Identification of Hybrid Systems with Application to Fault Detection of a Reverse-Flow Reactor System A. Ben-Zvi [1], S. Shah[2]

In this work, the suitability of several techniques for monitoring a reverse-flow reactor system are studied. Reverse reactor systems are operated by periodically reversing the direction of the flow inside the reactor [1],[2]. One benefit of a reverse-flow configuration is that, for exothermic reactions, the system exhibit a heat-trap effect [3] where the temperature profile across the reactor achieves a maximum near the centre of the reactor. This enhanced temperature profile allows the combustion of lean feed streams that could require pre-heating for combustion in a traditional, one-way reactor system.

The reverse-flow reactor system under study in this work is used for combustion of low concentration methane streams and has been modeled in the literature [3]. The data used for this work was obtained from the CANMET Energy Technology Centre at Varennes, Quebec Canada. Data from the reactor system under three distinct operating conditions will be studied. The three conditions are distinguished by the frequency at which the feed direction is switched and the concentration of methane in the feed stream. Table 1 lists the switch time and concentration associated with each condition. Plots of temperature versus time for selected thermocouples are shown in Figure 1. As can be seen from Figure 1, the switching flow direction induces temperature oscillations in the reactor. Furthermore, the period of the temperature oscillations is related to the period of switching. Less clear, however is the relationship between the feed concentration and the reactor temperature. As can be seen from Figure 1, the general trend of the mean temperature in the reactor is flat when operating at a feed concentration of 0.3% methane. However, when operating at a feed concentration of 0.7% methane, the averaged temperature increases with time.

Condition Number	Switch Period (s)	Methane Concentration mole %
1	300	0.3
2	100	0.3
3	100	0.7

Table 1: List of Reactor Operating Conditions

Traditional fault-detection schemes that rely on instantaneous process measurements [4] may fail to detect faults in the reverse flow reactor system due to the inherit temperature oscillations. Consider, for example, the problem of trying to determine if the reactor temperature is excessive or increasing rapidly. One cannot use any single instantaneous measurement of the system because, as shown in Figure 1, the temperature at any point in the reactor oscillates, and may therefore, at any single point in time, be much lower or much higher than the mean. Note that even if one was to implement an time-averaging scheme for each measurement, the period of averaging would have to depend on the operating condition of the reactor. A fast-switching operation would require fast averaging, while a slow-switching operation would require a slow averaging scheme.

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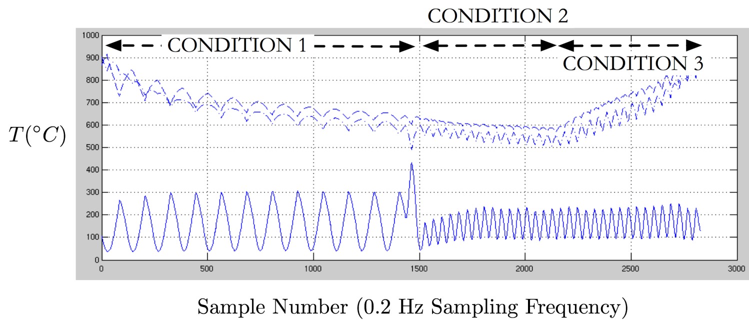

Figure 1: Temperature Plots for Selected Thermocouples.

To determine whether a standard latent-variable model is useful in monitoring the reactor system a PCA model of the reactor data using three latent variables was developed. Note that for the PCA analysis, as well as all other analysis done in this work the models developed are designed to explain 80% of the process variance unless otherwise stated. Figure 2 shows the sum of square error for the PCA model prediction. The PCA model is able to detect the transition from the first to the second operating condition (a change in the reactor switch time), but is not able to detect the transition from the second to the third operating condition (a change in the feed concentration).

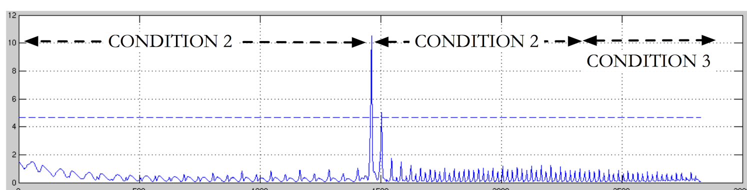

Figure 2: SSE for PCA Model; the dashed line corresponds to the 95^{th} percentile of residuals.

The score plots of the PCA model is shown in Figure 3. Note that the score plots cannot be easily divided into regions associated with the different operating conditions. That is, the score plots shown in Figure 3 cannot be used to identify the discrete state of the system.

One alternative to traditional PCA modeling and fault-detection techniques is the use of spectral PCA. In this approach, the power spectra of the data is computed using fast Fourier transform and analyzed using PCA. A plot of the projection of the process data, in the frequency domain on the principal components is shown in Figure 4 . As can be seen from Figure 4 (note that only two principal components were identified) there is indeed a change in the key frequencies of the system from Condition 1 to Condition 2. Furthermore, the data associated with each Condition appears to cluster in different locations in the principal component space. This technique is therefore superior to traditional PCA in its ability to categorize process data. However, this technique is limited as a real-time monitoring tool because the frequency data required to monitor the process cannot be collected in real time. As a result, the model prediction errors, for example, cannot be collected in real-time.

Recently, a hybrid identification procedure has been proposed [5] that is suitable for identification of linear relationships in systems with several discrete states. The general idea behind this

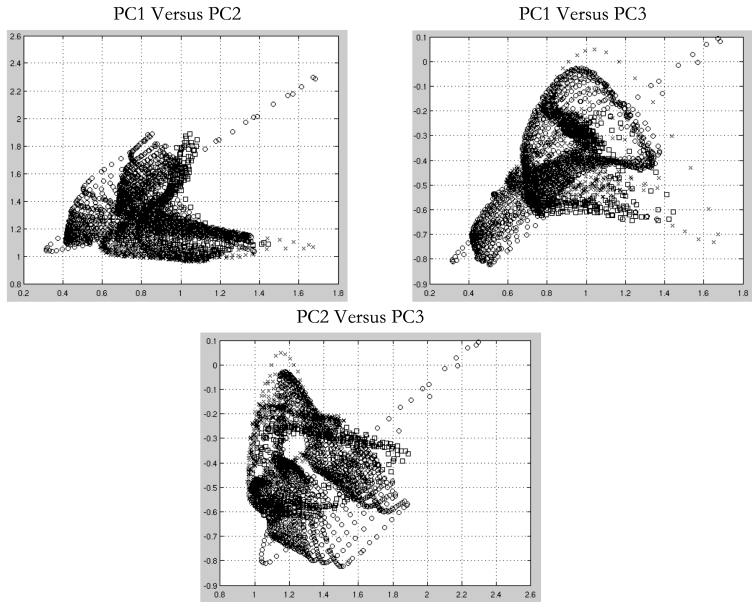

Figure 3: Score Plots of 3-Component PCA Model: $\circ$: Data from Condition 1; $\times$: Data from Condition 2; $\square$: Data from Condition 3

hybrid identification procedure is as follows. Let the system variables be z_i with $i = 1, 2, \ldots, n$. Any single linear discrete state is described by a constraint on the system variables given by $\sum_{i=1}^{n} \lambda_i z_i = 0$, with $\lambda_i \in \mathbb{R}$. Letting $\Lambda = [\lambda_1, \lambda_2, \ldots, \lambda_n]$, this sum can be written as $\Lambda z = 0$. For systems with m discrete states, we can write the linear constraint for each discrete state as $\Lambda_j z = 0$ for the j^{th} discrete state with $j = 1, 2, \ldots, m$. The hybrid system is described by the hybrid decoupling polynomial $\mathcal{P} = \prod_{j=1}^{m} \Lambda_j z$. This product can be expanded and expressed as the sum $\mathcal{P} = \sum_{i=1}^{M} \tilde{z}\tilde{\Lambda}$ where $\tilde{z}$ and $\tilde{\Lambda}$ are vectors made up of monomials in z and Λ, respectively, of degree m, and $M = \begin{pmatrix} m+n-1 \\ m \end{pmatrix}$. Note that for each sampling time $\mathcal{P} = 0$ for a noise-less system. For a stochastic system, one obtains an estimate for $\tilde{\Lambda}$ by finding the value of $\tilde{\Lambda}$ that minimizes $\mathcal{P}$.

Our approach is to use the hybrid decoupling polynomial to monitor the reactor system. The number of measured variables in this case is $n = 30$. With three discrete states ($m = 3$) the number of elements in $\tilde{\Lambda}$ is $M = \begin{pmatrix} m+n-1 \\ m \end{pmatrix} = 4960$, that is, more than the number of observations available to us. To overcome this difficulty, we use traditional PCA to reduce the number of model variables from 30 to three. A value of three for the reduced variables were chosen because three variables are sufficient to explain 80% of the variance in the original data.

After reducing the number of variables, we apply the hybrid identification procedure to the variables in the latent space. The degree of the hybrid decoupling polynomial was chosen as three because that is the number different conditions under which the reactor system was analyzed. A plot of the model data in the principal component space is shown in Figure 5. As can be seen from Figure 5, the hybrid model is able to separate the reactor data into areas populated by data corresponding to Conditions 1, 2 and 3 only slightly better than the traditional PCA model.

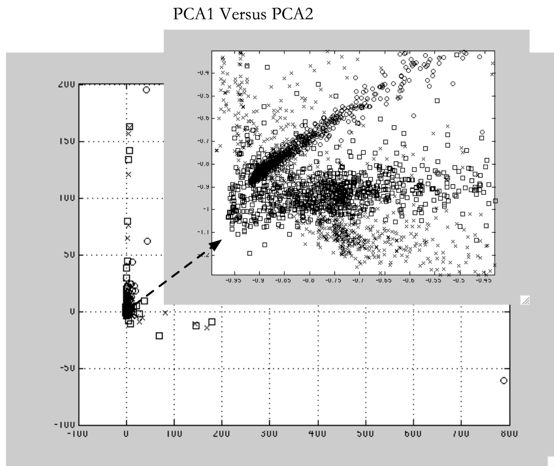

Figure 4: Score Plots of 2-Component Spectral PCA Model: ○: Data from Condition 1; ×: Data from Condition 2; □: Data from Condition 3

However, as shown in Figure 6, the hybrid approach allows us to monitor the reactor system by plotting the SSE as a function of time. This approach, therefore, is able to detect changes that would not normally be detected using a PCA-based approach for the system under study.

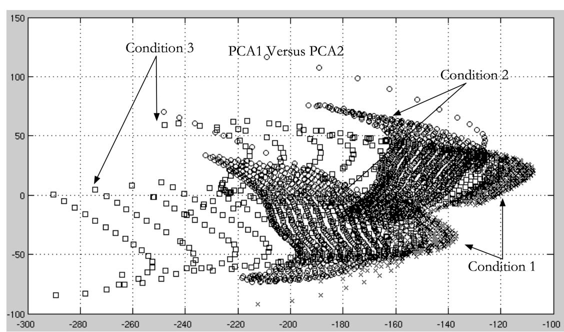

Figure 5: Score Plots of 2-Component Hybrid Polynomial Model: ×: Data from Condition 2; □: Data from Condition 3

In this work we consider three approaches for monitoring the operation of a reverse-flow reactor system. This system is challenging to monitor due to the lack of a steady state point. In addition, the dominant feature of data obtained from the reactor system is temperature oscillations which make monitoring and fault detection difficult. For this system traditional PCA techniques for monitoring may fail to identify a change of operating conditions. Frequency-based approaches can also be used to monitor the reactor system. However, these approaches may be difficult to implement in real-time. Using a hybrid-system monitoring approach it is possible to correctly identify changes in operating conditions in the reactor system. However, for systems with many measurements, it is necessary to reduce the number of variables in the data set before applying the hybrid identification algorithm.

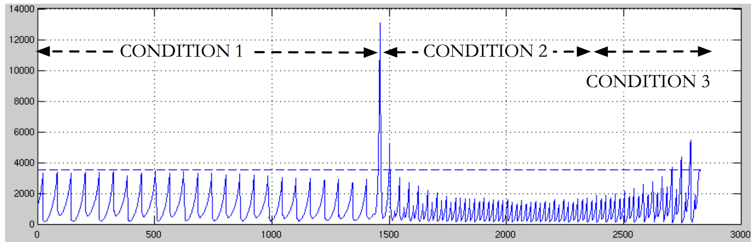

Figure 6: SSE Plot for the Hybrid Polynomial Model

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