CHEMICAL ENGINEERING TRANSACTIONS

VOL. 88, 2021

A publication of AIDIC
The Italian Association of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Yee Van Fan, Jiří J. Klemeš

ISBN 978-88-95608-86-0; **ISSN** 2283-9216

DOI: 10.3303/CET2188008

Heat Integrated Water Regeneration Network Synthesis via Graph-Theoretic Sequential Method

Bing Shen How[a,*], Ákos Orosz[b], Sin Yong Teng[c], Juin Yau Lim[d], Ferenc Friedler[e]

[a] Research Centre for Sustainable Technologies, Faculty of Engineering, Computing and Science, Swinburne University of Technology, Jalan Simpang Tiga, 93350, Kuching, Sarawak, Malaysia
[b] Department of Computer Science and Systems Technology, University of Pannonia, 8200, Veszprém, Egyetem u. 10, Hungary
[c] Radboud University, Institute for Molecules and Materials, P.O. Box 9010, 6500 GL, Nijmegen, the Netherlands
[d] Integrated Engineering, Dept. of Environmental Science and Engineering, College of Engineering, Kyung Hee University, 1732 Deogyeong-daero, Giheung-gu, Yongin-Si, Gyeonggi-do, 17104, Republic of Korea
[e] Széchenyi István University, 9026, Győr, Egyetem tér 1, Hungary
bshow@swinburne.edu.my

The integration of multiple resources conservation networks is necessary to attain the ever-stringent sustainable goals. This work takes initiatives to develop a heat integrated water network *via* a proposed P-graph-based sequential methodology. In the first step, a set of feasible water regeneration networks is generated using the conventional P-graph framework. Then, the obtained feasible networks will be used as the inputs in the second stage which aims to generate various sets of feasible heat exchanger networks. It is worth noting that the second model is solved by an extended P-graph framework (P-HENS) for combinatorial process network optimization. The solutions are then ranked based on the total network cost. To demonstrate the effectiveness of the proposed method, a typical water regeneration network (three sources and three sinks) with multi-contaminants is used. The results show a total of 103 feasible water network structures (water network cost ranging from 0.76 M$/y to 1.18 M$/y). Thereafter, a list of feasible HIWRN can be determined using P-HENS. The top four HIWRNs which offer similar total network cost (~1.639 M$/y) are demonstrated. This proposed method provides valuable insights that allow decision-makers to further select the optimal solution which may be more beneficial as compared to the one obtained *via* conventional methods.

1. Introduction

Both energy security and water scarcity issues have received growing concerns from both industrial and academic communities (Wang et al., 2020). Given the ever-growing world population, global water demand in 2050 is anticipated to increase to 5,800 km^3/y, i.e., about 26 % greater than that of in 2010 (IIASA, 2016); while energy demand, on the other hand, will rise nearly 50 % as compared to that of 2019 by 2050 (EIA 2020). As a countermeasure, one should explore the potential of resource conservation strategies, i.e., Heat-Integrated Water Networks (HIWN) for effective water and energy management.

There are two main classes of strategies opted for HIWN synthesis, i.e., (i) insight-based approach and (ii) mathematical programming. Insight-based approaches refer to the targeting tool which is based on the pinch analysis concept. These tools include, but not limited to, source-demand energy composite curves (Savulescu et al., 2002), two-dimensional grid diagram (Savulescu et al., 2005), Water Energy Balance Diagram (Leewongtanawit and Kim, 2009), modified Problem Table Algorithm (Bandyopadhyay and Sahu, 2010), temperature and concentration order composite curves (Hou et al., 2014), ΔH-F diagram (Liao et al., 2015), and T-H/H-F diagrams (Hong et al., 2018).

In terms of mathematical programming approaches, they can be classified into two main categories, i.e., simultaneous (accomplish the multi-objective optimization within a single step) and sequential (encompasses of multiple discrete optimization steps) models. Under the simultaneous model, both water allocation network (WAN) and heat exchanger network (HEN) are synthesized simultaneously with the consideration of the total network costs. One of the earliest documented works was conducted by Bogataj and Bagajewicz (2007),

Paper Received: 14 June 2021; Revised: 6 July 2021; Accepted: 9 October 2021
Please cite this article as: How B.S., Orosz Á., Teng S.Y., Lim J.Y., Friedler F., 2021, Heat Integrated Water Regeneration Network Synthesis via Graph-Theoretic Sequential Method, Chemical Engineering Transactions, 88, 49-54 DOI:10.3303/CET2188008

where a mixed-integer non-linear mathematical programming (MINLP) was developed to design a non-isothermal HIWN. Thereafter, a simultaneous model has been extended to cover regeneration and recycling (Cheng and Adi, 2018), splitting and mixing of freshwater and wastewater (Hong et al., 2016), inter-plant integration (Liu et al., 2018), etc. In contrast, under a sequential model, the optimal WAN with minimum water network cost will first be generated, while its optimal HEN is then synthesized subsequently. Its earliest implementation can be backdated to the early 21st Century (Bagajewicz et al., 2002). Due to its simplicity and greater flexibility, it has been widely applied even in some of the recently published works. For instance, Chauhan and Khanam (2021) proposed a three-step methodology to synthesize an optimal HIWN for a thermal power plant with the consideration of multiple contaminants. Kamat et al. (2019), on the other hand, claimed that their proposed three-stage sequential approach (minimization of (i) freshwater, (ii) regenerated water and (iii) utility) is preferable in areas that suffers from water scarcity issues.
Apart from that, a graph-theoretic method – P-graph has recently emerged to solve water and energy recovery problems. In contrast to other methods, P-graph is capable of generating multiple optimal and near-optimal solutions simultaneously, which are deemed useful for decision-makers (How and Lam, 2019). Notably, Lim et al. (2017) had demonstrated how P-graph can be used for water network synthesis. Its application is then extended by Foo et al. (2021) for batch water network. Orosz and Friedler (2020), on the other hand, developed an extension of P-graph (called “P-HENS”) for the HEN synthesis. Its effectiveness had been validated using three classic heat recovery problems. To the best of the authors' knowledge, the application of P-graph to solve heat-integrated water regeneration network (HIWRN) is still very limited. One recent work from Chin et al. (2019) had attempted to simultaneously solve the water and energy integration problem using P-graph. However, their model did not cover the alternative configurations of the HEN. This work aims to address this gap by proposing a P-graph-based sequential model, which integrate the use of conventional P-graph model and P-HENS to yield various sets of feasible HIWRNs to aid the decision-making.

2. Problem Statement

Given a set of water source (SR) *i* and a set of water sink (SK) *j* where each source is associated with a given flowrate of F_{SRi}, a source temperature of T_{SRi} and impurity (denoted as *k*) concentration of $C_{SRi,k}$; while each sink is associated with a required flowrate of F_{SKi}, a sink temperature of T_{SKj}, an input concentration of $C_{SKj,k}$, where $C_{SKj,k}$ must not exceed the maximum allowable impurity concentration, $C_{SKj,k}^{max}$. Freshwater (FW) with a concentration $C_{FW,k}$ and supply temperature T_{FW} can be used to supplement the water network. In addition, a fixed outlet type of regeneration unit is used to enhance the reusability of the generated water (RW), i.e., reduce the concentration to $C_{RW,k}$ (with temperature T_{RW}). Other unutilized water will be sent to the wastewater (WW) unit with a given temperature of T_{WW} .The work aims to determine the optimal HIWRN with the consideration of the total cost attributed from both water and heat exchanger networks.

3. Method

The proposed problem is solved using a two-step procedure (Figure 1). Both steps make use of the graph-theoretic algorithm which is embedded in the conventional P-graph model.

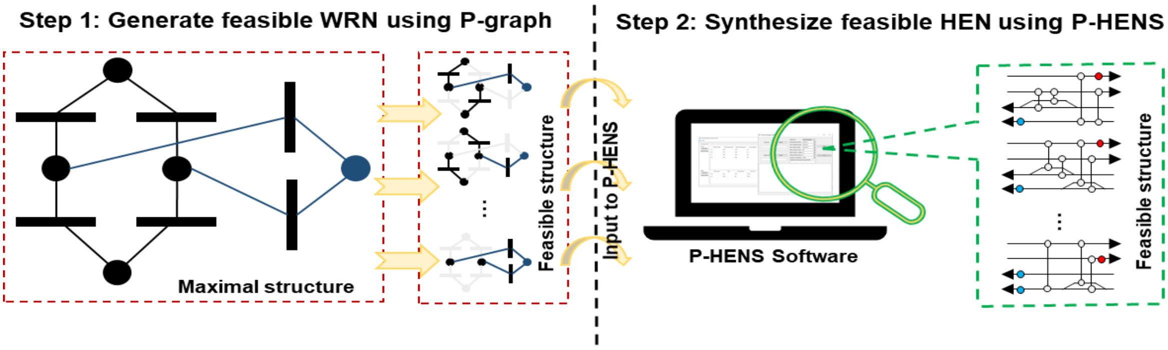

Figure 1: Schematic diagram for the proposed Graph-theoretic Sequential Method

3.1 Water regeneration network (WRN) synthesis using P-graph model

A P-graph model is first developed to synthesize all combinatorically feasible WRNs. The model is built based on the procedure outlined in Lim et al. (2017). Generally, the P-graph topology is specifically designed so that the following three mass balance equations are fulfilled:

$$F_{SRi} = \sum_j F_{SRi,SKj} + F_{SRi,RW} + F_{SRi,WW} \quad (1)$$

$$F_{SKj} = \sum_i F_{SRi,SKj} + F_{FW,SKj} + F_{RW,SKj} \quad (2)$$

$$\sum_i F_{SRi,SKj} \times C_{SRi,k} + F_{FW,SKj} \times C_{FW,k} + F_{RW,SKj} \times C_{RW,k} \leq F_{SKj} \times C_{SKj,k}^{max} \quad (3)$$

where $F_{SRi,SKj}$, $F_{SRi,RW}$ and $F_{SRi,WW}$ refer to the flowrate transferred from source *i* to sink *j*, to regeneration unit, and wastewater treatment; while $F_{FW,SKj}$ and $F_{RW,SKj}$ denote the flowrate of freshwater (FW) and regenerated water channelled to sink *j*. Note that the P-graph solver will rank the alternative networks based on the total water network cost (NC^{WRN}), which considers the unit freshwater cost (CF_{FW}), water regeneration cost (CF_{RW}) and wastewater treatment cost (CF_{WW}).

$$NC^{WRN} = \sum_j (F_{FW,SKj} \times CF_{FW}) + \sum_i (F_{SRi,RW} \times CF_{RW} + F_{SRi,WW} \times CF_{RW}) \quad (4)$$

3.2 Heat exchanger network (HEN) synthesis using P-HENS software

Based on the WRNs generated from the first model, the corresponding stream data (flowrate and temperature) will serve as the input for the P-HENS software developed by Orosz and Friedler (2020). The procedure of setting up the P-HENS follows the generic heuristic guide discussed in Orosz et al. (2021), where the main aim is to synthesise a list of feasible HENs which consume minimal energy with the need of minimum numbers of heat exchangers and stream splitting being installed. It is worth noting that, with the aid of the P-HENS software, all the combinatorically feasible HENs that require minimum utilities for each generated WRN can be synthesized at one go. The overall HEN cost (NC^{HEN}) is computed using Eq(5),

$$NC^{HEN} = Q_{HU}^{min} \times CF_{HU} + Q_{CU}^{min} \times CF_{CU} + 145.6A^{0.6} \quad (5)$$

where Q_{HU}^{min} and Q_{CU}^{min} refer to the minimum hot and cold utility required for the system, while their respective unit costs are denoted as CF_{HU} and CF_{CU}. The last term in Eq(5) indicates the capital cost associated with the heat transfer area (A) required (note that “145.6” is the assumed annualized area cost coefficient in \$/m^2).

4. Illustrative example

The illustrative case study is adapted from the work conducted by Kamat et al. (2018), where the limiting data are tabulated in Table 1, while the other assumed parameters are summarized in Table 2. Note that C_A, C_B, and C_C denote the concentration of contaminant A, B and C; T indicates the temperature of each stream; while ΔT_{min} refers to the assumed minimum temperature difference between the hot and cold streams.

Table 1: Limiting data, adapted from Kamat et al. (2018)

Sources	Flowrate (kg/s)	C_A (ppm)	C_B (ppm)	C_C (ppm)	T (°C)	Demand	Flowrate (kg/s)	C_A (ppm)	C_B (ppm)	C_C (ppm)	T (°C)
SR1	30	100	80	60	100	SK1	30	100	80	60	100
SR2	40	150	115	105	75	SK2	40	150	115	105	75
SR3	20	125	80	130	35	SK3	20	125	80	130	35
FW	-	0	0	0	80	WW	-	-	-	-	60
RW	-	60	80	30	60	RW	-	-	-	-	60

Table 2: Assumed parameters used in this case study, adapted from Kamat et al. (2018)

Item	Value	Item	Value
CF_{FW}	0.4500 \$/t FW	CF_{HU}	377 \$/kWy
CF_{WW}	0.0067 \$/t WW	CF_{CU}	189 \$/kWy
CF_{RW}	0.0067 \$/t RW	ΔT_{min}	10 °C

Figure 2 shows the P-graph model constructed for the WRN generation. On the illustration blue node refers to the FW allocation, while the red and green nodes denote the streams flow towards wastewater treatment and water regeneration units. In this work, there are 103 feasible WRN are generated from the developed P-graph model, in which the overall NC^{WRN} is ranging from 0.76 M\$/y to 1.18 M\$/y (assumed there are 8,000 h/y). The network information (i.e., flow allocation) of each feasible WRN is extracted, and insert into P-HENS software for HEN synthesis.

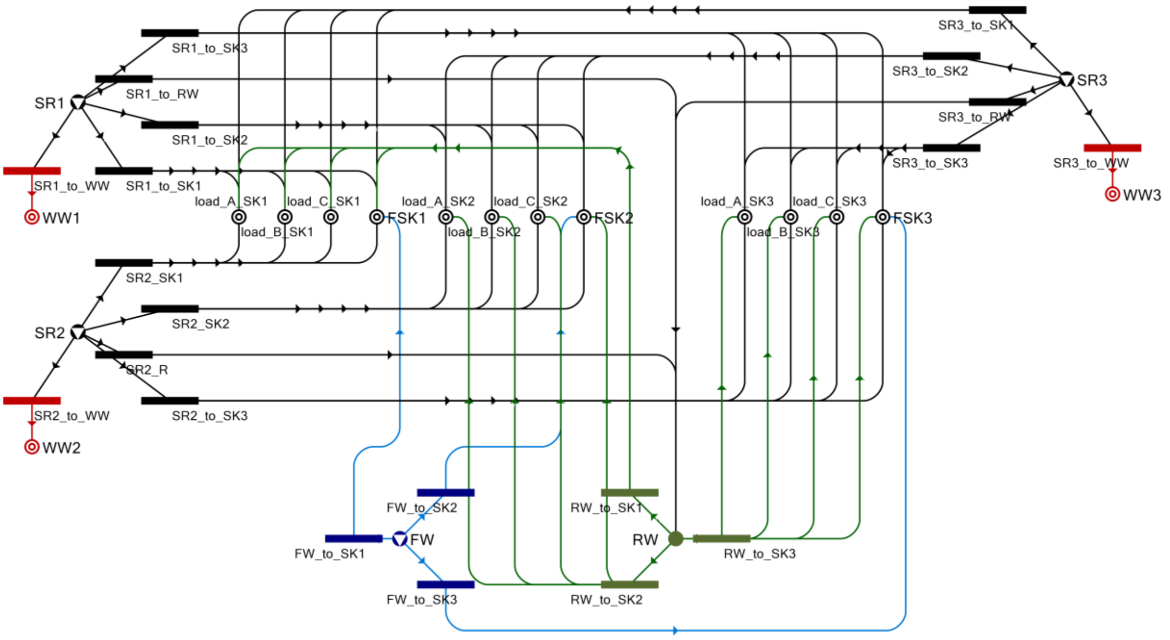

Figure 2: P-graph model for WRN synthesis

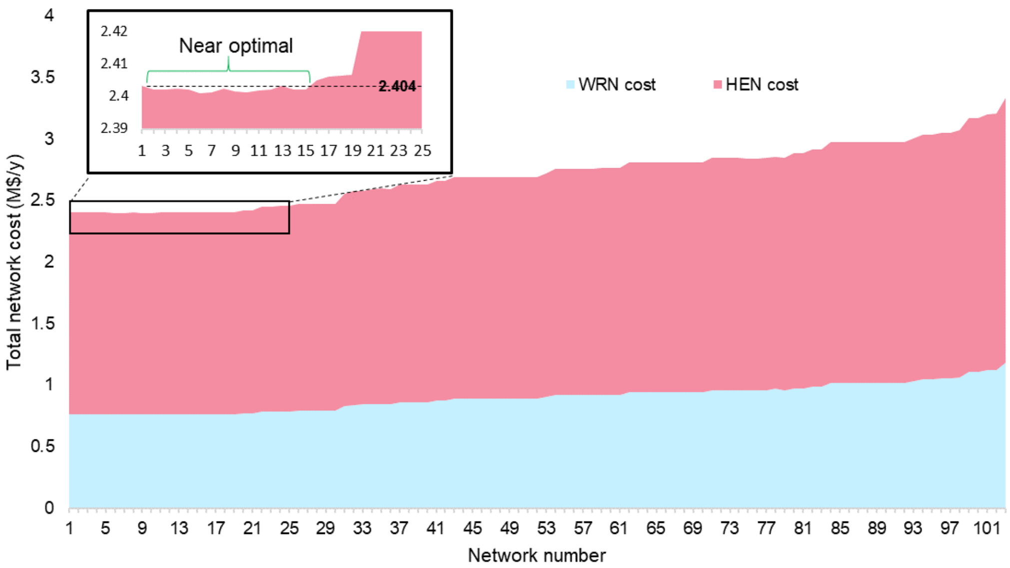

Figure 3: Total network cost for each generated network

The minimum NC^{HEN} required for each synthesized WRN can be extracted from P-HENS software. The resultant network costs for the feasible WRNs are illustrated in Figure 3. In general, the results show that the greater consumption in FW not only leads to a higher NC^{WRN}, but also causes higher NC^{HEN}. This is due to the greater Q_{CU}^{min} requirement (i.e., more energy is required to cool hot FW (80 °C) as compared to that of RW (60 °C). Based on the results, network 6 obtained from the P-graph model poses the minimal total network cost (i.e., 2.401 M$/y). Conventionally, this network design will be viewed as the sole optimal solution. However, its suitability of implementation is not guaranteed since the complexity of piping arrangement, safety consideration, and budget constraint (for retrofitting) were not considered by the model. Besides, the optimality of the network is also dependent on the unit prices (e.g., network 3 will become the optimal structure when CF_{FW} is increased by 3.8 folds). These show the necessity to consider the near-optimal structure in the decision-making process. For instance, aside from network 6, there are another 14 feasible networks (networks 1 to 15) that are within 0.1 % tolerance of the posed total network cost (i.e., less than 2.404 M$/y).

Apart from identifying the near-optimal WRN structures, another key feature of this proposed method is the capability of synthesizing near-optimal HEN designs for a given WRN structure. It is worth noting that all these generated structures are found as the multi pinch problem, where the pinch temperatures are 80 °C / 90 °C and 90 °C / 100 °C. Using the obtained optimal network (i.e., network 6) as an example, the computed Q_{HU}^{min} and Q_{CU}^{min} are 1,260 kW and 6,090 kW. Based on P-HENS, there are a total of 18 feasible configurations (18 below-Pinch region designs x 1 middle-pinch region design x 1 above pinch region design). The top four configurations based on NC^{HEN} are illustrated in Figure 4. As shown, these four designs offer competitive NC^{HEN} as the difference between them are less than 0.04 %. In other words, these designs are comparable and worth further consideration (e.g., considering the piping complexity and safety aspects).

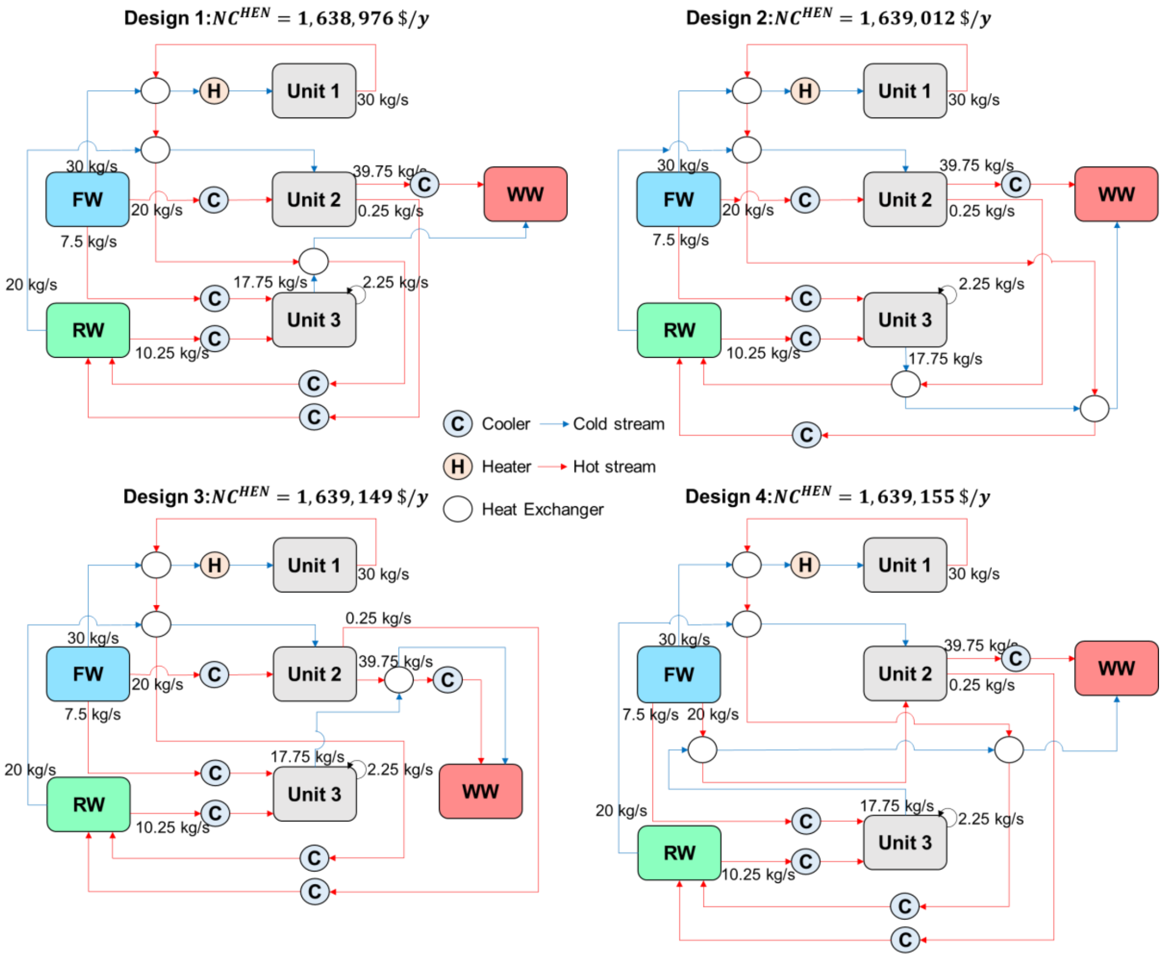

Figure 4: Top four HIWRN designs for network 6 obtained from P-graph model

5. Conclusions

A novel P-graph-based sequential model for the synthesis of HIWRN is proposed in this work. This is the first attempt of applying P-HENS in HIWRN generation. The effectiveness of the proposed method is demonstrated using a three source-three sink problem with the consideration of a fixed outlet type of regeneration unit. It shows that the proposed method is capable of identifying potential WRNs (103 networks) and their respective HEN design alternatives (a list of HIWRNs that offers similar total cost (~1.639 M\$/y)) which are invaluable for decision-makers. Nevertheless, solving more complex problems with the current framework may still be arduous. Future extension of P-HENS software (e.g., incorporating water conservation calculation into the software) can be made to enable simultaneous synthesis of WRNs and HENs.

Acknowledgements

This work was financially supported by Swinburne University of Technology Sarawak Campus *via* Early Career Researcher Award 2019. Besides, Project TKP2020-NKA-10 has been implemented with the support provided from the National Research, Development and Innovation Fund of Hungary, financed under the 2020-4.1.1-TKP2020 Thematic Excellence Programme 2020-National Challenges sub-program funding scheme. F. Friedler, on the other hand, would like to acknowledge the financial support from “National Laboratories 2020 Program – Artificial Intelligence Subprogram – Establishment of the National Artificial Intelligence Laboratory (MILAB) at Széchenyi István University (NKFIH-870-21/2020)” project. S.Y. Teng would like to acknowledge the financial support from Radboud Centre for Green Information Technology.

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