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Complete Partial Control Design for Extractive Fermentation Process

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Abstract: In this paper, the methodology for complete partial control design based on a novel PCA-based technique incorporating the inventory and constraint control objectives is described. Brief descriptions on the PCA-based technique, some definitions and criteria are also presented. The application of the methodology is demonstrated using a case study of extractive alcoholic fermentation process. Result shows that good understanding of the interaction among process variables is the key principle for designing partial control strategy. Interestingly the proposed methodology allows the designer to understand this interaction and hence to exploit its benefit in partial control design.

Keywords: partial control, plantwide control, extractive fermentation, PCA

1. INTRODUCTION

An eminent approach to bioprocess control has generally focused on the specific control methods or algorithms used to control certain variables of interest. In this regard, the control *philosophy* of the overall plant (Larsson and Skogestad, 2000) is frequently ignored in bioprocess control design i.e. which variables to be controlled and which variables to be manipulated - control structure problem.

One way to address this difficult problem in a theoretically-founded manner (Stephanopoulos and Ng, 2000) is by adopting the *partial control* framework introduced by Shinnar (1981). Since the number of manipulated variables is frequently smaller than that of output variables to be controlled (i.e. *thin* plant), partial control seems to be the natural choice in process industries. Reported examples of its applications are in fluidized catalytic cracker (Arbel et al., 1996) and Tennessee Eastman Process (Tyreus, 1999).

The key issue to be resolved in partial control is about the identification of the suitable *dominant variables,* which depend on the specified operating objectives. To date, the predominant technique for identifying the dominant variables is largely based on the engineering experience and process knowledge. Consequently such a practice has become the key obstacle in applying this concept to new processes where substantial experience about the processes is generally unavailable or limited.

In this paper, a novel PCA-based technique is briefly described, which can be used as a tool to design a complete partial control strategy incorporating inventory and constraint control objectives. Note that, the detail regarding the PCA-based technique for identifying the dominant variables is available in (Nandong et al., 2010). Note that, the proposed methodology allows the engineers to design partial control without the need for extensive experience or process knowledge. Moreover, the effectiveness of the technique is demonstrated based on its application to a case study of extractive alcoholic fermentation process.

2. PARTIAL CONTROL PROBLEM FORMULATION

Let a performance measure/operating objective be given by:

$$\phi_p = F_{D,p}(\Omega_p) + F_{M,p}(\Psi_p) \quad (1)$$

Where Ω_p and Ψ_p are the *dominant* and *minor* variable sets respectively. Here minor variables are the variables which have only small contribution to the performance measure. And $F_{D,p}$ and $F_{M,p}$ are functions that describe the contributions of dominant and minor variable sets to the performance measure ϕ_p respectively.

Assuming that the variation of the performance measure due to the disturbance occurrence can be written as:

$$\Delta\phi_p = \Delta F_{D,p} + \Delta F_{M,p} \quad (2)$$

Thus, for *n* performance measures one can write:

$$\Delta\Phi = [\Delta\phi_1 \; \Delta\phi_2 \; ... \; \Delta\phi_n]^T \quad (3)$$

Note that, the objective of partial control is to ensure that $\Delta\Phi \le \Delta\Phi_{max}$ in the face of external disturbance occurrence where $\Delta\Phi_{max}$ is the maximum allowable variations.

Therefore, based on (2) or (3) the dominant variables can be defined as:

Definition 1 (Dominant Variables). *The dominant variable set* Ω_p *for a given* ϕ_p *is defined as the smallest subset of variables that can (possibly) be formed from the set of all variables* (Σ) *describing the plant, so that when they are controlled,* $\Delta F_{D,p} = 0$ *and* $\Delta\phi_p = \Delta F_{M,p} \le \Delta\phi_{p,max}$.

Subsequently, the key problem in partial control can now be stated as (**P1**):

> Given a set of all variables Σ and ϕ_p, identify the set of dominant variables (Ω_p) that corresponds to ϕ_p.

Remark 1. *The dominant variables for a given performance measure is not necessarily the same as the dominant variables for another performance measure.*

Alternatively, the partial control problem can mathematically be represented as (**P2**):

$$\min_{\Omega_{CS} \in \Sigma} \left(\Delta\Phi(U, Y, B) \right)$$

Subject to the following constraints:

$$N_{\Omega_{CS}} \leq N_{U_{mv}} \quad (4)$$
$$\Delta\Phi \leq \Delta\Phi_{max} \quad (5)$$
$$U_{min} \leq U_{mv} \leq U_{max} \quad (6)$$
$$G(U, Y, B) = 0 \quad (7)$$

Where $N_{\Omega_{CS}}$ and $N_{U_{MV}}$ are number of dominant variables corresponding to a vector of performance measures and number of manipulated variables respectively. And U_{MV}, U, Y and B are vectors of manipulated variables, inputs, outputs and process parameters. Here G is a set of equations representing the plant model.

Remark 2. *It is rather unlikely that the set of dominant variables obtained in P2 will be the same as that obtained in P1 i.e. different approach leads to different results.*

3. FRAMEWORK FOR PCA-BASED TECHNIQUE

3.1 Concept of PCA-based Technique

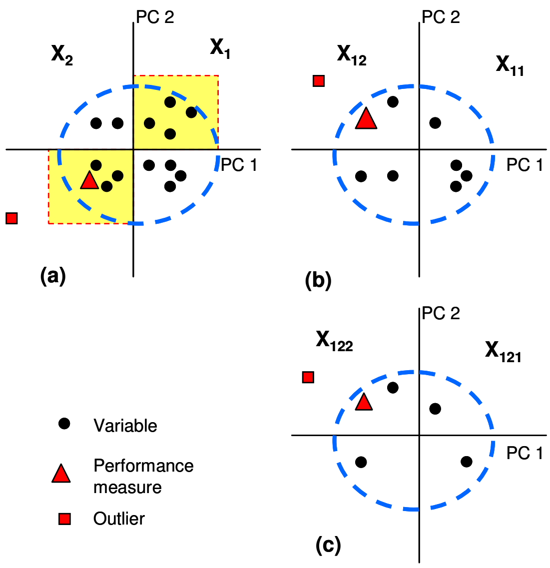

Fig. 1. Illustration of PCA-based technique for identifying the dominant variables (Nandong et al., 2010)

The concept assumes that the dominant variables can be identified through the successive dataset reduction process based on the Principal Component Analysis (PCA). Fig. 1(a) illustrates the idea where the original dataset X is first reduced using PCA into two uncorrelated sub-datasets X_1 and X_2.

The subscript "1" indicates the variables and performance measures which occupy the 1st and 3rd quadrants and "2" indicates those which occupy 2nd and 4th quadrants. The variables and performance measures occupying similar quadrant are bound to be positively correlated among each other but negatively correlated with those occupying the opposite quadrant. Notice that from Fig. 1(a), the performance measure is in the X_1 sub-dataset and which may correlate with 7 variables. Next, another PCA is applied to this sub-dataset in order to identify the critical variables that have strong influences on the performance measure. The scores and loadings of the first two principal components (PC 1 and PC 2) are plotted as in Fig. 1(b).

From Fig. 1(b) notice that, the performance measure and 4 variables are in the X_{12} sub-dataset. Note that, we have now reduced the number of variables from 7 to 4. Further PCA can be applied to the X_{12} sub-dataset which leads to Fig. 1(c). Now there are only 2 variables left which are deemed to correlate strongly with the performance measure. It can be concluded that these variables are the dominant variables for the given performance measure. However for this concept to be valid, some criteria and conditions must be fulfilled.

3.2 Dominant Variable Criteria

There are 3 important criteria which must be completely fulfilled. The sub-dataset must contain at least: (1) one variable, (2) one performance measure, and (3) one outlier. These are called the *dominant variable* (*DV*) *criteria*. The 1st and 2nd criteria arise naturally from the definition of dominant variable (Definition 1). Meanwhile, the 3rd criteria are important to ensure that the correlation between the dominant variable/s and the performance measure/s of interest is sufficiently strong i.e. dominant relationship exists.

Another *prerequisite* for the successive dataset reduction process to work is that at each level of dataset reduction, the DV criteria must be completely fulfilled. Otherwise the analysis is not consistent. This is termed as *successive dataset reduction* (*SDR*) *condition*. Recall the previous illustrative example (Fig. 1), the DV criteria is completely fulfilled throughout the 3 stages of dataset reduction process – thus, result is consistent.

3.3 Critical Dominant Variable (CDV) Condition

In order to determine at what level the dataset reduction process should be stopped, one needs to observe whether the *CDV condition* is achieved. The dataset reduction level which corresponds to CDV condition is called the *critical dataset reduction level.*

Definition 2 (CDV Condition). *The CDV condition is achieved once the sum of variances (SOV) of the principal components used to generate the PCA plot reaches a value that is at least equals to the threshold value* υ_{cric} *i.e. SOV* $\geq \upsilon_{cric}$.

It is recommended that the value of $\upsilon_{cric} \geq 80\%$. Significantly, the value of υ_{cric} indicates the strength of correlation or interaction among the variables and performance measure/s in the sub-dataset involved (Nandong et al., 2010). Hence, the higher the value of υ_{cric} the stronger is the correlation. Higher υ_{cric} could also mean that smaller number of dominant variables exist for a given performance measure.

4. METHODOLOGY

Fig. 2 shows the key steps that constitute the proposed PCA-based methodology for the complete partial control design. The controlled variables are divided into 3 categories based on their objectives as: (1) primary, (2) inventory, and (3) constraint variables. Whereas the primary variables are controlled to achieve the overall (implicit) operating objectives and which normally are subset of dominant variables, the inventory variables are controlled to prevent overflow or dry out. The constraint variables relate to the process constraints, e.g. maximum reactor temperature, maximum impurity, etc. These variables are controlled to ensure *safe, smooth* and *reliable* operation.

Step 1: Specify the performance measures or overall operating objectives (Φ). Normally Φ is an implicit function of the process variables e.g. optimum profit, maximum product yield, minimum cost, etc. Also, the maximum allowable variations $\Delta\Phi_{max}$ in the presence of external disturbance occurrence should be specified.

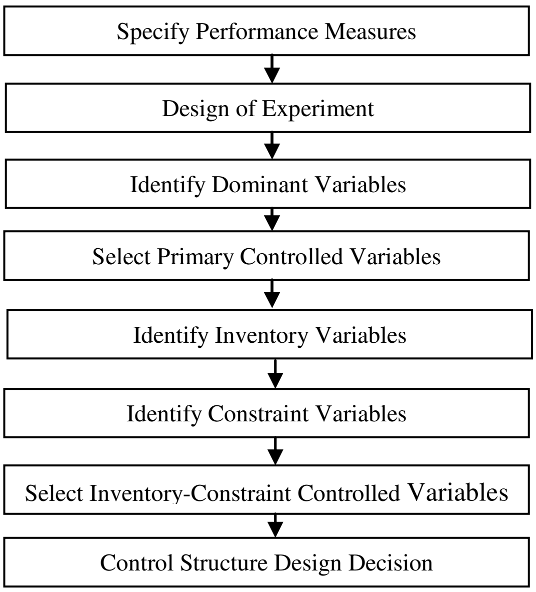

Fig. 2. The key steps in the complete partial control design methodology

Step 2: The inputs and size of their perturbations are selected and based on the Design of Experiment (DOE) concept; a number of experimental runs is generated. The plant is perturbed according to the experimental runs and the desired responses are calculated. The DOE can be performed on a *simulated* plant (process model required) if the existing plant is not running.

Step 3: Next, the successive dataset reduction process is then performed on the dataset X in order to identify the dominant variables. It is important that at this step, the DV criteria, SDR and CDV conditions are completely fulfilled to ensure consistency of the result as described in Section 3.

Step 4: Then, a set of primary variables (Y_{PM}) is selected from the set of dominant variables identified in step 3 ($Y_{PM} \subset \Omega_P$). Note that, it is not necessary to control all of the dominant variables because they might be tightly coupled. Thus, controlling one or two of the variables will indirectly control other closely related variables. The following *Primary Controlled Variable* (*PCV*) *Criteria* can be used as guidelines for the selection:

1) Select the most dominant variable/s as controlled variable/s for a given performance measure/s.
2) For the variables in series, select the most downstream variable/s because this implies the rejection of most of the disturbance effects.
3) Select a set of variables such that the diagonal elements of RGA are closed to unity i.e. leads to the most favourable pairings.
4) Select the variable/s that lead to dynamically fast disturbance rejection.

Step 5: Identify all of the variables (i.e. Y_I set) relating to the material balance e.g. liquid level in reactor.

Step 6: Identify all of the variables (i.e. Y_C set) relating to the safety, equipment limitations, environmental regulations and other operational issues e.g. flooding in distillation. Normally, this task can be carried out based on the *unit operation* knowledge and experience.

Step 7: Note that, there is no need to control all of the inventory and constraint variables because they are normally interrelated. Here, the PCA-based method can also be employed to understand the nature of interaction among these variables. The following criteria can be used as guidelines for the selection:

1) Select the most critical variables which are closed to their limits or based on the importance of constraints.
2) Select the variables which are easy to measure.
3) Select the variables which are the most susceptible to anticipated disturbances.

Step 8: Identify the available manipulated variables. Then, determine the manipulated-controlled variable pairings using the RGA analysis for the decentralized control architecture. More rigorous analysis can also be performed based on other quantitative analysis such as the conditional number, dynamic RGA (DRGA), performance RGA (PRGA) and Morari Resiliency Index (MRI). Finally, the controller tuning can be done based on the trial-and-error method (Lee et al., 1998).

5. CASE STUDY

5.1 Process Description – Extractive Fermentation

Figure 3 shows the flowchart of two-stage continuous extractive (TSCE) alcoholic fermentation process design which is adopted as a case study in this work. There are five interlinked units: (1) 2 bioreactors, (2) 1 centrifuge for separating cells from fermentation liquid, (3) 1 vacuum flash vessel to partially remove the ethanol from the fermentation liquid, and (4) 1 treatment tank in which the cells are treated with sulphuric acid solution before they are recycled back to the first bioreactor. Only the dynamics of bioreactors are considered in this study i.e. other units are assumed to be in pseudo steady-state. More details regarding this system can be found in Nandong et al. (2006).

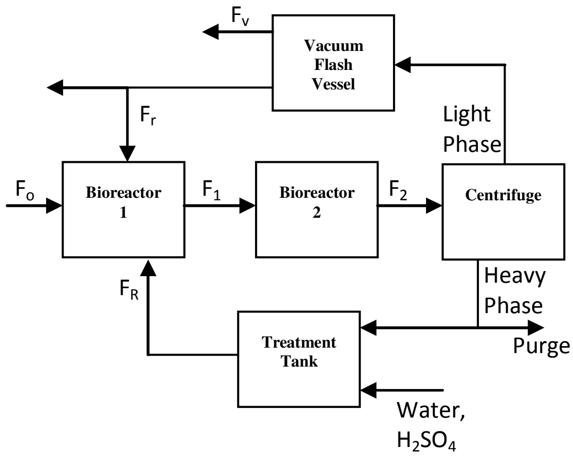

Fig. 3. Flowchart of the two-stage continuous extractive alcoholic fermentation process

Table 1. Set of manipulated variables (U_{MV})

Fresh substrate flow	F_o	*Cell recycle stream*	F_R
Flash liquid recycle	F_r	*Flash vapor flow*	F_v
Flow from bioreactor 1	F_1	*Flow from bioreactor 2*	F_2

There are 6 potential input variables that can be used for manipulations as shown in Table 1. The potential output variables to be controlled are 16 which are shown in Table 2. Note that, the subscript "1" indicates the first bioreactor and "2" the second bioreactor. In view of the limited number of manipulated variables, we can control only 6 of these outputs.

Table 2. Set of output variables

Viable cell conc. {Xv_1, Xv_2}	Substrate conc. {S_1, S_2}
Bioreactor T {T_1, T_2}	Ethanol conc. {Et_1, Et_2}
Bioreactor level {L_1, L_2}	Growth rate {rx_1, rx_2}
Consumption rate {rs_1, rs_2}	Formation rate {rp_1, rp_2}

Important overall performance measures for this process are the ethanol yield ($Yield$), substrate conversion ($Conv$) and ethanol volumetric productivity ($Prod$). Interestingly, the trends of $Yield$ and $Conv$ are opposite to that of $Prod$. In other words, the operating conditions that leads to the increase in $Yield$ and $Conv$ tends to decrease the $Prod$ (Costa et al., 2001).

For the TSCE alcoholic fermentation design the optimal trade-off values for $Yield, Conv$ and $Prod$ are 81%, 90% and 21 $kg/m^3.hr$ respectively (Nandong et al., 2006). This trade-off corresponds to 100 m^3/hr of fresh substrate flow (F_o), 120 kg/m^3 of fresh substrate concentration (S_o), 0.225 cell recycle ratio (R) and 0.270 flash liquid recycle ratio (r).

5.2 Complete Partial Control Design

The proposed methodology is applied to this case study.

Step 1: Let specify the performance measures as $\{\phi_1 = Yield, \phi_2 = Conv, \phi_3 = Prod\}$. Let the maximum allowable variation equals to 1.0% of their optimal trade-off value i.e. $\Delta\Phi_{max} = 1.0\%$.

Step 2: The inputs for DOE and their size of perturbations are shown in Table 3. Here, the selection of inputs is based on the process knowledge i.e. inputs which have strong influences on the process. There are 16 experimental runs corresponding to the perturbed operating levels and 1 experimental run at the nominal operating level. At every run, the outputs are recorded (16 outputs) and the performance measures are calculated. Thus, the dataset X consists of 17 rows (observations) and 23 columns (i.e. 4 inputs, 16 outputs and 3 performance measures).

Table 3. Real and coded values for factorial design

Input	Level (-1)	Level (0)	Level (+1)
F_o (m^3/hr)	80	100	120
S_o (kg/m^3)	96	120	144
R (-)	0.180	0.225	0.270
r (-)	0.216	0.270	0.324

Step 3: Let set the v_{cric} = 85% as the critical condition for the successive dataset reduction process. Application of PCA to the dataset X produces two sub-datasets X_1 and X_2. Due to space limitation, the PCA plot corresponds to this 1st level of dataset reduction is not shown here. The variables and performance measures that belong to X_1 and X_2 are shown in Table 4.

Table 4. Variables in X_1 and X_2

X_1	ϕ_1, ϕ_2, ϕ_3, S_o, Xv_1, Xv_2, S_1, S_2, rs_2, rp_2, rx_2, R
X_2	Et_1, Et_2, T_1, T_2, L_1, L_2, rx1, rs_1, rp_1, r, Fo

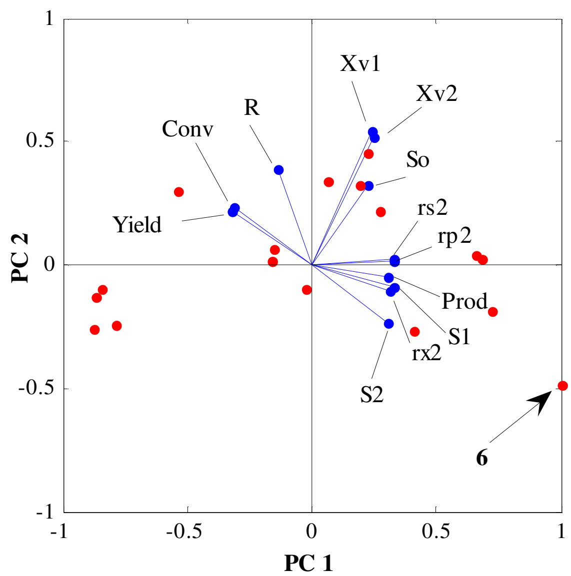

Fig. 4. PCA plot corresponding to X_1 sub-dataset

Notice that, all of the performance measures belong to the X_1 sub-dataset. The sum of variances of the first two principal components is 80%, which is a very high for the 1st level of dataset reduction process. Hence, this shows that the variables in each sub-dataset are strongly interrelated.

Next, another PCA is applied to the X_1 sub-dataset in order to reveal the dominant variables corresponding to the performance measures. Figure 4 shows the PCA plot that corresponds to this 2nd level of dataset reduction on X_1. Note that, the sum of PC-1 and PC-2 is 85%, which is equal to the specified v_{cric}. Thus, the critical level of dataset reduction has been reached and the dominant variables can now be identified.

Both *Yield* and *Conv* occupy the 2nd quadrant and *Prod* occupies the 4th quadrant i.e. they are negatively correlated. The set of dominant variables is {R, S_1, S_2, rx_2}. Note that, the observation #6 is an outlier implying that the DV criteria are completely fulfilled. Because both stages fulfil the DV criteria, thus the SDR condition is also fulfilled which indicates that the analysis is consistent.

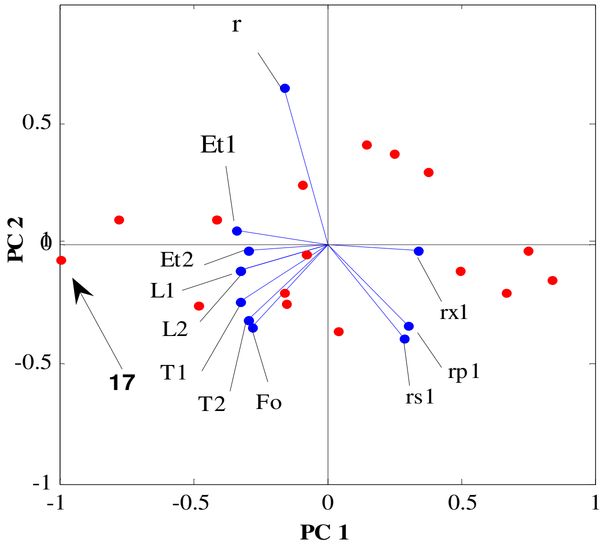

Fig. 5. PCA plot corresponding to X_2 sub-dataset

Step 4: The set of dominant variables consists of only 3 outputs. Because the variables are strongly related, that means we do not need to control all of the 3 variables. It is important to note that, if S_1 is chosen as one of the controlled variable, then one has the advantage of fast dynamic response to disturbance S_o. But in this case however, we select S_2 and rx_2 as the primary controlled variables because they fulfil the first 3 PCV criteria (see Methodology, step 4).

Step 5: Next, the inventory variables are identified. In this case, only 2 inventory variables are considered i.e. $Y_I = \{L_1, L_2\}$. Liquid levels in treatment tank and vacuum flash vessel are not considered because the dynamics of these two units are negligible. Our goal for inventory control is to keep the variations in L_1 and L_2 small so that we can operate closed to the maximum bioreactor volume.

Step 6: Two important constraint control objectives are to ensure that: (1) bioreactor temperatures do not exceed 33°C, and (2) ethanol concentrations do not drift too high above 40 kg/m^3, otherwise the growth and product formation rate will be significantly retarded. The set of variables corresponding to these constraints is $Y_C = \{T_1, T_2, Et_1, Et_2\}$.

Step 7: There are 6 outputs (2 inventory and 4 constraint variables) which should be considered as controlled variables to achieve the inventory and constraint control objectives. Since we already use two manipulated variables for primary control objectives, thus we can afford to control maximum 4 of the variables. Because these 6 variables are closely interrelated, we can afford to control only a few of them. To understand the nature of interaction among these 6 variables, we can also apply the PCA-based method to the sub-dataset containing the variables (i.e. to X_2). Application of PCA to the X_2 sub-dataset reduces it into two smaller sub-datasets X_{21} and X_{22}.

Figure 5 shows the PCA plot corresponding to the dataset reduction on X_2. The sum of variances of PC-1 and PC-2 is 90% implying very strong correlations among the variables in each sub-dataset. Fortunately, 5 out of 6 of the variables are strongly correlated in the X_{21} sub-dataset. Table 5 shows the nominal steady-state values of the inventory and constraint variables.

Table 5. Nominal values of inventory-constraint variables

Et_1 (kg/m^3)	30.6	*Et_2 (kg/m^3)*	41.2
T_1 (°C)	29.9	*T_2 (°C)*	31.0
L_1 (m)	5.2	*L_2 (m)*	4.2

Notice that, it is not likely that Et_1 value will drift too high above 40 kg/m^3 (i.e. its value is quite low). Thus, we can leave this variable out – no need to control it directly. In fermentation process, the temperature plays a very important role in biological activities. Thus, we give higher priority to temperature over the ethanol concentration. The temperature in bioreactor 2 is higher than that in bioreactor 1 i.e. only 2°C from the maximum allowable limit. Hence, we decide to choose T_2 as a constraint controlled variable. Furthermore, because T_2 is strongly coupled with T_1 and Et_2, we decide to control only T_2 to achieve the constraint control objectives overall. We could choose Et_2 as a controlled variable but it is harder to measure the ethanol concentration than the liquid temperature i.e. temperature sensor is also cheap.

As in the case of constraint variables, the inventory variables are also strongly correlated with each other. Hence, we need to control either one of them. From Table 5, we notice that L_1 is higher than L_2. Hence, assuming that both bioreactors have similar size, this means that L_1 is closer to the maximum limit than L_2. Consequently, it is more critical to directly control L_1 than L_2.

In summary our choice of controlled variables to meet the constraint and inventory control objectives are T_2 and L_1 respectively. As L_1 is also correlated with Et_2 and T_1, thus the inventory and constraint controls enhance each other.

Step 8: In total we have 4 controlled variables which are {S_2, rx_2, T_2, L_1}. Out of the 6 inputs which are available for manipulations, we choose (1) fresh substrate flow F_o, (2) cell recycle ratio R, vapor flow F_v, and (4) flow from bioreactor 1 F_1 as the manipulated variables. In this paper, for simplicity the pairings are determined based on the RGA analysis which gives the following loops: (1) R-S_2, (2) F_1-rx_2, (3) F_o-L_1, and (4) F_v-T_2. The PI controllers are used for R-S_2 and F_1-rx_2 and P-only controllers for F_o-L_1 and F_v-T_2 control-loops.

The controller tuning is based on the trial-and-error approach initially with the Ziegler-Nichols tuning formula and followed by detuning to achieve the desired dynamic responses. Lastly, the performance of the partial control design is tested against step changes in S_o with magnitude of 30 kg/m^3 or 25% of its nominal value.

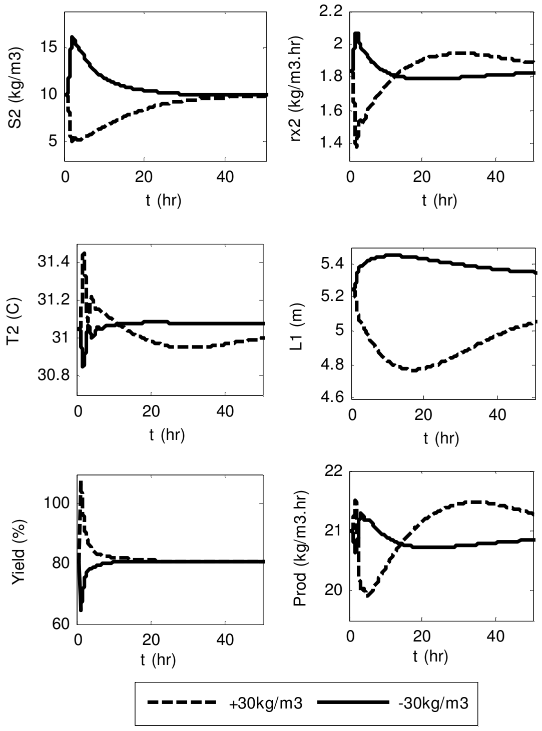

Fig. 6. Dynamic responses to step changes in S_o by ±30kg/m^3

5.3 Results and Discussion

Table 6. Summary of results of controlled variable (CV) and ϕ with step changes in S_o by ±30 kg/m^3

CV	T_2	T_1	Et_2	Et_1	L_2	L_1
Peak	31.5	30.7	43	33	6.5	5.5
ϕ	***Yield***	***Conv***	***Prod***			
$\Delta\phi(\%)$	0.01	0.01	0.35			

Figure 6 shows the dynamic responses of the controlled variables, *Yield* and *Prod* to step changes in fresh substrate concentration (S_o) by ±30 kg/m^3. Table 6 summarizes the constraint and inventory control results.

Notice that the peak value (i.e. during transient response) of the most critical constraint variable T_2 is less than 33^{o}C. Also, the peak value for the Et_2 is about 43 kg/m^3 which is still acceptable. Note that the threshold value of ethanol concentration is 12 %(v/v) or about 94 kg/m^3 beyond which the growth and product formation rates become very low (Minier and Goma, 1982). Thus, the partial control design meets the constraint control objectives. Meanwhile, the peak values of L_1 and L_2 are also acceptable (no snowball) which means that the inventory control objective is also achieved. For the performance measures, their variations (offsets) are *all less* than the maximum allowable limit of 1.0%. Hence, the control strategy achieves the overall operating objective, which is to maintain the performance measures around their optimal trade-off values.

6. CONCLUSION

It is important to note that, while the limited number of manipulated variables necessitates the use of partial control, it is the interaction among the variables that allows such strategy to work in real practice. Without the strong interaction among the variables, it becomes necessary to control more variables in order to achieve the same objectives. Consequently, it is important to understand the nature of interaction among the variables in order to exploit its benefit in partial control design. Luyben (1988) claimed that the approach to minimize the interaction among loops is flawed. What is more important is the structure that can minimize the impact of external disturbance where he proposed eigenstructure concept to address this problem. Essentially the key to identifying this structure lies in the understanding of variable interaction which is the missing link in the concept of eigenstructure. In this manner, the PCA-based method described in this paper serves as a valuable tool not only to understand the variable interaction but also to identify the dominant variables for the overall operating objectives, which are normally implicit in nature.

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