Automated synthesis of control configurations for process networks based on structural coupling

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Abstract

In this paper, a method to systematically synthesize control configurations with favorable structural coupling is developed, using relative degree as a measure of such coupling. Initially, an integer optimization problem is formulated to identify optimal distributions of inputs and outputs (decentralized control configurations) that minimize the overall structural coupling in the network. Then, a hierarchical clustering procedure, which allows identifying groups of inputs and outputs that are strongly connected topologically (block decentralized control configurations), is proposed. The application of the method is illustrated through an example process network.

Keywords: Control structure selection, Plantwide control, Process networks, Integer programming, Hierarchical clustering

1. Introduction

Control structure design, i.e. the selection and pairing of manipulated inputs and controlled outputs, is a classic problem in control that has received a lot of attention in the literature (see e.g. van de Wal and de Jager, 2001). In process control in particular, this problem has been studied extensively in the context of plantwide control design (see e.g. Rangaiah and Kariwala, 2012). Examples include: (a) heuristics-based approaches whereby the selection and pairing are performed following logical rules (e.g. Price and Georgakis, 1993; Ng and Stephanopoulos, 1996; Luyben et al., 1997); (b) the concept of self-optimizing control for selecting controlled outputs

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as the basis for control structure design (e.g. Skogestad, 2000a,b; Baldea et al., 2008); (c) the concept of relative gain array (RGA) (e.g. Chang and Yu, 1990) and block RGA (e.g. Manousiouthakis et al., 1986; Kariwala et al., 2003); and (d) optimization based approaches using for example economic criteria (e.g. Heath et al., 2000; Psaltis et al., 2013; Ellis and Christofides, 2014; Psaltis et al., 2014).

The problem of control structure selection becomes particularly challenging for tightly integrated process networks, which are the rule rather than the exception in modern chemical and energy plants, and also in the context of smart manufacturing (Christofides et al., 2007). Integration results in significant economic benefits, but also limits the available degrees of freedom and leads to significant interactions that need to be addressed in controller design (including the selection of the control configuration). In a series of papers (Kumar and Daoutidis, 2002; Baldea et al., 2006; Jogwar et al., 2009), we have documented that whenever integration results in large rates of recovery and recycle of material and/or energy (compared to the input/output flows), a time-scale hierarchy develops: individual units evolve in a fast time scale (and are affected by the large internal and recycle flows) and slower network-level dynamics emerge (that are affected by the small external flows). This particular feature can be exploited for the selection of manipulated inputs acting in appropriate time scales to address individual process control objectives and network level objectives, in the context of hierarchical control.

However, integrated process networks are not necessarily characterized by a segregation of material and/or energy flows. The design of control systems for such networks is a challenging, open problem, that has been addressed, for example, using passivity-based control (e.g. Ydstie, 2002; Hudon and Bao, 2012; Tippet and Bao, 2013), distributed control (e.g. Rawlings and Stewart, 2008; Liu et al., 2009; Scattolini, 2009) and quasi-decentralized control (e.g. Mhaskar et al., 2007; Sun and El-Farra, 2008). Central to this problem is the pairing of manipulated inputs and controlled outputs, either in the form of single-input single-output controllers or multivariable ones. A promising approach to this end is to exploit the extensive work in network theory and graph theory towards identifying “communities” (of manipulated inputs and controlled outputs, in our case) whose members interact strongly among them, yet are weakly coupled to the rest of the network members (e.g. Girvan and Newman, 2002; Jiang et al., 2007). This community detection problem can be pursued using optimization of clustering parameters that capture the network connectivity (e.g. Newman, 2004, 2006) or through spectral graph theory (e.g. Varigonda et al., 2004). The former approaches are generally more easily scalable to larger networks.

For the pairing of manipulated inputs and controlled outputs, which we will

refer to as the control configuration synthesis problem, a meaningful approach is to seek potential inputs and outputs that are strongly connected topologically. One measure of topological closeness is the concept of relative degree (Daoutidis and Kravaris, 1992). Relative degree essentially captures the directness of the effect of an input on an output, or the physical closeness between the two variables, and can be used to identify input/output clusters with favorable “structural coupling” in the above sense (Daoutidis and Kravaris, 1992; Schné and Hangos, 2011). Its generic calculation requires only structural information on the dynamic interactions in the network, and can be automated on the basis of an equation graph that captures these dynamic interactions.

In this paper, we develop a method to systematically synthesize control configurations with favorable structural coupling, using relative degree as a measure of such coupling. Initially, we formulate an integer optimization problem to identify optimal distributions of inputs and outputs (essentially decentralized control configurations) that minimize the overall structural coupling in the network. We then propose a hierarchical clustering procedure which allows identifying groups of inputs and outputs that are strongly connected topologically, and are thus block decentralized control configuration candidates. The proposed approach is flexible as it allows generating control configurations that span the entire gamut from fully decentralized ones to the fully centralized one. It can also be automated for ease of implementation. Its application is illustrated through a case study on an integrated energy system.

2. Relative degree as a measure of structural coupling

Let us consider a general state space model of the form:

$$\begin{aligned}\dot{x} &= f(x) + \sum_{i=1}^{n_u} g_i(x)u_i \\ y_j &= h_j(x), \quad j = 1, \dots, n_y\end{aligned}\tag{1}$$

where $x \in \mathbb{R}^{n_x}$ denotes the state variables, and $u_i, y_j \in \mathbb{R}$ denote the input variables and the output variables, respectively. f, g_i are vector fields on $\mathbb{R}^{n_x}$, and h_j are scalar fields on $\mathbb{R}^{n_x}$.

The relative degree between u_i and y_j , r_{ij} , is defined as the smallest integer that satisfies (Khalil, 2002):

$$\mathcal{L}_{g_i}\mathcal{L}_f^{r_{ij}-1}h_j(x) \neq 0\tag{2}$$

where $\mathcal{L}$ represents the Lie derivative, defined as:

$$\mathcal{L}_{f(x)}h(x) = \frac{\partial h(x)}{\partial x}f(x)$$

In Daoutidis and Kravaris (1992), it was shown that the relative degree can be interpreted as a measure of how *direct* the effect of an input is on an output, as it represents the number of integrations needed for an input to affect an output. It was also argued that the relative degree can be used as a measure of *physical closeness* between an input and an output as it captures the sluggishness of the input/output response (in effect representing an apparent dead time). Also, it was shown that the generic calculation of relative degree requires only structural information of a process, i.e. knowledge of the interdependencies among the process variables. This can be used to construct an *equation graph* where nodes represent the state, input and output variables, and edges represent the interdependencies among the process variables. Edges are added based on the following rules:

- there is an edge from node x_k to node x_l if $\partial f_l(x)/\partial x_k \neq 0$
- there is an edge from node u_i to node x_l if $g_{il}(x) \neq 0$
- there is an edge from node x_k to node y_j if $\partial h_j(x)/\partial x_k \neq 0$

where $f_l(x)$, $g_{il}(x)$ are the l -th element of $f(x)$, $g_i(x)$, respectively.

In such a graph, a *path* is defined as an open walk of nodes and edges of a graph such that no node is repeated. The *length* of a path is the number of edges contained in the path. An *input-to-output path* (IOP) is a path which starts from an input node and terminates at an output node. The relative degree r_{ij} is then related to the length of the shortest IOP connecting u_i and y_j of the equation graph as follows (Daoutidis and Kravaris, 1992):

$$r_{ij} = l_{ij} - 1 \tag{3}$$

Based on the above, relative degree can be used as a measure of structural coupling, i.e. coupling among the input/output variables based on their structural interdependencies, to provide guidelines for the design and evaluation of multi-loop control configurations. The procedure described in Daoutidis and Kravaris (1992) involves the following steps:

1. Compute the relative degrees between all the inputs and the outputs to form a relative degree matrix (RDM) whose elements are the relative degrees between

the inputs and the outputs:

$$M_r = \begin{bmatrix} r_{11} & \cdots & r_{1n_y} \\ \vdots & \ddots & \vdots \\ r_{n_u1} & \cdots & r_{n_un_y} \end{bmatrix}$$

2. Rearrange the outputs such that the minimum relative degree in each column of the RDM falls on the major diagonal. Then, the diagonal elements of the rearranged RDM represent the relative degrees between the input/output pairs forming the control configuration with a favorable structural coupling. The off-diagonal relative degrees in a row capture the coupling between a specific input and the other outputs, while the off-diagonal relative degrees in a column capture the coupling between a specific output and the other inputs.
3. Evaluate the overall structural coupling for the particular input/output assignment by comparing the diagonal and the off-diagonal relative degrees. Specifically, the differences between off-diagonal and diagonal relative degrees in a row (i.e. $r_{ij} - r_{ii}$) and in a column (i.e. $r_{ji} - r_{ii}$) provide a measure of the overall structural coupling. The larger these differences are, the more favorable the control configuration is.

The above procedure is time consuming to apply to large scale process networks as each step needs to be executed manually. Also, only fully decentralized control configurations are considered. In what follows, we exploit the graph theoretic interpretation of relative degrees to propose a generally applicable and easy to automate framework to synthesize optimal control configurations (ranging from fully decentralized to fully centralized) for process networks.

3. Control configuration synthesis based on structural coupling

In this section, we develop an optimization-based framework to synthesize control configurations based on structural coupling. We define a control configuration synthesis problem as a distribution problem, where the inputs and the outputs are distributed to the controllers. The assumption is that the controllers are square, i.e. the same numbers of inputs and outputs are distributed to each controller. We define the size of a controller as the number of inputs (or outputs) that are distributed to the controller. Initially, we limit the size of all the controllers to 1 (i.e. we consider fully decentralized control configurations only), and formulate an optimization problem to generate such decentralized control configurations so as to minimize the

overall structural coupling between the different loops. Starting from such decentralized control configurations, we then describe the synthesis of block decentralized control configurations by hierarchical clustering of the input/output pairs.

3.1. Synthesis of decentralized control configurations

Let us consider a system with n_u inputs and n_y outputs, and the corresponding RDM, M_r . We assume that we have more inputs than outputs which is typically the case in practical problems (i.e. $n_u > n_y$). For a given input/output assignment, consider the RDM rearranged such that the relative degrees between the chosen input/output pairs fall on the main diagonal. The structural coupling of this configuration can be evaluated using the differences between the diagonal and off-diagonal relative degrees of the first n_y rows of the RDM, and noting that the relative degrees in the remaining $n_u - n_y$ rows do not affect the structural coupling of the system as they represent the relative degrees between the unselected inputs (i.e. the inputs that are not distributed to any controller) and the outputs. The overall structural coupling for the given control configuration can thus be evaluated based on the value of the following term:

$$J_{DC} = \sum_{i=1}^{n_y} \sum_{j=1}^{n_y} (r_{ij} - r_{ii}) \quad (4)$$

The larger the above term is (i.e. the smaller the diagonal relative degrees and the larger the off-diagonal ones), the more favorable the control configuration is.

We note that the relative degrees in a column can be classified into three classes, diagonal ($\mathbf{r}_d$), off-diagonal ($\mathbf{r}_o$) and the remaining ones ($\mathbf{r}_r$). The relative degree r_{ij} is:

- in $\mathbf{r}_d$ if u_i and y_j are distributed to the same controller
- in $\mathbf{r}_r$ if u_i is not distributed to any controller
- in $\mathbf{r}_o$ otherwise

Let us now define two different sets of binary variables that will allow us to capture this classification without rearranging the RDM:

$$p_{ij} = \begin{cases} 1, & \text{if } u_i \text{ is distributed to the same controller with } y_j \\ 0, & \text{otherwise} \end{cases} \quad (5)$$

$$q_i = \begin{cases} 0, & \text{if } u_i \text{ is not distributed to any controller} \\ 1, & \text{otherwise} \end{cases} \quad (6)$$

Note that, by definition, p_{ij} cannot be equal to 1 if q_i is equal to 0, leaving three possible combinations of p_{ij} and q_i , corresponding to the classes of relative degrees defined above:

$$\begin{aligned}\mathbf{r}_d &= \{r_{ij} \in M_r | p_{ij} = 1, q_i = 1\} \\ \mathbf{r}_o &= \{r_{ij} \in M_r | p_{ij} = 0, q_i = 1\} \\ \mathbf{r}_r &= \{r_{ij} \in M_r | p_{ij} = 0, q_i = 0\}\end{aligned}$$

Also note that, for systems with more outputs than inputs, q_j , instead of q_i , can be defined such that q_j is equal to 0 if y_j is not distributed to any controller.

The optimization problem for decentralized control configuration synthesis corresponds to an exhaustive search over all possible input/output distributions such that the term in Eq.(4) is maximized. Using the binary variables defined in Eqs.(5)-(6), this optimization problem can be stated as follows:

$$\text{maximize } J_{DC} = \sum_{i=1}^{n_u} \sum_{j=1}^{n_y} r_{ij} q_i - n_y \sum_{i=1}^{n_u} \sum_{j=1}^{n_y} r_{ij} p_{ij} \quad (7)$$

where the first and the second terms of the objective function represent the corresponding terms in Eq.(4), and the decision variables are p_{ij} and q_i . We now describe a set of constraints to complete the problem.

The number of input/output pairs needs to be equal to the number of outputs to ensure that all the outputs are distributed to a controller:

$$\sum_{i,j} p_{ij} = n_y \quad (8)$$

The following set of constraints states that any input or output can be distributed to one controller at most:

$$\sum_j p_{ij} \leq 1 \quad \forall i \quad (9)$$

$$\sum_i p_{ij} \leq 1 \quad \forall j \quad (10)$$

Finally, since any input u_i can be distributed to at most one output y_i :

$$q_i \leq \sum_j p_{ij} \quad \forall i \quad (11)$$

This formulation (Eqs.(7)-(11)) corresponds to a bipartite matching problem Leiserson et al. (2001), where a set of variables is divided into two disjoint subsets (in this case, the set of inputs and the set of outputs), and the variables from each set are matched so as to minimize/maximize the objective function. For such a problem, the existence of a global optimum is guaranteed, although in general there does not exist a unique solution (Leiserson et al., 2001). This optimization problem can be solved within the environment of GAMS using the CPLEX Optimizer (IBM, 2011). We can also find alternative solutions with the same objective value by excluding the optimal solutions that have been already found and resolving the optimization problem.

The output of the optimization problem is the $n_u \times n_y$ matrix P_{opt} whose i, j -th element is p_{ij} . Note that P_{opt} is a variant of a permutation matrix whose i -th row sum is 1 if u_i is distributed to a controller, and 0 otherwise. Using P_{opt} , we can obtain the *optimal* RDM ($n_y \times n_y$), $M_{r,opt}$, as:

$$M_{r,opt} = P_{opt}^T M_r \quad (12)$$

Note that, by premultiplying M_r by P_{opt}^T , we eliminate the $n_u - n_y$ rows of M_r , whose elements represent the relative degrees between the unselected inputs and the outputs, while rearranging the remaining n_y rows with respect to the optimal decentralized control configuration.

Example. For a simple illustration, let us consider a continuous stirred tank reactor (CSTR) shown in Figure 1. Feed streams of A and B with molar flow rates F_A , F_B , temperatures T_A , T_B , and concentrations c_{A0} , c_{B0} , respectively, are fed to the reactor, where a reaction $A + B \rightarrow C + D$ occurs, to produce a product stream with molar flow rate F , temperature T , and concentrations c_A , c_B , c_C , c_D . We assume that the reaction is endothermic, and heat is supplied to the reactor at a rate Q to facilitate the reaction.

Assuming constant density ρ and heat capacity C_p , the energy/material balances

of the system can be described by the following equations:

$$\begin{aligned}
\frac{dM}{dt} &= F_A + F_B - F \\
\frac{dc_A}{dt} &= \frac{F_A}{M}(c_{A0} - c_A) - \frac{F_B}{M}c_A - k c_A c_B \exp\left(\frac{-E}{RT}\right) \\
\frac{dc_B}{dt} &= \frac{F_B}{M}(c_{B0} - c_B) - \frac{F_A}{M}c_B - k c_A c_B \exp\left(\frac{-E}{RT}\right) \\
\frac{dc_C}{dt} &= -\frac{F_A + F_B}{M}c_C + k c_A c_B \exp\left(\frac{-E}{RT}\right) \\
\frac{dT}{dt} &= \frac{F_A}{M}(T_A - T) + \frac{F_B}{M}(T_B - T) + \frac{Q}{MC_p} - \frac{\Delta H}{\rho C_p} k c_A c_B \exp\left(\frac{-E}{RT}\right)
\end{aligned}$$

where M is the molar holdup of the reactor, and k and E are the rate constant and the activation energy of the reaction. ΔH represents the heat of reaction.

We define the following sets of the inputs and the outputs:

$$\begin{aligned}
\mathbf{u} &= \{F_A, F_B, F, Q\} \\
\mathbf{y} &= \{M, c_A, c_C, T\}
\end{aligned}$$

Then, the equation graph of the system can be obtained as shown in Figure 2. The RDM of the system can be computed as follows:

$$M_r = \begin{matrix} & M & c_A & c_C & T \\ \begin{matrix} F_A \\ F_B \\ F \\ Q \end{matrix} & \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ \infty & 2 & 2 & 1 \end{bmatrix} \end{matrix}$$

and the shortest IOPs between all input/output pairs are provided in Table 1.

By solving the optimization problem defined by Eqs.(7)-(11), we get two optimal solutions as follows:

$$\begin{aligned}
P_{opt,1} &= \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
P_{opt,2} &= \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}
\end{aligned}$$

which translate into the following optimal RDMs:

$$\begin{aligned}
M_{r,opt,1} &= \begin{array}{c} \\ F \\ F_B \\ F_A \\ Q \end{array} \begin{array}{c} M \quad c_A \quad c_C \quad T \\ \left[\begin{array}{cccc} 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \infty & 2 & 2 & 1 \end{array} \right] \end{array} \\
M_{r,opt,2} &= \begin{array}{c} \\ F \\ F_A \\ F_B \\ Q \end{array} \begin{array}{c} M \quad c_A \quad c_C \quad T \\ \left[\begin{array}{cccc} 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \infty & 2 & 2 & 1 \end{array} \right] \end{array}
\end{aligned}$$

In both control configurations, the molar holdup and the temperature of the reactor is controlled by manipulating the outlet flowrate and the heat input rate, respectively. The flowrates of the feed streams of A and B are respectively manipulated to control the concentrations of C and A of the outlet stream in the control configuration given by $M_{r,opt,1}$, and to control the concentrations of A and C of the outlet stream in the control configuration given by $M_{r,opt,2}$.

3.2. Hierarchical clustering of input/output pairs

In this subsection, we propose a systematic way to cluster the input/output pairs hierarchically, by considering the structural coupling between different input/output *pairs* (rather than simply inputs and outputs). The goal is to generate a hierarchy of block decentralized control configurations with increasing controller sizes, whereby in each level we form clusters of input/output pairs which are structurally close in a sense that will be made precise shortly. The result of clustering can be visualized as a dendrogram where each level of the dendrogram represents a block decentralized control configuration.

Let us consider the following optimal RDM obtained as a solution to the optimization problem discussed above (in the case of multiple optimal solutions, each

one can be considered separately):

$$M_{r,opt} = \begin{matrix} & y_1 & \cdots & y_i & \cdots & y_j & \cdots & y_{n_y} \\ \begin{matrix} u_1 \\ \vdots \\ u_i \\ \vdots \\ u_j \\ \vdots \\ u_{n_y} \end{matrix} & \begin{bmatrix} r_{11} & \cdots & r_{1i} & \cdots & r_{1j} & \cdots & r_{1n_y} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ r_{i1} & \cdots & r_{ii} & \cdots & r_{ij} & \cdots & r_{in_y} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \\ r_{j1} & \cdots & r_{ji} & \cdots & r_{jj} & \cdots & r_{jn_y} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \\ r_{n_y1} & \cdots & r_{n_yi} & \cdots & r_{n_yj} & \cdots & r_{n_yn_y} \end{bmatrix} \end{matrix} \quad (13)$$

Two input/output pairs, $\{u_i, y_i\}$ and $\{u_j, y_j\}$, will be structurally close if the inputs u_i, u_j have comparable structural effect on the outputs y_i, y_j , i.e. the values of the off-diagonal relative degrees r_{ij} and r_{ji} are close to the values of the diagonal relative degrees r_{ii} and r_{jj} . Motivated by this, we define a distance between the two input/output pairs as the sum of the *largest* differences between the off-diagonal and diagonal relative degrees:

$$\begin{aligned} d(\{u_i, y_i\}, \{u_j, y_j\}) &= (\max\{r_{ij}, r_{ji}\} - r_{ii}) + (\max\{r_{ij}, r_{ji}\} - r_{jj}) \\ &= 2\max\{r_{ij}, r_{ji}\} - r_{ii} - r_{jj} \end{aligned} \quad (14)$$

Proposition 3.1. *The distance defined in Eq.(14) is a pseudo-semi-metric (Kunen and Vaughan, 1984), satisfying the following properties:*

$$\begin{aligned} d(\{u_i, y_i\}, \{u_j, y_j\}) &\geq 0 \\ d(\{u_i, y_i\}, \{u_i, y_i\}) &= 0 \\ d(\{u_i, y_i\}, \{u_j, y_j\}) &= d(\{u_j, y_j\}, \{u_i, y_i\}) \end{aligned}$$

Proof. The objective function value computed from the above optimal RDM is:

$$\begin{aligned} J_{DC,opt} &= \sum_{k=1}^{n_y} \sum_{l=1}^{n_y} (r_{kl} - r_{ll}) \\ &= [(r_{11} - r_{11}) + \cdots + (r_{1i} - r_{11}) + \cdots + (r_{1j} - r_{11}) + \cdots + (r_{1n_y} - r_{11})] + \cdots \\ &\quad + [(r_{i1} - r_{ii}) + \cdots + (r_{ii} - r_{ii}) + \cdots + (r_{ij} - r_{ii}) + \cdots + (r_{in_y} - r_{ii})] + \cdots \\ &\quad + [(r_{j1} - r_{jj}) + \cdots + (r_{ji} - r_{jj}) + \cdots + (r_{jj} - r_{jj}) + \cdots + (r_{jn_y} - r_{jj})] + \cdots \\ &\quad + [(r_{n_y1} - r_{n_yn_y}) + \cdots + (r_{n_yi} - r_{n_yn_y}) + \cdots + (r_{n_yj} - r_{n_yn_y}) + \cdots + (r_{n_yn_y} - r_{n_yn_y})] \end{aligned}$$

Let us swap the i, j -th rows to get the following RDM:

$$M'_r = \begin{matrix} & y_1 & \cdots & y_i & \cdots & y_j & \cdots & y_{n_y} \\ \begin{matrix} u_1 \\ \vdots \\ u_j \\ \vdots \\ u_i \\ \vdots \\ u_{n_y} \end{matrix} & \left[\begin{array}{cccccc} r_{11} & \cdots & r_{1i} & \cdots & r_{1j} & \cdots & r_{1n_y} \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ r_{j1} & \cdots & r_{ji} & \cdots & r_{jj} & \cdots & r_{jn_y} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \\ r_{i1} & \cdots & r_{ii} & \cdots & r_{ij} & \cdots & r_{in_y} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots \\ r_{n_y1} & \cdots & r_{n_yi} & \cdots & r_{n_yj} & \cdots & r_{n_yn_y} \end{array} \right] \end{matrix}$$

The objective function value computed from the above RDM is:

$$\begin{aligned} J'_{DC} = & [(r_{11} - r_{11}) + \cdots + (r_{1i} - r_{11}) + \cdots + (r_{1j} - r_{11}) + \cdots + (r_{1n_y} - r_{11})] + \cdots \\ & + [(r_{j1} - r_{ji}) + \cdots + (r_{ji} - r_{ji}) + \cdots + (r_{jj} - r_{ji}) + \cdots + (r_{jn_y} - r_{ji})] + \cdots \\ & + [(r_{i1} - r_{ij}) + \cdots + (r_{ii} - r_{ij}) + \cdots + (r_{ij} - r_{ij}) + \cdots + (r_{in_y} - r_{ij})] + \cdots \\ & + [(r_{n_y1} - r_{n_yn_y}) + \cdots + (r_{n_yi} - r_{n_yn_y}) + \cdots + (r_{n_yj} - r_{n_yn_y}) + \cdots + (r_{n_yn_y} - r_{n_yn_y})] \end{aligned}$$

The difference between the objective function values is:

$$\begin{aligned} J_{DC,opt} - J'_{DC} = & [(r_{i1} - r_{ii}) + \cdots + (r_{ii} - r_{ii}) + \cdots + (r_{ij} - r_{ii}) + \cdots + (r_{in_y} - r_{ii}) \\ & + (r_{j1} - r_{jj}) + \cdots + (r_{ji} - r_{jj}) + \cdots + (r_{jj} - r_{jj}) + \cdots + (r_{jn_y} - r_{jj})] \\ & - [(r_{j1} - r_{ji}) + \cdots + (r_{ji} - r_{ji}) + \cdots + (r_{jj} - r_{ji}) + \cdots + (r_{jn_y} - r_{ji}) \\ & + (r_{i1} - r_{ij}) + \cdots + (r_{ii} - r_{ij}) + \cdots + (r_{ij} - r_{ij}) + \cdots + (r_{in_y} - r_{ij})] \\ = & n(r_{ij} + r_{ji} - r_{ii} - r_{jj}) \end{aligned}$$

Recall that $M_{r,opt}$ is the optimal RDM, implying that the above difference should be greater than or equal to 0, i.e.:

$$n(r_{ij} + r_{ji} - r_{ii} - r_{jj}) \geq 0$$

Then,

$$d(\{u_i, y_i\}, \{u_j, y_j\}) = 2\max\{r_{ij}, r_{ji}\} - r_{ii} - r_{jj} \geq r_{ij} + r_{ji} - r_{ii} - r_{jj} \geq 0$$

The second and third properties can be shown easily from Eq.(14). $\square$

The main idea behind the proposed clustering procedure is to identify the input/output pairs that are structurally close (i.e. have a small distance) and merge them to form a cluster of input/output pairs that will form a new controller block in a block decentralized configuration. At each level of clustering, the number of controllers is decreased by 1 (although more general formulations are possible), and the clustering procedure stops when there is only one controller (i.e. when we have fully centralized control configuration).

Let us first consider the merging of individual input/output pairs. Note that there is always the possibility that there can be multiple pairs with identical distance. Let us consider the following example RDM:

$$M_{ex} = \begin{array}{c} \begin{array}{ccc} & y_1 & y_2 & y_3 \\ \begin{array}{c} u_1 \\ u_2 \\ u_3 \end{array} & \begin{bmatrix} 1 & 5 & 5 \\ 4 & 3 & 6 \\ 3 & 4 & 3 \end{bmatrix} \end{array} \end{array} \quad (15)$$

Note that $d(\{u_1, y_1\}, \{u_2, y_2\}) = d(\{u_2, y_2\}, \{u_3, y_3\}) = d(\{u_1, y_1\}, \{u_3, y_3\}) = 6$, i.e. all three input/output pairs are equally spaced in terms of the distance defined in Eq.(14). However, different pairs of input/output pairs (e.g. $\{u_1, y_1\}/\{u_2, y_2\}$ and $\{u_1, y_1\}/\{u_3, y_3\}$) have different structural coupling. In such a case, we need to impose additional criteria to determine the input/output pairs to be merged. A natural first such criterion is to use the sum of the *smallest* differences between off-diagonal and diagonal relative degrees, i.e.:

$$\delta(\{u_i, y_i\}, \{u_j, y_j\}) = 2\min\{r_{ij}, r_{ji}\} - r_{ii} - r_{jj} \quad (16)$$

Additionally, we could use the actual values of the off-diagonal elements to further discriminate between different pairs of input/output pairs. To this end, we define:

$$\Delta(\{u_i, y_i\}, \{u_j, y_j\}) = \max\{r_{ij}, r_{ji}\} \quad (17)$$

We can now define the distance matrices, D_d , D_δ and D_Δ , whose i, j -th elements are $d(\{u_i, y_i\}, \{u_j, y_j\})$, $\delta(\{u_i, y_i\}, \{u_j, y_j\})$ and $\Delta(\{u_i, y_i\}, \{u_j, y_j\})$, respectively. We can also define a *distance triplet* as (d, δ, Δ) . For the example in Eq.(15), D_d , D_δ

and D_Δ take the form:

$$\begin{aligned}
D_d &= \begin{matrix} & \{u_1, y_1\} & \{u_2, y_2\} & \{u_3, y_3\} \\ \begin{matrix} \{u_1, y_1\} \\ \{u_2, y_2\} \\ \{u_3, y_3\} \end{matrix} & \begin{bmatrix} 0 & 6 & 6 \\ 6 & 0 & 6 \\ 6 & 6 & 0 \end{bmatrix} \end{matrix} \\
D_\delta &= \begin{matrix} & \{u_1, y_1\} & \{u_2, y_2\} & \{u_3, y_3\} \\ \begin{matrix} \{u_1, y_1\} \\ \{u_2, y_2\} \\ \{u_3, y_3\} \end{matrix} & \begin{bmatrix} 0 & 4 & 2 \\ 4 & 0 & 2 \\ 2 & 2 & 0 \end{bmatrix} \end{matrix} \\
D_\Delta &= \begin{matrix} & \{u_1, y_1\} & \{u_2, y_2\} & \{u_3, y_3\} \\ \begin{matrix} \{u_1, y_1\} \\ \{u_2, y_2\} \\ \{u_3, y_3\} \end{matrix} & \begin{bmatrix} 0 & 5 & 5 \\ 5 & 0 & 6 \\ 5 & 6 & 0 \end{bmatrix} \end{matrix}
\end{aligned}$$

Note that $\delta(\{u_1, y_1\}, \{u_2, y_2\}) > \delta(\{u_2, y_2\}, \{u_3, y_3\}) = \delta(\{u_1, y_1\}, \{u_3, y_3\})$. Furthermore, $\Delta(\{u_2, y_2\}, \{u_3, y_3\}) > \Delta(\{u_1, y_1\}, \{u_3, y_3\})$. Based on these criteria, $\{u_1, y_1\}$ and $\{u_3, y_3\}$, with the distance triplet of (6,2,5), are the input/output pairs to be merged into a cluster.

We can now proceed to discuss the merging of input/output clusters. Let us consider the set of all optimal input/output pairs, $IO_i = \{u_i, y_i\}$, and denote it as IO . Any subset of this set will be an input/output cluster, and be denoted by $C(A)$ where A is the set of indices of the input/output pairs in the cluster (e.g. $C(\{k, l, m\}) = \{IO_k, IO_l, IO_m\}$). Note that a single input/output pair can be considered as a (trivial) cluster by itself (e.g. $C(\{k\}) = \{IO_k\}$). The closeness between input/output clusters can be assessed through an exhaustive search over all possible pairs of input/output pairs from the two clusters, such that their distance is maximized. This leads naturally to the following definition of the distance between clusters $C(A)$ and $C(A')$:

$$d(C(A), C(A')) = \max\{d(IO_k, IO_l) | k \in A, l \in A'\} \quad (18)$$

Note that, in this case too, there is the possibility that there can be multiple pairs of input/output clusters with the same distance. These can be further discriminated using the criteria that we defined previously. Specifically, we can define:

$$\delta(C(A), C(A')) = \delta(IO_k, IO_l) \quad (19)$$

$$\Delta(C(A), C(A')) = \Delta(IO_k, IO_l) \quad (20)$$

where IO_k, IO_l are the input/output pairs identified in Eq.(18). The corresponding distance matrices, D_d, D_δ and D_Δ , can then be formed at each step of the procedure and used to determine the clusters to be merged.

For the example in Eq.(15), the distances d, δ and Δ between the newly formed cluster, $C(\{1, 3\})$, and $C(\{2\})$ can be evaluated yielding the following distance matrices:

$$\begin{aligned}
D_d^{(1)} &= \begin{matrix} & C(\{1, 3\}) & C(\{2\}) \\ \begin{matrix} C(\{1, 3\}) \\ C(\{2\}) \end{matrix} & \begin{bmatrix} 0 & 6 \\ 6 & 0 \end{bmatrix} \end{matrix} \\
D_\delta^{(1)} &= \begin{matrix} & C(\{1, 3\}) & C(\{2\}) \\ \begin{matrix} C(\{1, 3\}) \\ C(\{2\}) \end{matrix} & \begin{bmatrix} 0 & 4 \\ 4 & 0 \end{bmatrix} \end{matrix} \\
D_\Delta^{(1)} &= \begin{matrix} & C(\{1, 3\}) & C(\{2\}) \\ \begin{matrix} C(\{1, 3\}) \\ C(\{2\}) \end{matrix} & \begin{bmatrix} 0 & 5 \\ 5 & 0 \end{bmatrix} \end{matrix}
\end{aligned}$$

where the superscript represents the number of updates in the calculation of the distance matrices or equivalently the number of mergings implemented. Note that at the i -th update, the distance matrices are of dimension $(n_y - i) \times (n_y - i)$, i.e. they contain $n_y - i$ clusters.

The procedure for hierarchical clustering of the input/output pairs described above can be summarized and generalized as follows:

1. At each level of clustering (including the initial optimal decentralized configurations), compute the distance matrices, D_d, D_δ and D_Δ .
2. Find the smallest off-diagonal value in D_d (i.e. the shortest distance between distinct input/output clusters). If there exist multiple pairs of input/output clusters with the smallest value, compare the following values in order:
 - (a) δ
 - (b) Δ
Choose the pair with the smallest distance triplet values and merge the clusters to form a new cluster.
3. Repeat steps 1 and 2. Terminate when a single cluster is formed.

Remark 3.1. There is the possibility that there can be multiple pairs of the input/output clusters with the same distance triplet values. In such case, each choice

can be considered separately, proceeding to the subsequent levels to complete the clustering. Multiple dendrograms will be generated to summarize the results in this case.

Example (continued). Let us consider one of the optimal RDMs obtained for the CSTR example:

$$M_{r,opt,1} = \begin{array}{c} F \\ F_B \\ F_A \\ Q \end{array} \begin{array}{c} M \quad c_A \quad c_C \quad T \\ \left[\begin{array}{cccc} 1 & 2 & 2 & 2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ \infty & 2 & 2 & 1 \end{array} \right] \end{array}$$

The initial input/output clusters are formed as follows:

$$\begin{aligned} C(\{1\}) &= \{IO_1\} = \{F, M\} \\ C(\{2\}) &= \{IO_2\} = \{F_B, c_A\} \\ C(\{3\}) &= \{IO_3\} = \{F_A, c_B\} \\ C(\{4\}) &= \{IO_4\} = \{Q, T\} \end{aligned}$$

The corresponding distance matrices are:

$$\begin{aligned}
D_d &= \begin{array}{c} C(\{1\}) \\ C(\{2\}) \\ C(\{3\}) \\ C(\{4\}) \end{array} \begin{array}{c} C(\{1\}) \quad C(\{2\}) \quad C(\{3\}) \quad C(\{4\}) \\ \left[\begin{array}{cccc} 0 & 2 & 2 & \infty \\ 2 & 0 & 0 & 2 \\ 2 & 0 & 0 & 2 \\ \infty & 2 & 2 & 0 \end{array} \right] \end{array} \\
D_\delta &= \begin{array}{c} C(\{1\}) \\ C(\{2\}) \\ C(\{3\}) \\ C(\{4\}) \end{array} \begin{array}{c} C(\{1\}) \quad C(\{2\}) \quad C(\{3\}) \quad C(\{4\}) \\ \left[\begin{array}{cccc} 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \end{array} \right] \end{array} \\
D_\Delta &= \begin{array}{c} C(\{1\}) \\ C(\{2\}) \\ C(\{3\}) \\ C(\{4\}) \end{array} \begin{array}{c} C(\{1\}) \quad C(\{2\}) \quad C(\{3\}) \quad C(\{4\}) \\ \left[\begin{array}{cccc} 0 & 2 & 2 & \infty \\ 2 & 0 & 1 & 2 \\ 2 & 1 & 0 & 2 \\ \infty & 2 & 2 & 0 \end{array} \right] \end{array}
\end{aligned}$$

The smallest off-diagonal element in D_d is $D_d(2, 3) = D_d(3, 2) = 0$. Thus, we merge $C(\{2\})$ and $C(\{3\})$ to form a new cluster $C(\{2, 3\})$. The updated distance

matrices are:

$$\begin{aligned}
D_d^{(1)} &= \begin{array}{c} C(\{1\}) \\ C(\{2,3\}) \\ C(\{4\}) \end{array} \begin{array}{ccc} C(\{1\}) & C(\{2,3\}) & C(\{4\}) \\ \left[\begin{array}{ccc} 0 & 2 & \infty \\ 2 & 0 & 2 \\ \infty & 2 & 0 \end{array} \right] \end{array} \\
D_\delta^{(1)} &= \begin{array}{c} C(\{1\}) \\ C(\{2,3\}) \\ C(\{4\}) \end{array} \begin{array}{ccc} C(\{1\}) & C(\{2,3\}) & C(\{4\}) \\ \left[\begin{array}{ccc} 0 & 0 & 2 \\ 0 & 0 & 0 \\ 2 & 0 & 0 \end{array} \right] \end{array} \\
D_\Delta^{(1)} &= \begin{array}{c} C(\{1\}) \\ C(\{2,3\}) \\ C(\{4\}) \end{array} \begin{array}{ccc} C(\{1\}) & C(\{2,3\}) & C(\{4\}) \\ \left[\begin{array}{ccc} 0 & 2 & \infty \\ 2 & 0 & 2 \\ \infty & 2 & 0 \end{array} \right] \end{array}
\end{aligned}$$

The distance triplets between $C(\{1\})$ and $C(\{2,3\})$ and between $C(\{2,3\})$ and $C(\{4\})$ are equal to $(2,0,2)$. Therefore, we can choose to merge either, and the results can be summarized as dendrograms shown in Figure 3, along with the distance triplet values between the clusters to be merged at each level of the dendrogram. Note that these triplets are identical for both dendrograms, indicating similar coupling characteristics. We can now draw a horizontal line at any height to cut the dendrogram, resulting in a block decentralized control configuration. The number of intersections between the horizontal line and the vertical lines represent the number of controllers. For example, the dendrogram shown in Figure 3(a) can be cut at a height between $(2,1,2)$ and $(\infty,2,2)$, to generate a block decentralized control configuration with IO_1, IO_2, IO_3 assigned to one controller, and IO_4 assigned to the other. Note that such a control configuration is reasonable since the first controller addresses the control of material balance variables, while the energy balance variable is assigned to the other controller.

Remark 3.2. In the case of multiple dendrograms, the distance triplet values at each level are not always the same for all the dendrograms. Different dendrograms can be evaluated noting that larger distance triplet values imply more weakly coupled block decentralized control configurations.

3.3. Algorithm for automation of synthesis procedure

The proposed framework can be automated using the algorithm provided below.

Algorithm: *AutomatedControlConfigurationSynthesis*

```

1:  $\mathcal{EG} = \text{ConstructEquationGraph}$ 
2:  $[M_r, SIOP] = \text{Floyd-Warshall}(\mathcal{EG})$ 
3:  $[J_{DC,opt}, P_{opt}] = \text{DesignDC}(M_r)$ 
4: Add  $P_{opt}$  to ODC
5:  $P'_{opt} = P_{opt}$ 
6: while  $J_{DC} = J_{DC,opt}$  do
7:   Exclude  $P'_{opt}$ 
8:    $[J_{DC}, P'_{opt}] = \text{DesignDC}(M_r)$ 
9:   if  $J_{DC} = J_{DC,opt}$  then
10:    Add  $P'_{opt}$  to ODC
11:   end if
12: end while
13: for  $i = 1$  to  $\text{Size}(\text{ODC})$  do
14:    $M_{r,opt} = \text{ODC}[i]^T M_r$ 
15:   HC =  $\text{HierarchicalClustering}(M_{r,opt})$ 
16:   Add HC to DEND
17: end for
18: return ODC, DEND

```

The input to the algorithm is the equations which describe the dynamic behavior of the energy/material balances variables. By default, the material/energy flow rates are marked as the manipulated inputs, and the molar holdups, temperatures and concentrations of the process units are marked as the controlled outputs. An additional input can be provided to the algorithm to define specific sets of manipulated inputs and controlled outputs. The outputs of the algorithm are the optimal decentralized control configurations, and the dendrograms.

The subroutine *ConstructEquationGraph* configures the equation graph of the given network, $\mathcal{EG}$, from the input. The RDM of the network (M_r), and the shortest IOPs between all input/output pairs (SIOP) are computed using the Floyd-Warshall algorithm (Leiserson et al., 2001). The Floyd-Warshall algorithm initially sets the length of the path between different nodes to 1 if the nodes are directly connected, otherwise to a very large finite integer, which, in our case, is chosen to be 10001, so that the relative degree of 10^4 represents a relative degree of infinity.

The subroutine *DesignDC* computes the optimal objective function value, $J_{DC,opt}$, and P_{opt} by solving the optimization problem defined by Eqs.(7)-(11). P_{opt} is added to

ODC , the set of optimal decentralized control configurations. The *while* loop is added to find the alternative solutions. Then, for each configuration in ODC , hierarchy of input/output clusters HC , which is built in a form of dendrogram, is generated using the subroutine *HierarchicalClustering* which automates the procedure proposed in the previous section. HC is added to $DEND$, the set of dendrograms.

In what follows, we illustrate the application of the above algorithm using an example process network.

4. Case study – energy integrated solid oxide fuel cell (SOFC) system

4.1. Process description

Let us consider the energy integrated SOFC system with an external reformer proposed in Georgis et al. (2011). The process flow diagram of the system is shown in Figure 4. In this system, the feed stream of water is vaporized in HE1 and HE2, and it is mixed with the methane stream which is preheated in HE7. Then, the fuel mixture is heated in HE3 before entering the steam reformer to facilitate the following reactions:

The outlet of the steam reformer is heated in HE5, and supplied into the anode of the fuel cell. The air feed stream is heated in HE4 and HE6, then fed into the cathode of the fuel cell. In the fuel cell, electrochemical potential is generated through the following redox reactions:

Both the outlet streams of the fuel cell are then fed into the catalytic burner where methane, carbon monoxide and hydrogen are completely combusted. The outlet stream of the catalytic burner, which is at high temperature, provides energy to the stream reformer and the feed streams as it passes through the jacket of the stream reformer and the heat exchangers.

Important control objectives for this system are:

- control the temperature of the fuel cell (y_1) to prevent material damages while sustaining the ioninc conductivity of the electrolyte

- control the fuel utilization of the fuel cell (y_2) to ensure efficient usage of fuel while preventing fuel starvation
- control the fuel cell air inlet temperature (y_3) to enhance the operation of the fuel cell
- control the conversion of the steam reformer (y_4) to generate hydrogen-rich stream
- control the inlet temperature of the steam reformer (y_5) to facilitate the reactions

Also, we have the following potential manipulated inputs:

- the flow rate of air stream entering the fuel cell (u_1)
- the flow rate of fuel stream entering the fuel cell (u_2)
- the duty of HE6
- the jacket flow rate of the steam reformer (u_4)
- the duty of HE3

Since the duty of heat exchangers cannot be manipulated directly, the bypass ratio around the hot channel of HE6 (u_3) and the bypass ratio around the hot channel of HE3 (u_5) will be used as manipulated inputs.

4.2. Automated synthesis of control configurations

Let us now apply the developed graph-theoretic framework to this energy integrated SOFC system. The original equation graph consists of 224 nodes and 529 edges, and for brevity, only a part of the original equation graph, which contains the nodes for the inputs and the outputs mentioned previously, and the nodes for the state variables that are included in the IOPs, is shown in Figure 5. Table 2 shows the list of the nodes in this graph. The RDM is obtained as:

$$M_r = \begin{matrix} & y_1 & y_2 & y_3 & y_4 & y_5 \\ \begin{matrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{matrix} & \begin{bmatrix} 1 & 1 & 2 & 7 & 7 \\ 1 & 1 & 4 & 6 & 6 \\ 3 & 4 & 2 & 5 & 5 \\ 4 & 5 & 5 & 3 & 3 \\ 5 & 6 & 4 & 4 & 2 \end{bmatrix} \end{matrix}$$

Two optimal solutions are returned by the algorithm:

$$P_{opt,1} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$P_{opt,2} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

which translate into the following optimal RDMs:

$$M_{r,opt,1} = \begin{array}{c} \begin{matrix} & y_1 & y_2 & y_3 & y_4 & y_5 \end{matrix} \\ \begin{matrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{matrix} \begin{bmatrix} 1 & 1 & 2 & 7 & 7 \\ 1 & 1 & 4 & 6 & 6 \\ 3 & 4 & 2 & 5 & 5 \\ 4 & 5 & 5 & 3 & 3 \\ 5 & 6 & 4 & 4 & 2 \end{bmatrix} \end{array}$$

$$M_{r,opt,2} = \begin{array}{c} \begin{matrix} & y_1 & y_2 & y_3 & y_4 & y_5 \end{matrix} \\ \begin{matrix} u_2 \\ u_1 \\ u_3 \\ u_4 \\ u_5 \end{matrix} \begin{bmatrix} 1 & 1 & 4 & 6 & 6 \\ 1 & 1 & 2 & 7 & 7 \\ 3 & 4 & 2 & 5 & 5 \\ 4 & 5 & 5 & 3 & 3 \\ 5 & 6 & 4 & 4 & 2 \end{bmatrix} \end{array}$$

From both solutions, we note that, for each row, the diagonal element has the smallest value, implying that each input is paired with the output that it has the most direct effect on. The process flow diagram with the control loops determined by $P_{opt,1}$ is shown in Figure 6. In this configuration, the temperature and the fuel utilization of the fuel cell are controlled by manipulating the flow rates of the air and fuel inlet stream, respectively, and the air inlet temperature is controlled by manipulating the bypass ratio around the hot channel of HE6. The jacket flow rate of the steam reformer and the bypass ratio around the hot channel of HE3 are manipulated to control the conversion and the inlet temperature of the steam reformer. Note that

this control configuration matches the control strategy proposed and evaluated via simulations in Georgis et al. (2011). By switching the manipulated inputs which are used to control the temperature and the fuel utilization of the fuel cell in the previous configuration, we get the control configuration determined by $P_{opt,2}$. This change is reasonable since u_1 and u_2 have the same structural effect on y_1 and y_2 (i.e. $M_r(1,1) = M_r(1,2) = M_r(2,1) = M_r(2,2) = 1$).

For the control configuration determined by $P_{opt,1}$, we have the following initial clusters:

$$\begin{aligned} C(\{1\}) &= IO_1 = \{u_1, y_1\} \\ C(\{2\}) &= IO_2 = \{u_2, y_2\} \\ C(\{3\}) &= IO_3 = \{u_3, y_3\} \\ C(\{4\}) &= IO_4 = \{u_4, y_4\} \\ C(\{5\}) &= IO_5 = \{u_5, y_5\} \end{aligned}$$

and the distance matrix D_d :

$$D_d = \begin{array}{c} \begin{matrix} C(\{1\}) \\ C(\{2\}) \\ C(\{3\}) \\ C(\{4\}) \\ C(\{5\}) \end{matrix} \end{array} \begin{array}{ccccc} C(\{1\}) & C(\{2\}) & C(\{3\}) & C(\{4\}) & C(\{5\}) \\ \left[\begin{array}{ccccc} 0 & 0 & 3 & 10 & 11 \\ 0 & 0 & 5 & 8 & 9 \\ 3 & 5 & 0 & 5 & 6 \\ 10 & 8 & 5 & 0 & 3 \\ 11 & 9 & 6 & 3 & 0 \end{array} \right] \end{array}$$

Note that there is only one pair of clusters with the shortest distance ($C(1)$ and $C(2)$), thus the additional criteria are not required at this level. $C(\{1\})$ and $C(\{2\})$ are the clusters to be merged, and D_d is updated accordingly:

$$D^{(1)} = \begin{array}{c} \begin{matrix} C(\{1,2\}) \\ C(\{3\}) \\ C(\{4\}) \\ C(\{5\}) \end{matrix} \end{array} \begin{array}{cccc} C(\{1,2\}) & C(\{3\}) & C(\{4\}) & C(\{5\}) \\ \left[\begin{array}{cccc} 0 & 5 & 10 & 11 \\ 5 & 0 & 5 & 6 \\ 10 & 5 & 0 & 3 \\ 11 & 6 & 3 & 0 \end{array} \right] \end{array}$$

Again, we have only one pair of clusters with the shortest distance, $C(\{4\})$ and

$C(\{5\})$, which are merged yielding the following distance matrix:

$$D^{(2)} = \begin{matrix} & C(\{1,2\}) & C(\{3\}) & C(\{4,5\}) \\ \begin{matrix} C(\{1,2\}) \\ C(\{3\}) \\ C(\{4,5\}) \end{matrix} & \begin{bmatrix} 0 & 5 & 11 \\ 5 & 0 & 6 \\ 11 & 6 & 0 \end{bmatrix} \end{matrix}$$

We finally merge $C(\{1,2\})$ and $C(\{3\})$, and then $C(\{1,2,3\})$ and $C(\{4,5\})$ to complete the clustering. Note that, in this case, the additional criteria are not used as we have only one pair of clusters with the shortest distance at each level of clustering. The hierarchical clustering results obtained from $M_{r,opt,1}$ and $M_{r,opt,2}$ are shown in Figures 7 and 8, respectively.

The dendrograms shown in both figures can be cut at different heights to generate the block decentralized control configurations summarized in Tables 3 and 4, respectively. We can compare the block decentralized configurations at the same level (e.g. solution 1-1 and solution 2-1) based on the distance triplet values shown in Figures 7 and 8. In solution 1-1 and solution 2-1, the distance triplets of the closest clusters are (3,1,4). Thus, the block decentralized control configurations in both solutions are equally good from a structural point of view. In solution 1-2 and solution 2-2, the distance triplets of the closest clusters are (5,5,4) and (5,3,4), respectively. Since solution 1-2 has a greater δ , it represents a more weakly coupled control configuration than solution 2-2. Similarly, the control configuration in solution 2-3 is more weakly coupled than the one in solution 1-3. Note that, although the additional criteria (i.e. δ and Δ) are not used to complete the clustering, they can be used to further analyze the results.

Noting that the manipulated inputs and the controlled outputs represent physical properties of process units and the flows connecting them, the hierarchical clustering results can also be used to identify subnetworks of closely coupled and decoupled process units. By identifying the process units associated with the inputs and outputs in each cluster, different subnetworks are detected as shown in Figure 9. For example, as shown in Figure 10, solution 1-3 suggests to address the control problem around the fuel cell (i.e. control of the temperature, the fuel utilization and the air inlet temperature of the fuel cell) using a MIMO controller with the flow rates of the air and fuel inlet streams, and the bypass ratio around the hot channel of HE6 as the manipulated inputs, while the control problem around the steam reformer (i.e. control of the temperature and the conversion of the steam reformer) is addressed by another MIMO controller manipulating the jacket inlet flowrate and the bypass ratio around the hot channel of HE3. These choices look reasonable but of course will need to be evaluated using additional criteria as well, and ultimately via simulations.

5. Conclusions

In this paper, a method for optimal control configuration synthesis based on structural coupling (physical closeness) has been developed. Specifically, we proposed an integer optimization problem formulation to synthesize optimal decentralized control configurations using the relative degree as a measure of structural coupling. Then, we proposed a hierarchical clustering procedure to identify groups of inputs and outputs such that the variables in the same group interact strongly with each other, while different groups are loosely coupled. This was based on a distance metric defined between input/output clusters, and additional distance measures to differentiate among clusters with the same distance. The proposed method was automated within a graph theoretic framework and was illustrated through an example process network. This procedure can be used to generate block decentralized control configuration candidates, to be further evaluated by the control designer. The proposed framework can be further developed to incorporate i) additional process information such as gains and time constants, and ii) heuristics so that specific pairings are included in or excluded from the optimal control configuration.

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Figure 1: A simple CSTR

Figure 2: Equation graph of the simple CSTR example

Figure 3: Hierarchical clustering results for the simple CSTR example

Figure 4: Process flow diagram of the energy integrated SOFC system

Figure 5: Part of the equation graph of the energy integrated SOFC system

Figure 6: Control configuration for solution 1

Figure 7: Hierarchical clustering result for the energy integrated SOFC system, solution 1

Figure 8: Hierarchical clustering result for the energy integrated SOFC system, solution 2 ($C(\{6\}) = \{u_2, y_1\}$, $C(\{7\}) = \{u_1, y_2\}$)

Figure 9: Subnetworks of the energy integrated SOFC system

Figure 10: Subnetworks controlled by different controllers, solution 1-3

	$y_1(M)$	$y_2(c_A)$	$y_3(c_C)$	$y_4(T)$
$u_1(F_A)$	$F_A \rightarrow M \rightarrow y_1$	$F_A \rightarrow c_A \rightarrow y_2$	$F_A \rightarrow c_C \rightarrow y_3$	$F_A \rightarrow T \rightarrow y_4$
$u_2(F_B)$	$F_B \rightarrow M \rightarrow y_1$	$F_B \rightarrow c_A \rightarrow y_2$	$F_B \rightarrow c_C \rightarrow y_3$	$F_B \rightarrow T \rightarrow y_4$
$u_3(F)$	$F \rightarrow M \rightarrow y_1$	$F \rightarrow M \rightarrow c_A \rightarrow y_2$	$F \rightarrow M \rightarrow c_C \rightarrow y_3$	$F \rightarrow M \rightarrow T \rightarrow y_4$
$u_4(Q)$	No path	$Q \rightarrow T \rightarrow c_A \rightarrow y_2$	$Q \rightarrow T \rightarrow c_C \rightarrow y_2$	$Q \rightarrow T \rightarrow y_4$

Table 1: Shortest paths between the inputs and the outputs of the simple CSTR example

Input nodes			
Index	Variable	Index	Variable
115	u_5	119	u_1
116	u_2	123	u_3
118	u_4		
State nodes			
Index	Variable	Index	Variable
22	$T_{HE3,cold}$	51	$T_{HE5,cold}$
26	$T_{HE3,hot}$	58	$T_{HE5,hot}$
31	$T_{HE4,cold}$	62	$M_{HE6,cold}$
34	$T_{HE4,hot}$	63	$T_{HE6,cold}$
39	T_{SR}	66	$T_{HE6,hot}$
42	$c_{CH_4,SR}$	71	T_{SOFC}
46	T_{SRJ}	73	$c_{H_2,SOFC}$
50	$M_{HE5,cold}$	79	T_{CB}
Output nodes			
Index	Variable	Index	Variable
153	y_5	202	y_1
173	y_4	204	y_2
194	y_3		

Table 2: Node list of the energy integrated SOFC system equation graph in Figure 5

Solution	Number of Controller	Input/output clusters
1-1	4	$C(\{1, 2\}), C(\{3\}), C(\{4\}), C(\{5\})$
1-2	3	$C(\{1, 2\}), C(\{3\}), C(\{4, 5\})$
1-3	2	$C(\{1, 2, 3\}), C(\{4, 5\})$

Table 3: Block decentralized control configurations generated from the energy integrated SOFC system, solution 1

Solution	Number of Controller	Input/output clusters
2-1	4	$C(\{6, 7\}), C(\{3\}), C(\{4\}), C(\{5\})$
2-2	3	$C(\{6, 7\}), C(\{3\}), C(\{4, 5\})$
2-3	2	$C(\{3, 6, 7\}), C(\{4, 5\})$

Table 4: Block decentralized control configurations generated from the energy integrated SOFC system, solution 2