CHEMICAL ENGINEERING TRANSACTIONS
VOL. 61, 2017
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.aidic.it/cet
Guest Editors: Petar S Varbanov, Rongxin Su, Hon Loong Lam, Xia Liu, Jiří J Klemeš

ISBN 978-88-95608-51-8; **ISSN** 2283-9216
DOI: 10.3303/CET1761283

Design of Control Structure for Integrated Process Networks Based on Graph-theoretic Analysis

Lixia Kang, Yongzhong Liu*

Xi'an Jiaotong University, Dept. of Chemical Engineering, Xianning West Rd. 28,710049 Shannxi, China
yzliu@mail.xjtu.edu.cn

A novel graph representation is developed to address the control structure selection of the process networks featuring multiple scale material and energy dynamics, which is a combination of the process flow graph and energy flow graph so that both the material and energy flow structures of the process networks in each time scale can be captured and analysed at the same time using a graph theory based procedure. The control structure of the network evolved in each time scale is then optimally designed by employing a graph-theoretic approach, which can be used as the basis for hierarchical control structure of the whole process networks. The effectiveness of the proposed graph-theoretic procedure for control structure selection is finally verified via an example of a vinyl acetate process.

1. Introduction

High efficiencies of energy and material utilization are critical for modern chemical plants (Lee et al, 2015), which generally benefit from energy and material integration technologies. However, it is not uncommon that challenges in operations are encountered. Significant efforts have been made to overcome the difficulties in analysis and control of these process networks, passivity/dissipative-based methods (Tippett and Bao, 2013), distributed control (Rawlings and Stewart, 2008) and quasi-decentralized control (Sun and El-Farra, 2008), for examples.

It has been reported that the most integrated process networks, comprising of multiple integration loops that result in large rates of recovery and recycle of energy (Jogwar et al. 2009) and/or material (Jogwar et al., 2012), tend to exhibit multiple time scale dynamics. Alternative methods for exploiting this time scale multiplicity can be either singular perturbation based methods (Kumar et al., 1998) where an energy/material dynamic model for the network of interest is required, or graph theory based methods where only the magnitude of the energy (Heo et al., 2014) /material (Heo and Daoutidis, 2015) flows in the network is required. Due to the generic and scalable natures, the graph theory based methods have become effective approaches to reduce the complexity of tightly integrated networks, and can be used as the basis for hierarchical control.

It is also worth noting that the graph-theoretic frameworks and graph theory based approaches have been extensively used to solve the control relevant problems in chemical and energy networks, smart manufacturing systems, electrical power systems, transportation networks and biological networks (Kang et al., 2016). The investigations are mainly focused on the decomposition and partitioning of the system's digraphs into specific subgraphs so that the communication cost or interaction energy are minimized (Ge et al., 2017). In addition, alternative graph-theoretic representations have been developed to facilitate the process dynamic analysis and control structure selection. Examples of them are cause-and-effect graph, P-graph and equation graph (Wal and Jager, 2001).

In spite of the successful application of the graph representation of the networks with energy integration loops or the networks with material integration loops, a graph-theoretic framework of process networks that combines simultaneously energy and material integration loops has not been reported. In addition, although the potential manipulations acting in different time scales and the form of the reduced order models in each time scale can be obtained, the input/output pairs or control structure within each time scale need to be further determined.

Please cite this article as: Kang L., Liu Y., 2017, Design of control structure for integrated process networks based on graph-theoretic analysis, Chemical Engineering Transactions, 61, 1711-1716 DOI:10.3303/CET1761283

Therefore, the major objective of this work is to develop a design method for complex process networks in which multiple time scale dynamics are present due to combination of energy and material integration loops. The rest of the paper is organized as follows: in section 2, the multiple time scale dynamics of energy integrated networks are first introduced. The graph-theoretic procedure for control structure design of the process network featuring integrated material and energy dynamics is given in section 3 and an example is used to verify the effectiveness of the proposed procedure in section 4. Section 5 gives our conclusions.

2. Multiple time scale dynamics of complex energy integrated networks

For a generic complex energy-integrated process network where the energy flows h_i, spanning m orders of magnitude, the energy dynamics can be described by the following equations,

$$\frac{d\mathbf{H}}{dt} = \sum_{i=1}^{m} \frac{1}{\varepsilon_i^e} \mathbf{F}_i \mathbf{g}_i(\mathbf{H}, \mathbf{u}_i) \tag{1}$$

and the dynamics of a general process networks featuring multiple interconnected material recycle structures, where different material flows span n orders of magnitude take the form:

$$\frac{d\mathbf{x}}{dt} = \sum_{j=1}^{n} \frac{1}{\varepsilon_j^f} \mathbf{g}_j(\mathbf{x}, \mathbf{u}_j) \tag{2}$$

where H is the vector of the enthalpy of N process units and x is the vector of the material balance variables. The subscripts *i* and *j* are the indices to the energy flows and material flows of different orders of magnitude, respectively. ε_i^e and ε_j^f are small parameters such that $\varepsilon_i^e, \varepsilon_j^f << 1$, $\varepsilon_{i+1}^e / \varepsilon_i^e << 1, \varepsilon_{j+1}^f / \varepsilon_j^f << 1$ and $\varepsilon_1^e, \varepsilon_1^f \approx 1$.We assume that the flows of the *i*-th magnitude, ε_i^e are of $\mathrm{O}(1/\varepsilon_i^e)$, and t represents the time scale where the slowest dynamic evolves. $\mathbf{g}_i$ and $\mathbf{g}_j$ are the vectors with contributions from the energy flows of $\mathrm{O}(1/\varepsilon_i^e)$ and material flows of $\mathrm{O}(1/\varepsilon_j^f)$. $\mathbf{F}_i$ are the selector matrices; u_i and u_j represent the scaled energy flows and material flows that can be considered the potential manipulated inputs.

Specifically, when the enthalpies of the flows are expressed as the products of molar flow rates and molar enthalpies of the flows, the orders of magnitude of enthalpy can be expressed as the products of the orders of magnitude of molar enthalpy and those of molar flowrates. In this case, the energy dynamics of a process where different material flows span n orders of magnitude and the molar enthalpies span m orders of magnitude can thus be rewritten as:

$$\frac{d\mathbf{H}}{dt} = \sum_{i=1}^{m} \sum_{j=1}^{n} \frac{1}{\varepsilon_{ij}} \mathbf{F}_{ij} \mathbf{g}_{ij}(\mathbf{H}, \mathbf{u}_{ij}) \tag{3}$$

where ε_{ij} are small parameters that are calculated as the products of ε_i^e and ε_j^f. Note that, the small parameters, ε_{ij} satisfy $\varepsilon_{i,j+1} / \varepsilon_{i,j} << 1$, $\varepsilon_{i+1j} / \varepsilon_{ij} << 1$ and $\varepsilon_{11} \approx 1$. To keep consistent with the definition of small parameters in Eqs. (1) and (2), ε_{ij} are ranked and clustered to K clusters so that $\varepsilon_k << 1$, $\varepsilon_{k+1} / \varepsilon_k << 1$, and $\varepsilon_1 = \varepsilon_{11} \approx 1$. The system determined by Eq. (3) is then a singularly perturbed system with multiple small parameters, like those determined by Eqs.(1) and (2). The reduced dynamic models of such systems can thus be obtained by considering each time scale, $\tau_k = t / \varepsilon_k$ and setting the small parameters to zeros sequentially, starting from the fastest time scale, τ_K and proceeding all the way to the slowest, *t.* The potential manipulated inputs, the state variables and the controlled variables evolved in each time scale are accordingly identified for subsequent analysis of the hierarchical control. It should be pointed out that both the multi-time scale material and energy dynamics of the process can thus be analysed in each time scale.

3. Graph-theoretic control structure selection of integrated material and energy networks

3.1 Graph representation of integrated material and energy networks

Motivated by the above analysis, a novel graph representation of the process networks should be developed to capture the material and energy flow structures simultaneously due to the limited utilization of the energy flow graph and process flow graph.

In energy flow graph, the relationship between material flows and energy flows is neglected, and thus the large energy flows caused by pure energy flows (with small flow rate), large material flows or by both cannot be distinguished. In process flow graph, some energy transfer units are usually omitted (i.e. heat exchangers,

heaters, coolers, compressors. etc.), which may result in an incomplete energy flow graph when using process flow graph to capture the energy and material dynamics.
To this end, in what follows, a proper combination of the energy flow graph and process flow graph would be a natural and promising way to capture the energy and material flow structures of the networks simultaneously. A novel graph representation of process networks is thus defined as follows:
A generic process network, including N process units, n_s chemical species, is defined as a weighted digraph G (V, E), where V and E are the set of nodes and the set of edges, respectively. In G, the following subsets of V and E are defined:

V_{normal} : the set of normal nodes which represent individual process units. The process units where the enthalpies of the streams are changed while the flow rates remain unchanged are defined as pure energy transfer units and are marked as red solid rectangular. Otherwise, they are marked as a black solid rectangular.

V_{source}: the set of auxiliary nodes which represent material sources (e.g. feed streams) and energy sources (e.g. heat, cold and electricity). The nodes of pure energy sources are drawn as the red dashed circulars and the others are black dashed circulars.

V_{sink}: the set of auxiliary nodes which represent material or energy sinks. These nodes for material sinks are marked as black dashed rectangular while those for energy sinks are red dashed rectangular.

$V_{reaction}$: the set of auxiliary nodes which represent the chemical reactions. This kind of nodes are drawn as black solid circular nodes.

E_{normal}: the set of normal edges which represent material or energy flows. Note that the pure energy flows are marked as red solid arrows, and black solid arrows otherwise.

$E_{auxiliary}$: the set of auxiliary edges which represent formation/consumption of chemical species and these edges are drawn as black dashed arrows.
The edge weights are given as:

For a normal edge the weights represent the order of magnitude of total flow rate and those of different chemical species flow rates.

For an auxiliary edge, the weights represent the order of magnitude of the chemical reaction rate.
The energy flows of different orders of magnitude are distinguished using edges of different thickness. The larger is the order, the thicker is the edge. Unlike the conventional energy flow graph, the order of magnitude for an energy flow in G will be determined by the orders of magnitude of molar flow rate and that of molar enthalpy, as has mentioned in section 2.

3.2 Graph-theoretic analysis of multiple scale material and energy dynamics

Once the novel graph representation of the process network is constructed, the energy dynamics are analysed through the same procedure provided in literature (Heo et al. 2014), and the material dynamics are also analysed using the edge weights using the corresponding approach (Heo and Daoutidis, 2015).
During the multi-time scale analysis, two basic building blocks are commonly involved, i.e. large recycle and large throughput. In addition, it is also possible to have a partial material recycle/throughput. All these basic blocks can be replaced by a composite unit in the graph so that the complexity of the graph is reduced and the subsequent dynamic analysis is simplified. The graph algorithms to identify these basic building blocks and replace them with their corresponding composite units, to determine the potential manipulated variables, state variables and controlled variables in each time scale have been developed, which will be improved to analyse the multiple scale dynamics in integrated material and energy networks in this work.

3.3 Graph-theoretic approach for control structure selection

Given the potential manipulated variables, state variables and controlled variables, we can obtain the optimal input/output pairs in each time scale by finding a maximum weighted matching in a bipartite graph, taking the input set, U and the output set, Y as two disjoint vertex subsets, and the structural decoupling matrix, S as the weight matrix. The elements of S, s_{pq} are calculated as

$$s_{pq} = \left(\sum_{q'=1}^{n_y} r_{pq'} + \sum_{p'=1}^{n_u} r_{p'q}\right) - (n_u + n_y) r_{pq} \tag{4}$$

where r_{pq} is the relative degree of the output, y_q with respect to the input, u_p, which can be obtained from the equation graph of the process networks. n_u and n_y are the numbers of the inputs and outputs respectively.
The procedure to design a control structure for integrated material and energy networks that developed in this work can thus be organized as
(1) Construct the proposed graph representation according to the process networks;
(2) Analysis multiple material and energy dynamics by graph theory-based procedures;
(3) Control structure selection of the process networks via the bipartite matching.

4. Case study-vinyl acetate (VAc) process

4.1 Process description

In this section, a vinyl acetate (VAc) process (Luyben and Tyréus, 1998), is adopted to illustrate the procedure of the proposed method. In this process, three raw materials, ethylene, acetic acid and oxygen are converted into the vinyl acetate product and it is assumed that a small component of an inert component, ethane enters with the fresh ethylene feed stream. More details of this process can be found elsewhere in literature.
It is noted that following features of this process may arise a potential of multiple scale material and energy dynamics: (1) a large amount of unreacted reactants is recycled; (2) a small purge exists in this process; (3) both vapor phase and liquid phase are involved, which may cause a separation in orders of magnitude of molar enthalpy of the streams.

4.2 Graph-theoretic control structure selection of VAc process

According to the above analysis, following small parameters are defined below:
for molar flow rate: $\varepsilon_1^f = 1$, $\varepsilon_2^f = P_s / F_{in,s}$, $\varepsilon_3^f = P_s / R_s$ with $\varepsilon_3^f << \varepsilon_2^f << \varepsilon_1^f \approx 1$

for molar enthalpy: $\varepsilon_1^e = 1$ $\varepsilon_2^e = h_s^l / h_s^v$ with $\varepsilon_2^e << \varepsilon_1^e \approx 1$

where P, Fin, R are the molar flow rates of purge, feed and recycled streams, respectively. h^l and h^v are the molar enthalpy of liquid and vapour phases. The subscript s denotes the steady state value.
By calculating the products of the orders of molar flowrate and those of molar enthalpy, five clusters corresponding to five orders of magnitude are obtained as follows when assume that $\varepsilon_2^f / \varepsilon_2^e \approx 1$.

$$O(1/\varepsilon_3^f \varepsilon_2^e) << O(1/\varepsilon_2^f \varepsilon_2^e) << O(1/\varepsilon_3^f) << O(1/\varepsilon_2^e) << O(1)$$

According to the process data provided in literature (Luyben and Tyréus,1998), the graph representation of vinyl acetate process is constructed and given in Figure 1. The list of nodes is presented in Table 1. Figure 1 shows that the energy flows in this process span three orders of magnitude, which are $O(1/\varepsilon_3^f \varepsilon_2^e)$, $O(1/\varepsilon_2^f \varepsilon_2^e)$ and $O(1)$. Note that when the energy transfer related nodes and edges (red nodes and edges) are removed, Figure 1 will reduce to the process flow graph of VAc process. Thus, the multiple scale material dynamics can also be analysed using the edge weights.

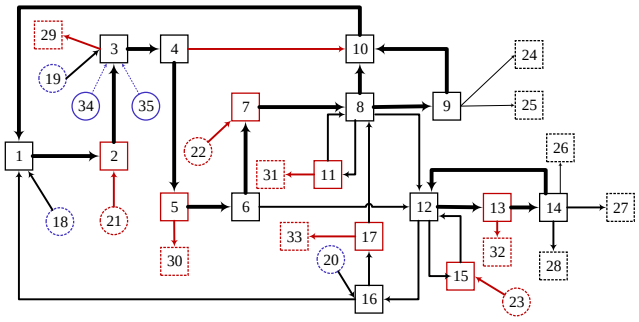
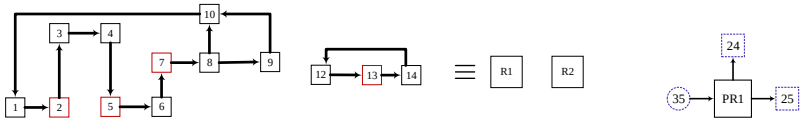


Figure 1: The graph representation of VAc process

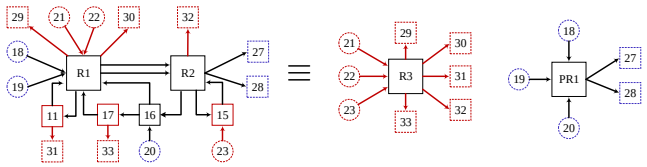
Taking the graph in Figure 1 and the edge weights as the input, the graph theory based algorithms can then be used to analyse the multiple scale material and energy dynamics via subgraph generation and graph simplification, as shown in Figure 2.
The subgraph with the largest energy flows is given in Figure 2(a). The process units evolving in this time scale are P3 = {1,2,3,4,5,6,7,8,9,10,12,13,14}. In this subgraph, three recycles are identified in both energy and material flow structures, and are simplified as two composite nodes, R1 and R2. Figure 2(b) shows the subgraph with the intermediate energy flows. The units are P2 = {R1, R2, 11, 15, 16, 17}. In energy flow structure, this subgraph contains four recycles and can be simplified to be a composite unit R3, while in material dynamic analysis, these four recycles are determined as the partial material recycles and thus reduced to be a composite unit PR1. By comparing the composites of the internal and external flows of PR1, the material flow structure around the recycle loop for CO_2 forms a large recycle, and the total holdup of CO_2 in the recycle loop evolves in the slow time scale while the holdup of CO_2 in individual unit evolves in this time scale. In the subgraph with the smallest energy flows, corresponding to the time scale, *t* is given in Figure 2(c). The subset of process units related to this time scale is P1= {1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17}. Note that only the material flows with the order of magnitude of O (1) are connected to PR1.

Table 1: Node list of graph representation of Vac process

Normal nodes							
nodeunit		node	unit	nodeunit		nodeunit	
1	vaporizer	5/11	cooler	9	FEHE-cold	14	decanter
2	heater	6	separator	10	CO_2 removal	15	reboiler
3	reactor	7	compressor	12	distillation column	16	HA_C tank
4	FEHE-hot	8	absorber	13	condenser	17	cooler
Source/sink nodes							
18	ethylene feed	22	electricity	26	vent	30	cold
19	oxygen feed	23	heat	27	organic product	31	cold
20	HAc feed	24	purge	28	Aqueous product	32	cold
21	heat	25	CO_2 purge	29	reaction enthalpy	33	cold
Reaction nodes							
node	reactions						
34	$2C_2H_4+2CH_3COOH+O_2$—>$2CH_2$=$CHOCOCH_3+2H_2O$						
35	$C_2H_4+3O_2$—>$2CO_2+2H_2O$						



(a) with the largest energy flows *(c)with the smallest energy flows*



(b) with the intermediate energy flows

Figure 2: Subgraphs of the graph representation of VAc process

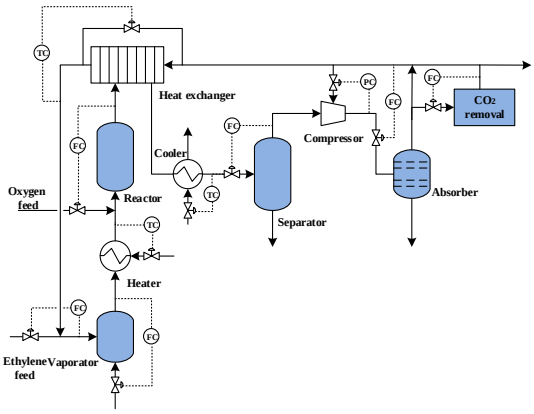


Figure 3: The control structure of part of process networks evolved in the fast time scale

According to the above results, the VAc process will exhibit three-time scale dynamics. The dynamics of different chemical species evolving in these time scales are the same as those obtained in literature (Heo and Daoutidis, 2015). In addition, the controlled outputs and potential manipulated inputs available in each time scale are determined using the graph theory based algorithms (Heo et al. 2014) and more recently (Heo and Daoutidis, 2015). In the fast time scale (τ_2), the energy balance variables of the individual process units and

the material balance variables of the individual process units (i.e. 1, 3, 4, 6, 8, 9, 10, 12, 14) need to be controlled, and all but one out of ten units can be controlled simultaneously in R1 and all but one out of three units can be controlled simultaneously in R2. Noting that this subgraph has no auxiliary node. Potential manipulated inputs in this time scale include all the edges in both R1 and R2. The material balance variables associated with HAc tank, the enthalpies of coolers, reboiler as well as the total enthalpy of the R1 and R2 need to be controlled in the intermediate time scale (τ_1). This can be achieved using any external flows in this time scale. In the slow time scale (t), the holdup of CO_2 needs to be controlled and this can also be realized using the small external flows.

Taking the process units evolved in the fast time scale as an example, we apply the graph-theoretic approach to synthesize the control structure of this part of process on the basis of the mathematical model developed in literature (Chen et al., 2013), as shown in Figure 3.

5. Conclusions

In this paper, the graph-theoretic control structure design of the process networks is addressed, which features multiple scale material and energy dynamics. A novel graph representation of the process networks is developed through the combination of the process and energy flow graphs. A graph-theoretic analysis of the multiple scale material and energy dynamics is then performed to determine the potential manipulated inputs and controlled outputs evolved in each time scale. The hierarchical control structure can thus be obtained by combining the control structures obtained by bipartite matching in each time scale. The proposed graph method is finally examplified as an effective tool to design control structures for the process networks coupling energy and material integration loops.

Acknowledgments

Financial support from the Natural Science Foundation of China (No. 21376188 and No. 21676211) is highly acknowledged.

References

Bunse K., Vodicka M., Schönsleben P., Brülhart M., Ernst F.O., 2011, Integrating energy efficiency performance in production management – gap analysis between industrial needs and scientific literature. Journal of Cleaner Production, 19, 667-679.

Chen R., Dave K., McAvoy T., 2003, A Nonlinear Dynamic Model of a Vinyl Acetate Process, Industrial & Engineering Chemistry Research, 42, 4478-4487.

Ge X., Yang F., Han QL., 2017, Distributed networked control systems: A brief overview, Information Sciences, 380, 117-131.

Heo S., Rangarajan S., Daoutidis P., Jogwar S.S., 2014, Graph reduction of complex energy-integrated networks: Process systems applications, AIChE Journal, 60, 995-1012.

Heo S., Daoutidis P., 2015, Graph-Theoretic Analysis of Multitime Scale Dynamics in Complex Material Integrated Plants, Industrial & Engineering Chemistry Research, 54, 10322-10333.

Jogwar S.S., Baldea M., Daoutidis P., 2009, Dynamics and Control of Process Networks with Large Energy Recycle, Industrial & Engineering Chemistry Research, 48, 6087-6097.

Jogwar S.S., Torres A.I., Daoutidis P., 2012, Networks with large solvent recycle: Dynamics, hierarchical control, and a biorefinery application, AIChE Journal, 58, 1764-1777.

Kang L., Tang W., Liu Y., Daoutidis P., 2016, Control configuration synthesis using agglomerative hierarchical clustering: A graph-theoretic approach, Journal of Process Control, 46, 43-54.

Kumar A., Christofides P.D., Daoutidis P., 1998, Singular perturbation modelling of nonlinear processes with nonexplicit time-scale multiplicity, Chemical Engineering Science, 53, 1491-1504.

Lee J.-Y., Seid E.R., Majozi M., 2015, Heat integration of material transfer streams in batch processing plants, Chemical Engineering Transactions, 45, 127-132.

Luyben M. L., Tyréus B.D., 1998, An industrial design/control study for the vinyl acetate monomer process, Computer & Chemical Engineering, 22, 867-877.

Rawlings J.B., Stewart B.T., 2008, Coordinating multiple optimization-based controllers: New opportunities and challenges, Journal of Process Control, 18, 839-845.

Sun Y., El-Farra N.H., 2008, Quasi-decentralized model-based networked control of process systems, Computer & Chemical Engineering, 32, 2016-2029.

Tippett M.J., Bao J., 2013, Distributed model predictive control based on dissipativity, AIChE Journal, 59, 787-804.

Wal M.V.D., Jager B.D., 2001, A review of methods for input/output selection, Automatica, 37, 487-510.