_q^T \Delta x_i}{\|\Delta x_q\|_2 \cdot \|\Delta x_i\|_2} \tag{6}$$

$$\Delta x_q = x_q - x_{q-1} \tag{7}$$

$$\Delta x_i = x_i - x_{i-1} \quad (8)$$

3.3. Correlation based similarity factor

There are two existing correlations based similarity factor. These two correlations were proposed for Gaussian and non-Gaussian distributed data. Here, similarity factor J is used instead of s_i. Details of J are explained in the following.

For Gaussian-distributed data [10, 13 – 15, 21]

$$J = \lambda T^2 + (1 - \lambda)Q \quad (9)$$

where $0 \leq \lambda \leq 1$ and T^2 and Q are Hotelling's T^2 and Q statistics derived and obtained from principal component analysis (PCA).

For non-Gaussian distributed data [30]

$$J = \lambda D + (1 - \lambda)T^2 \quad (10)$$

where $0 \leq \lambda \leq 1$ and T^2 and Q are Hotelling's T^2 and D statistics derived and obtained from support vector data description (SVDD).

Table 1. Summary of the developments of JIT models in recent years.

JIT model version	Similarity factor	Shortcoming	Ref
Original model	Eucledian distance	Correlations among variables are neglected; applicable for Gaussian data only; badly influenced by an outlier if new data is an outlier	[5, 20, 24, 31]
N/A	Weighted Eucledian distance	Correlations among variables are neglected; applicable for Gaussian data only; badly influenced by an outlier if new data is an outlier	[20]
Cheng's enhanced model	Combined Eucledian distance and angle	For orthogonal pairs of samples, the angle does not always describe the correlation among variables; difficulties in tuning the weight parameter (γ); applicable for Gaussian data only; badly influenced by an outlier if new data is an outlier	[19, 29]
CoJIT	Correlation using Raich and Cinar index (combination between Q statistic from PCA and Hotelling's T^2)	Difficulty in setting parameter ($\boldsymbol{\lambda}$) by trial-and-error; applicable for Gaussian data only; badly influenced by an outlier if new data is an outlier	[10, 13 – 15]
MJIT	Mahalanobis distance	applicable for Gaussian data only; badly influenced by an outlier if new data is an outlier; the estimation results can be discontinuous	[21]
Non-Gaussian JIT model	Correlation using Raich and Cinar index (combination between measure distance from SVDD and Hotelling's T^2)	Difficulty in setting parameter ($\boldsymbol{\lambda}$) by trial-and-error; badly influenced by an outlier if new data is an outlier	[30]

4. Recommendations and Future Research Directions

During the past decade, considerable process has been in the theory and practice of JIT model based adaptive soft sensor. Few reports have indicated that JIT models are able to cope with process nonlinearity and changes in process characteristics (10, 13 – 15, 17 – 19). Nevertheless, there are still some open issues and future steps for the development of improved and more practical JIT model based adaptive soft sensor.

4.1. Selection of the relevant training data set

Despite owing some good performances, the original version of JIT modeling which is based on distance measure has also few shortcomings. These shortcomings are mainly related to the selection of relevant training data set. During the selection, correlations among variable are neglected. Consequently, some good data may not be selected. These situations have motivated researchers to propose variants of JIT modeling technology. Table 1 provides a summary of different variants of JIT models. Cheng's enhance model, CoJIT and non-Gaussian JIT model have proven to perform better than the original model [10, 13 – 15, 19, 29 – 30]. However, these approaches face challenges in obtaining the optimum parameters of γ and λ. For practical applications, easily tuned parameters would be desirable. For this purpose, distance measures based JIT modeling technology can be good options since there are no parameters to be tuned. Modifications into the calculation of distance, however, are necessary to take into account the relations between variables as successfully demonstrated by Galvão et al. [32] and Saptoro et al. [33] in the applications of data partition for empirical modelling.

All existing approaches as outlined in Table 1 are also not robust against the presence of outliers. Thus, new frameworks of incorporation of data cleaning and/or robustification the algorithm against outliers are required. In this regard, robust PCA can possibly be implemented for correlation based JIT instead of standard PCA proposed by Fujiwara et al. [10, 13 – 15]. Robust Eucledian and Mahalanobis distances can also be tested for this purpose. Among existing algorithms of JIT modeling, there is only one algorithm which can deal with non-Gaussian data [30]. Therefore, there is also a space for improvement to develop an approach which is able to accommodate both Gaussian and non-Gaussian data.

4.2. Process applications

As mentioned earlier, in the last decade, JIT models have been applied as soft sensors in various units and processes: blast furnace [20], methane steam reforming process [21], CSTR 10, 13 - 15, 19, 22 - 23), waste water plant [16], water heating process [24], fuel cell engine [25], polymerization reactor [19], rolling mill process [26], Tennessee Eastman process [5] and debutanizer column [5]. Meanwhile, incorporations into control systems have been proposed in adaptive decentralized PID controller [27] and robust PID controller [23] and statistical process control [28]. Since JIT model performs well in the process systems above, it would also be interesting and promising to see its application in other processes/units. Beside applications in general chemical and petroleum process industries, future studies should be directed toward wider applications of JIT models based adaptive soft sensors in bioprocesses, pharmaceutical industries and steel-making and semi-conductor industries since these related processes exhibit nonlinearity and frequent process changes.

5. Conclusions

This paper provides an overview of existing JIT models based adaptive soft sensors. The paper mainly focuses on current status of the JIT modeling approaches and their applications to arrive at the proposal for future research directions and recommendations. Critical review to the current JIT modeling approaches indicate that despite owing promising performances, the future of JIT models based adaptive soft sensors depends on the continued development of effective and robust selection of relevant training data set. Further applications of this technology into other nonlinear processes such bioprocesses, pharmaceutical industries and steel-making and semi-conductor industries are still wide open beside its other and wider implementations in the traditional chemical and petroleum processing industries.

Acknowledgements

The authors acknowledge the financial support from National Institute of Technology (ITENAS) Bandung.

References

1. Fortuna L, Graziani S, Rizzo A Xibilia MG. Soft Sensors for Monitoring and Control of Industrial Processes. London: Springer; 2007.
2. Kaneko H, Funatsu K. Maintenance-free soft sensor models with time difference of process variables. *Chemometr Intell Lab* 2011; **107**: 312 – 317.
3. Kadlec P, Gabrys B, Strandt S. Data-driven Soft Sensors in the process industry. *Comput Chem Eng* 2009; **33**: 795 -834.
4. Karlsson, CP, Avelin A, Dahlquist E. New Methods for Adaptation to Degeneration in Process Models for Process Industries. *Chem Prod Process Model* 2009; **4** (1): Article 25.
5. Ge Z, Song Z. A comparative study of just-in-time-learning based methods for online soft sensor modeling. *Chemometr Intell Lab* 2010; **104**: 306 – 317.
6. Kano M, Ogawa M. The state of the art in chemical process control in Japan: Good practice and questionnaire survey. *J Process Contr* 2010; **20**: 969 – 982.
7. Ljung L. Theory and practice of recursive identification. MIT Press; 1985.
8. Nakabayashi A., Nakaya M, Ohtani T, Chen D, Wang D, Li X. A process simulator based on hybrid model of physical model and Just-In-Time model. *Proceedings of the SICE Annual Conference, August 18 – 21, 2010, Taipei, Taiwan*.
9. Kadlec P, Grbic R, Gabrys B. Review of adaptation mechanism for data-driven soft sensors. *Comput Chem Eng* 2011; **35**: 1 – 24.
10. Fujiwara K, Kano M, Hasebe S. Development of correlation-based pattern recognition algorithm and adaptive soft sensor design. *Control Eng Pract* 2012; **20**: 371 – 378.
11. Li W, Yue HH, Valle-Servantes S, Qin SJ. Recursive PCA for adaptive process monitoring. *J Process Contr* 2000; **10**: 471 – 486.
12. Qin SJ. Recursive PLS algorithms for adaptive data modeling. *Comput Chem Eng* 1998; **22**: 503 – 514.
13. Fujiwara K, Kano M, Hasebe S. Correlation-Based Just-In-Time Modeling for Soft-Sensor Design. *Proceedings of the 18th European Symposium on Computer Aided Process Engineering – ESCAPE 18, June 1 – 4, 2008, Lyon, France*.
14. Fujiwara K, Kano M, Hasebe S, Takinami A. Soft-Sensor Development Using Correlation-Based Just-in-Time Modeling. *AIChE J* 2009; **55** (7): 1754 – 1765.
15. Fujiwara K, Kano M, Hasebe S. Development of Correlation-Based Pattern Recognition and Its Application to Adaptive Soft-Sensor Design. *Proceedings of the ICROS-SICE International Joint Conference, August 18-21, 2009, Fukuoka, Japan*.
16. Liu Y, Huang D, Li Y. Development of Interval Soft Sensors Using Enhanced Just-In-Time Learning and Inductive Confidence Predictor. *Ind Eng Chem Res* 2011; **51**: 3356 – 3367.
17. Bontempi G, Birattari M, Bersini H. Lazy Learning for Local Modeling and Control Design. *Int J Contr* 1999; **72**: 643 – 658
18. Atkeson CG, Moore AW, Schaal S. Locally Weighted Learning. *Artif Intell Rev* 1997; **11**: 11 – 73.

19. Cheng C, Chiu MS. A new data-based methodology for nonlinear process modeling. *Chem Eng Sci* 2004; **59**: 2801 – 2810.
20. Ito M, Matsuzaki S, Odate N, Uchida K, Ogai H, Akizuki K. Large scale database Online Modeling for Blast Furnace. *Proceedings of the IEEE International Conference on Control Applications, September 2-4, 2004, Taipei, Taiwan*.
21. Nakabayashi A, Nakaya M, Ohtani T, Chen D, Wang D, Li X. A process simulator based on hybrid model of physical model and Just-In-Time model. *Proceedings of the SICE Annual Conference, August 18 – 21, 2010, Taipei, Taiwan*.
22. Su QL, Kano M, Chiu, MS. A new strategy of locality enhancement for Just-in-Time learning method. In: Karimi IA, Srinivasan R, editors. *Proceedings of the 11th International Symposium on Process Engineering, 15 – 19 July 2012, Singapore*. p. 1662 – 1666.
23. Cheng C, Chiu MS. Robust PID controller design for nonlinear processes using JITL technique. *Chem Eng Sci* 2008; **63**: 5141 – 5148.
24. Stenman A, Gustafsson F, Ljung L. Just In Time Models for Dynamical Systems. *Proceedings of the 35th Conference on Decision and Control, December 11-13, 1996, Kobe, Japan*.
25. Chuqi S, Xiang L. Just-in-time Learning Theory-based Study on the Dynamic Model of Fuel Cell Engine System. *Proceedings of the 2nd International Workshop on Computer Science and Engineering, October 28-30, 2009, Qingdao, China*.
26. Zheng Q, Kimura H. Just-in-Time modeling for function prediction and its applications. *Asian J Contr* 2001; **3** (1): 35 - 44.
27. Yang X, Jia L, Chiu MS. Adaptive decentralized PID controllers design using JITL modeling methodology. *J Process Contr* 2012; **22**: 1531 – 1542.
28. Kano M., Sakata T., Hasebe S. Just-in-time statistical process control for flexible fault management. *Proceedings of the SICE Annual Conference, August 18 – 21, 2010, Taipei, Taiwan.*
29. Cheng C, Hashimoto Y, Chiu MS. An Enhanced Just-in-Time Learning Methodology for Process Modeling. *Proceedings of the 5th Asian Control Conference, July 20-23, 2004, Melbourne, Australia*.
30. Zeng J, Xie L, Gao C, Sha J. Soft Sensor Development Using Non-Gaussian Just-In-Time Modeling. *Proceedings of the 50th IEEE Conference on Decision and Control and European Control Conference (CDC-ECC), December 12-15, 2011, Orlando, FL, USA*.
31. Chen D, Li X, Xiang K, Wang D, Nakabayashi A, Nakaya M, Ohtani T. Hybrid Plant Model of Physical and Statistical Model with Robust Updating Method. *Proceedings of the International Conference on Intelligent Control and Information Processing, August 13-15, 2010, Dalian, China*.
32. Galvão RKH., Araujo, MCU, José GE, Pontes MJC, Silva EC, Saldanha TCB. A method for calibration and validation subset partitioning. *Talanta* 2005; **67**: 736-740.
33. Saptoro A, Tadé MO, Vuthaluru HB. A modified Kennard-Stone Algorithm for optimal division of data for developing artificial neural network models. *Chem Prod Process Model* 2012; **7** (1): Article 13.