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Fault Detection of Multi-Rate Two-Phase Reactor-Condenser System with Recycle Using Multiple Probabilistic Principal Component Analysis †

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Abstract: Fault detection in multi-rate process systems is a challenging task. Common techniques used for fault detection include threshold-based detectors, statistical detectors, and machine learning-based detectors. One such statistical detector technique is Multiple Probabilistic Principal Component Analysis (MPPCA). MPPCA uses probabilistic PCA to detect fault signals from multiple sensors without down-sampling or up-sampling. This paper uses MPPCA to detect faults in a Two-Phase Reactor-Condenser system with Recycle (TPRCR) with three measurement classes. These measurement data are used to build the MPPCA model using Expectation Maximization (EM). Based on this, T^2 and SPE statistics are generated for fault detection in TPRCR systems, and the MPPCA approach's effectiveness for fault detection is satisfactory.

Keywords: fault detection; multi-rate process; MPPCA

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1. Introduction

Modern chemical industries focus on detecting and diagnosing faults as early as possible to increase production yield [1]. Effective fault detection techniques available in the literature require regular availability of measurements [2]. However, some variables in chemical processes are measured online, while other quality variables are measured offline. Measurement of these offline quality variables requires human involvement, which makes the system an irregularly sampled multi-rate system [3]. Fault detection techniques for multi-rate systems include state space estimation techniques and data-based modelling methods. State space estimation techniques require accurate system models, which are difficult to model for complex chemical engineering systems. Compared to the above methods, another data-driven approach uses measurement data to model the system's behaviour. These data-driven methods for multi-rate systems require down-sampling, up-sampling and re-sampling. While the down-sampling approaches will lose essential information during modelling, the up-sampling methods heavily rely on the correctness of the predictions [4]. In most chemical processes, the variation in sample rates is also too significant, resulting in unmanageable complexity in the re-sampling models. The MPPCA method does not require down-sampling, up-sampling and re-sampling of multi-rate data. It uses multi-rate data to build an inferential model that can handle multiple measurement classes. MPPCA method is an extension of Probabilistic Principal Component Analysis (PPCA) which uses the EM algorithm for parameter tuning.

In this study effectiveness of the MPPCA method in detecting various faults for multi-rate nonlinear chemical process TPRCR is studied, and fault detection is done by using T^2 and SPE statstics.

The remainder of this paper is organised as follows. Section 2 gives detail about the MPPCA method and model parameter estimation. Then Section 3 details about TPRCR model. Section 4 implements a fault detection technique on TPRCR. Finally, conclusions are made in the last section

2. MPPCA Method

The MPPCA model combines several rate data into a single model without down or up sampling. In our article, we have considered the MPPCA model with three different classes of measurements, and it is given by the following equations

$$x_1 = \emptyset_1 t + \epsilon_1 \quad (1)$$

$$x_2 = \emptyset_2 t + \epsilon_2 \quad (2)$$

$$x_3 = \emptyset_3 t + \epsilon_3 \quad (3)$$

In Equations (1)–(3) $x_1 \in R^{K1\times M1}$, $x_2 \in R^{K2\times M2}$, $x_3 \in R^{K3\times M3}$ are three different rate measurements classes in which x_3 is the slowest and x_1 is the fastest measurement. $\emptyset_1 \in R^{M1\times D}$, $\emptyset_2 \in R^{M2\times D}$ and $\emptyset_3 \in R^{M3\times D}$ are loading matrices with three different sampling rates. $t \in R^D$ is a latent variable which extracts a restricted link between data with varied sampling rates and helps to develop one single model. The latent variable is assumed to have a Gaussian distribution with zero means and unit variance. $\varepsilon_1 \in R^{M1}$, $\varepsilon_2 \in R^{M2}$ and $\varepsilon_3 \in R^{M3}$ are used to model the corresponding isotropic Gaussian noises.

The sequence of the measurements can be altered for easier notation and visualisation on the premise that all sample variables are independent. The whole observation (V) comprises three divisions of the observed data. The first sample contains all observations with dimensions M1 + M2 + M3 (V_3), the following sample variables have dimensions M1 + M2 (V_2), and the last one contains only M1 (V_1) variables. As a result, the entire observation set is expressed as a union of all three.

$$V = V_3 \cup V_2 \cup V_1 \quad (4)$$

The EM technique is used to estimate model parameters for the MPPCA model. The method repeats the expectation step (E-step) and the maximisation step (M-step) until convergence. In the E-step, the current model parameters are utilised to estimate the posterior distributions of the latent variables. The model parameters are then adjusted in the M-step by maximising log likelihood. The reference contains a detailed step of the EM algorithm for MPPCA training [5].

SPE statistics can be used to detect abnormal behaviour in measurements. There are three different classes of measurements, so three different SPE statistics are used to detect any anomaly in measurement.

$$SPE_1 = x_1 - \emptyset_1 t \quad (5)$$

$$SPE_2 = x_2 - \emptyset_2 t \quad (6)$$

$$SPE_3 = x_3 - \emptyset_3 t \quad (7)$$

since each SPE statistic is compiled based on the prediction errors of different classes of measurements, it clearly shows that a given fault is caused by which class of measurements. The confidence bound of SPE statistics can be predicted by χ^2 distributed approximation: $SPE \sim g.\chi_h^2$ in which g and h are the parameters of χ^2 distribution, and they are given by [6].

$$gh = mean(SPE) \quad (8)$$

$$2g^2h = var(SPE) \quad (9)$$

3. Two-Phase Reactor Condenser System with Recycle

The process depicted in Figure 1 includes a two-phase reactor and condenser [7]. Reactants A and B are introduced into the reactor at molar flow rates F_A and F_B and temperatures T_A and T_B, respectively, in the vapour and liquid phases. Reactant A diffuses into the liquid phase at rate N_{A1}, where an exothermic reaction occurs, which is given by Equation (10).

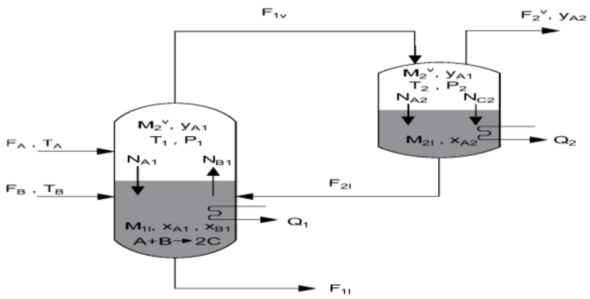

Figure 1. Schematic Diagram of TPRCR system.

$$A + B \rightarrow 2C \quad (10)$$

Product C diffuses into the vapour phase at a rate Nc1, whereas reactant B is non-volatile. The interphase mass transfer resistance is assumed to be minimal, and the Arrhenius equation provides the reaction rate in the bulk liquid phase, which is given by Equation (11).

$$r_A = k_{10}\exp\left(\frac{-E_a}{RT_1}\right) M_1^l \rho x_{A1} x_{B1} \quad (11)$$

where r_A is the rate at which reactant A is consumed at temperature T_1. The preexponential factor and activation energy are denoted by k_{10} and E_a, respectively. M_{1l} is the liquid molar holdup in the reactor, and ρ is the liquid density. x_{A1} and x_{B1} are A and B mole fractions in the liquid phase. For the sake of simplicity, heat capacity, density, and molar heat of vaporisation are considered to be constant and equal for all species. The liquid and vapour phases are suitable combinations. The liquid stream from the reactor is withdrawn at a constant flow rate F_{1l}, while the vapour stream enters the condenser at a flow rate F_{1v}. The vapour in the condenser is cooled to T_2 to improve product purity by eliminating reactant A from the liquid.

The reactant A-rich liquid phase in the condenser is returned to the reactor at a flow rate of F_{2l}, while the product vapour phase departs the condenser at a flow rate of F_{2v} and a composition of y_{A2}.

Equations (12) to (29) give a detailed Differential Algebraic Equation (DAE) model used to train the MPPCA model for data generation.

$$\dot{M}_1^l = F_B - F_{1l} + F_{2l} + N_{A1} - N_{C1} \quad (12)$$

$$\dot{x}_{A1} = \left(\frac{1}{M_1^l}\right)[-F_B x_{A1} + F_{2l}(x_{A2} - x_{A1}) + N_{A1}(1 - x_{A1}) + N_{C1}x_{A1} - r_A] \quad (13)$$

$$\dot{x}_{B1} = \left(\frac{1}{M_{1l}}\right)[F_B(1 - x_{B1}) - F_{2l}x_{B1} - N_{A1}x_{B1} + N_{C1}x_{B1} - r_A \quad (14)$$

$$\dot{M}_1^v = F_A - F_{1v} - N_{A1} + N_{C1} \quad (15)$$

$$\dot{y}_{A1} = \left(\frac{1}{M_1^v}\right)[F_A(1 - y_{A1}) - N_{A1}(1 - y_{A1}) - N_{C1}y_{A1}] \tag{16}$$

$$\dot{T}_1 = \left(\frac{1}{M_1^l + M_1^v}\right)[F_A(T_A - T_1) + F_B(T_B - T_1) + F_{2l}(T_2 - T_1) + (N_{A1} - N_{C1})\frac{\Delta H^v}{C_P} - \frac{Q_1}{C_P} + r_A\left(\frac{-\Delta H_r}{C_P}\right)] \tag{17}$$

$$\dot{M}_2^l = N_{A2} + N_{C2} - F_{2l} \tag{18}$$

$$\dot{x}_{A2} = \left(\frac{1}{M_2^l}\right)[N_{A2}(1 - x_{A2}) - N_{C2}x_{A2}] \tag{19}$$

$$\dot{M}_2^v = F_{1v} - F_{2v} - N_{A2} - N_{C2} \tag{20}$$

$$\dot{y}_{A2} = \left(\frac{1}{M_2^v}\right)[F_{1v}(y_{A1} - y_{A2}) - N_{A2}(1 - y_{A2}) + N_{C2}y_{A2}] \tag{21}$$

$$\dot{T}_2 = \left(\frac{1}{M_2^l + M_2^v}\right)[F_{1v}(T_1 - T_2) + (N_{A2} + N_{C2})\frac{\Delta H^v}{C_p} - \frac{Q_2}{C_P}] \tag{22}$$

$$0 = N_{A1} - k_A a(y_{A1} - y_{A1}^*)\frac{M_1^l}{\rho} \tag{23}$$

$$0 = N_{C1} - k_C a(y_{c1}^* - (1 - y_{A1}))\ \frac{M_1^l}{\rho} \tag{24}$$

$$0 = N_{A2} - k_A \mathrm{a}(y_{A2} - y_{A2}^*)\ \frac{M_2^l}{\rho} \tag{25}$$

$$0 = N_{C2} - k_C a * (1 - y_{A2} - y_{C2}^*)\ \frac{M_2^l}{\rho} \tag{26}$$

$$0 = P_1\left(V_{1T} - \frac{M_1^l}{\rho}\right) - M_1^v R T_1 \tag{27}$$

$$0 = P_2\left(V_{2T} - \frac{M_2^l}{\rho}\right) - M_2^v R T_2 \tag{28}$$

$$0 = P_1 - P_2 - \frac{1}{0.09}(F_{1v})^{\frac{7}{4}} \tag{29}$$

The system parameter values are given in Table 1.

Table 1. TPRCR system parameter.

Parameter	Description	Value	Unit
a	Interfacial mass transfer area/unit liquid holdup	1000	m^2/m^3
C_p	Molar heat capacity	80	J/mol K
E_a	Activation energy	110	kJ/mol
K	Proportional gain of pressure controller	−8	mol/s atm
K_{10}	Preexponential factor	2.88×10^{11}	m^3/mol s
k_a	overall mass transfer coefficient for A	0.2	mol/m^2 s
k_c	overall mass transfer coefficient for C	0.8	mol/m^2 s
M_1^l	Liquid molar holdup in reactor	14.52	kmol
M_2^l	Liquid molar holdup in condenser	15	kmol

M_1^v	vapour molar holdup in reactor	3.75	kmol
M_2^v	vapour molar holdup in condenser	3.90	Kmol
P_1	Pressure in reactor	50	atm
P_2	Pressure in condenser	48.69	atm
P^*	Set point for reactor pressure	50	atm
T_A	Temperature of feed A	315	K
T_B	Temperature of feed B	300	K
T_1	Temperature in reactor	330	K
T_2	Temperature in Condenser	304.16	K
V_{1T}	Volume of reactor	3	m^3
V_{2T}	Volume of condenser	3	m^3
ρ	Liquid molar density	15000	mol/m^3
ΔH_r	Heat of reaction	−50	kJ/mol
ΔH^v	Heat of vaporization	10	kJ/mol

4. Fault Detection Using MPPCA for the TPRCR System

Three types of measurements are used to train the MPPCA model. Fast-rate measurements include temperature, pressure, and flow rates available every second (x_1). Medium-rate measurements include molar holdups available every fifteen seconds (x_2), and slow-rate measurements include mole fractions available every one minute (x_3).

The MPPCA model is trained with 7200 samples of fast rate measurements, 480 samples of medium rate measurements, and 120 samples of slow rate observations. The fault identification capability of the MPPCA approach is assessed using the six categories of faults indicated in Table 2.

Table 2. Fault description in the TRPCR system.

Fault No.	Fault Type	Fault Introduced (s)
1	Step jump in flow rate of A (F_A)	2400
2	Step jump in flow rate of B (F_B)	2400
3	Step jump in Temperature of A (T_A)	2400
4	Step jump in Temperature of B (T_B)	2400
5	Ramp jump in flow rate of A(0.0004*t)	2400
6	Ramp jump in Temperature of A(0.003*t)	2400

For a fair comparison, all detection models in this work have a level of significance of 0.99 for SPE and T^2 statistics. Table 3 shows the false alarm rates for normal data and the missing detection rates for faults, where Fault 0 represents normal test data and monitoring results are false alarm rates. The false alarm rate is the fraction of normal data that is interpreted as problem data. Similarly, the missing detection rate is the fraction of the defect data that is treated as normal data. Table 3 shows the monitoring results of all faults using T^2 and different SPE statistics for the MPPCA model.

Table 3. Fault Monitoring Results Using T^2 and SPE Statistics.

Fault No	T^2	SPE_1	SPE_2	SPE_3
0	0.021	0.001	0.004	0.0001
1	0.035	0.023	0.09	0.008
2	0.067	0.065	0.011	0.034
3	0.001	0.001	0.001	0.001
4	0.854	0.673	0.765	0.231
5	0.313	0.452	0.023	0.045

6	0.201	0.121	0.111	0.201

Three different SPE statistics are used to see what kind of fault wil have effect on which SPE statistics. Figure 2 shows SPE statistics for fault in flow rate of A (F_A), which suggests that this fault affects all three SPE statistics.

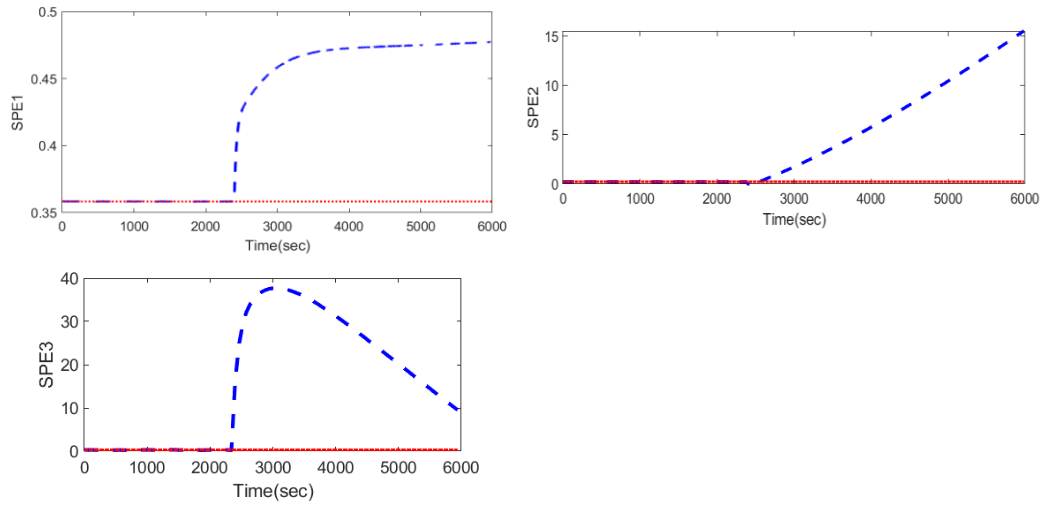

Figure 2. Monitoring Results of Fault 1.

4. Conclusion

In this paper, the TPRCR system is modelled as a multi-rate system due to the involvement of quality variables, including three different classes of measurements. These measurements are used to develop the MPPCA model using EM algorithm. This developed MPPCA model is used to detect faults by developing T^2 and three different SPE statistics for each measurement class. Six different types of faults are used to check the effectiveness of the developed MPPCA model, and from monitoring results, we can clearly say that the MPPCA model can detect faults with a high detection rate.

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