Design technologies for eco-industrial parks: from unit operations to processes, plants and industrial networks

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Abstract

The concept of eco-industrial park (EIP) has recently become the subject of a great deal of attention from industry and academic research groups. This paper proposes a series of systematic approaches for multi-level modelling and optimisation in EIPs. The novelties of this work include, (1) building a four-level modelling framework (from unit level to process level, plant level and industrial network level) for EIP research, (2) applying advanced mathematical modelling methods to describe each level operation, (3) developing efficient methodologies for solving optimisation problems at different EIP levels, (4) considering symbiotic relations among the three networks (material, water and energy networks) at the top EIP level with the boundary conditions of economic, social and legal requirements. For methodology demonstration, two cases at process level and industrial network level respectively are tested and solved with the developed modelling and optimisation strategies. Finally, the challenges and applications in future EIP research are also discussed, including data collection, the extension of the current networks to EIPs, and the feasibility of the proposed methodologies for complex EIP problems. The extended EIPs include the combination of material exchanges, energy systems and waste-water treatment networks. The aspects considered for future industrial ecology are carbon emission, by-product reuse, water consumption, and energy consumption. The main object of this paper is to explain the detailed model construction process and the development of optimisation approaches for a complex EIP system. In future work, this system is expected to share services, utility, and product resources among industrial plants to add value, reduce costs, improve environment, and consequently achieve sustainable development in a symbiosis community.

Keywords: Eco-industrial parks (EIPs); Resource and energy efficiency; Multi-level modelling and optimisation; Mathematical programming

1. Introduction

Numerous aspects of eco-industrial parks (EIPs) have been widely studied over the past decades. According to Chertow [1], in an EIP system, businesses cooperate with each other and the local community to reduce waste and pollution, efficiently share resources (such as information, materials, water, energy, infrastructure, and natural resources), and minimize environmental impact to increase business success. Several definitions for the concept of EIP have been reported in the literature. However, a basic principle for EIP is that the total benefit (improvements to social, economic and environmental impacts) achieved by working cooperatively is higher than working as a standing alone facility [2]. Kastner et al. [3] reviewed the recent developed quantitative tools and methods identifying and cultivating industrial symbiotic exchanges in existing industrial parks to minimize overall energy and material consumption. EIP application is a systematic approach, where the eco-industrial intent can be realised with a new EIP design, or developed through retrofits in the existing industrial system.

In many EIP studies, life cycle thinking is a very important principle in industrial ecology. It implies that all environmental impacts caused by a product, system, or project during its life cycle are taken into account, including raw material extraction, material processing, manufacture, use, maintenance and disposal. Dong et al. [4] used the tiered hybrid LCA (life cycle analysis) method to evaluate the carbon footprint of an industrial park. They concluded that the two largest sectors for life cycle carbon footprint were chemical industry sector and machinery manufacture sector. Recently, Chen and Chen [5] and Lu et al. [6] proposed ecological network analysis for urban systems and industrial parks. Their methods can help to (1) understand the interactive processes within an existing system (the energy and resource flows between each sector), (2) evaluate its sustainability (carbon metabolism and other environmental problems), (3) figure out the sectors affecting the system significantly, and (4) provide suggestions for improving the whole system performance. Thus, life cycle analysis and network analysis can provide a guideline for selecting key sectors for optimisation in an industrial park to improve the park's overall performance. That is, the chemical and manufacture industry are the two largest sectors for life cycle carbon footprint analysis in an industrial park [4]; Dom (domestic sector) and ITS (industry, trade and service sector) represent the main carbon outflow of the metabolic system [5]; External environment and energy providers are the most dominating inflows of the carbon metabolic system [6]. These sectors will be considered to achieve the economic and environmental benefits of an industrial park in this paper.

Based on the recent studies on EIP optimisation, the main way to design an EIP includes exchanges of materials, water and energy through a sharing network between the companies of an EIP. As stated by Boix et al. [7], these studies focus most of time on the optimisation of single style network, namely considering material, energy and water separately. Regarding the material exchanges in an EIP, the materials can be products, by-products and wastes. These materials from a company might serve as a feedstock to other companies of the park. The main challenge of optimising material networks is how to exchange various materials between plenty of companies in a park to achieve industrial symbiosis. Connelly and Koshland [8, 9] provided an exergy-based definition of resource depletion in EIPs, and proposed a Depletion number (Dp) for quantitative analysis of system sustainability including resource usage and conservation. Cimren et al. [10] developed a novel decision support tool to analyse BPS (by-product synergy) network for material processing and transporting among companies in an EIP. They used mathematical programming techniques to determine the optimal network structure and material flows to minimize total cost or environmental impacts, which also can be extended to analyse dynamic industrial and ecological processes. Haslenda and Jamaludin [11] presented a systematic framework for optimal utilization of by-products from palm oil refining processes. They formulated the material network as a mixed integer linear programming (MILP) model with the objective of maximizing total refinery profit towards Zero Waste. Lim et al. [12] developed a mathematical model for the optimal design and planning of an integrated and resource-efficient rice mill complex. The issues they addressed included product demands, resource availability and energy supply. Most recently, Tan and Aviso [13] proposed a bi-level linear integer programming model for optimising waste exchange between power plants, palm oil mills and bio-refineries in an EIP. Their EIP method dealt with the conflict of interest between EIP authority and industrial plants when economic and environmental benefits could not be achieved simultaneously.

For optimising energy networks in EIPs, many researchers have investigated total site heat integration with graphical and numerical methods. Karimkashi and Amidpour [14] developed a new graphical method based on the R-curve concept, which can be used to retrofit the utility system of a total site and select the cleanest and most economical fuel for boilers. Liew et al. [15] proposed an algorithm to efficiently perform utility targeting for a large-scale TSHI (total site heat integration) system considering renewable energy and variable energy supply/demand. They stated that heat integration analysis utilising a numerical algorithm typically provided higher precision and more rapid calculations compared with the graphical approach. Chae et al. [16] presented a mathematical model to synthesize a waste heat utilization network including nearby companies and communities in an eco-industrial park. They used an existing petro-chemical complex in case study to illustrate the economic and environmental benefits due to the reduction of the regional energy consumption with waste heat recycle. Karlsson [17] used MIND method (Method for analysis of INDustrial energy systems) to optimise industrial energy systems from the food industry to the pulp and paper industry, where the main issues stated by the European Commission were considered, such as reduction of greenhouse gas emissions, improvements regarding security of supply and increased use of renewable energy. Furthermore, Maes et al. [18] investigated different literature energy management strategies in eco-industrial parks in Flanders. They found that energy management on industrial parks can be integrated in the entire development process and park management, and local synergies can be enhanced with energy clustering.

Water network is the most common type for EIP problems reported in the literature. Mathematical programming optimisation has been widely used to study large-scale and multi-objective optimisation problems of water networks at EIPs. Keckler and Allen [19] built a linear program model for exchanging water between several collocated industrial facilities and an industrial water treatment plant, which allowed blending water streams to obtain various degrees of purity to feed different plants. Their results demonstrated that a number of economical water reuse opportunities might exist with water network optimisation. Chew et al. [20] proposed an MILP model for direct interplant water integration (where water from different plants is integrated directly via cross-plant pipelines), and an MINLP model for indirect interplant water integration (where water from different plants is integrated indirectly via a centralized utility hub). They stated that the implementation of centralized utility hub improves the overall water network practicability and flexibility when serving a greater numbers of plants comprising the individual water network. Lovelady and El-Halwagi [21] developed an optimisation approach of the water management among multiple processes in a common EIP facility. Recycle, reuse, and separation using interception devices were considered as possible strategies for managing waste-water to minimise the total EIP annual cost associated with interception operation, fresh water consumption and waste treatment. Montastruc et al. [22] gave some guidelines for performing a flexibility analysis of an existing EIP, including implementing linear multi-objective optimisation for identifying the best solutions corresponding to different scenarios, and using two indicators (the equivalent number of connections (ENC) which reflects the piping and pumping costs in the EIP infrastructure, and the Global Equivalent Cost (GEC) expressed as an equivalent of freshwater flow rate) for performing the choice of some particular solutions.

As discussed above, various strategies have been reported to achieve EIP optimisation. However, the optimisation of EIP lies on the decoupling of networks at the present state, and the existing research is based on either the material exchanges [8-13], or the energy links [14-18] or water reuse facilities [19-22], typically focusing on a single aspect of the three. The optimal symbiotic relations among industries in an EIP require considering all resources simultaneously within the whole system. This will increase the difficulty of solving EIP problems with conventional optimisation approaches, as too many potential resource exchanging options are addressed in the mathematical programming models, which leads to computational difficulties (curse of dimensionality) for finding an optimal or even feasible solution. Focusing on the study of solving the computational difficulties for large scale and complex industrial optimisation problems, this paper presents a novel multi-level modelling and optimisation approach for EIPs. Firstly, a hierarchy framework is structured to describe the four levels of an EIP from bottom to top (namely from unit operations, to processes, plants and industrial networks), which has not been addressed in the existing research previously. Secondly, advanced mathematical modelling approaches are utilized to accurately predict the object performance at each EIP level. Efficient optimisation methodologies are then developed to find the optimal performance or designs for different level problems. Finally, the combination of the three networks (material, water and energy networks) at the top EIP level is recommended to increase the symbiotic relations among the industries in an EIP. An important development is to consider the surrounding environment of an EIP, including the available natural resources, social and economic situation of the region, which is fundamental to evaluate total impacts of the EIP.

This paper is structured as follows: methodology developments for EIP modelling and optimisation are introduced in Section 2, followed by the method demonstrations in a process-level problem and a network-level problem in Sections 3 and 4. Section 5 presents the discussion of challenges and applications in future EIP research, including data collection, the combination of material exchanges, energy systems and waste-water treatment networks to achieve industrial symbiosis, and the feasibility of the proposed methodologies for EIP optimisation under the above complex situations.

2. Methodology development for EIP modelling and optimisation

In this section, a holistic approach is proposed towards the fulfilment of the outlined goals accomplished through research and development at multiple levels with an integrated framework, which includes a hierarchy model (four levels) of EIPs, advanced mathematical modelling approaches for describing each level performance, and efficient optimisation methodologies for solving complex EIP problems.

2.1 The hierarchy model of EIPs

This work addresses the symbiosis of energy and resource management for enhancing energy efficiency, improving cost effectiveness, and increasing sustainability and environmental benefits in EIPs. In order to achieve this, an EIP is described in a four-level framework (from unit level, to process level, plant level and industrial network level), and it is proposed to associate the technical components at each level with its own representation which include executable models and optimisation approaches. Fig. 1 briefly shows the hierarchy model and the overall symbiosis network of an EIP, where the models at industrial network level are composed of the models from the plant level, and the models of lower levels (unit level, process level and plant level) are built using High Dimensional Model Representation (HDMR) surrogate modelling methods based on the simulation results provided by commercial software tools or the practical data from industries. At each lower level (units, processes and plants), efficient optimisation approaches are developed to find the best performance of each surrogate model. Finally, the whole industrial symbiosis can be achieved with the optimal interaction across the resource, energy and waste networks at the top level.

The main object of this paper is to explain the detailed model construction process and the development of optimisation approaches for the above four-level EIP system. The sustainability can be achieved at each EIP level, including (1) optimal unit operations with minimal electrical consumption, (2) optimal processes producing minimum waste, (3) flexible plant planning and scheduling under varying market and environmental requirements, and (4) optimal EIP networks with the lowest emission and waste discard. It is envisaged that this system will make it possible to facilitate the process of planning, commissioning, and controlling optimal energy and resource exchanging among the industrial plants and infrastructures in an EIP with the consideration of economic, social, and legal requirements as the boundary conditions. However, the difficulties of considering such detailed EIP performances must be sorted out, including model accuracies, model simplifications, and the optimisation of complex mathematical problems. These will be introduced in the following sections.

2.2 Surrogate models for describing unit, process and plant operations

In practical modelling work, detailed models of units, processes and plants are complex to be coded. Many specialised simulation software packages have been used in the existing studies. At unit level, the literature models for heat exchangers [23] are updated and compared with the simulation results given by the commercial software tools (HTRI® and HEXTRAN®), which can be applied to predict exchanger performances at process level [24-26]. At plant level, the analysis of integrating power plant with CO_2 capture plant is carried out using the software packages (GateCycle^{TM} and Aspen Plus^{TM}), which provides detailed plant operating data for the further optimisation in plant integration [27]. However, these simulation software packages appear to the users as black boxes. To tackle the complexity of building very detailed models based on the explicit knowledge of the physical behaviour of the system, surrogate models are adopted to find the connections between the system state variables (input, internal and output variables). The experiment data from references [28, 29] or the data generated with applying commercial software packages are used to construct simpler but accurate models which include accurate empirical approximation describing the relation between input variables and response values of a system. The HDMR method not only takes into account the inherent uncertainties in the input parameters but also potential non-linearities and contributions due to interactions between input parameters. This method has been applied to analyse the economic viability of a chemical process under technical and economic uncertainties [30] and its global sensitivity analysis [31].

As presented in Fig. 1, the system information at lower EIP levels is obtained from commercial software simulation, practical industrial data and literature results. The problems at these levels then can be modelled with the used of surrogate models. It is noticed that an EIP includes many units, processes and plants which do not have published models in the literatures, and the simulation models supplied by the commercial software are commercial confidentiality. This is not suitable for optimizing energy and resource management in an EIP without the consideration of detailed operations from unit to plant levels. In order to build the surrogate models for various units, processes and plants, High Dimensional Model Representation (HDMR) method developed by Brownbridge et al. [30] is used to generate surrogate models which have been demonstrated as the most efficient and actual models in industrial applications. The main feature of HDMR is the decomposition of the full function into a sum of functions that only depend on subsets of the input variables such that:

$$y = f_0 + \sum_{i=1}^{N} f_i(x_i) + \sum_{i=1}^{N}\sum_{j=i+1}^{N} f_{ij}(x_{i,}x_j) + \cdots + f_{12\ldots N}(x_{1,}x_{2,} \ldots, x_N) \quad (1)$$

where N is the number of input parameters, i and j index the input parameters, and f_0 is the mean value of $f(x)$.

The expansion given in Eq. (1) has a finite number of terms and exactly represents f(x), however for most practical applications terms containing functions of more than two input parameters can often be ignored due to their negligible contributions compared to the lower order terms [32, 33]. Therefore the truncated approximation (Eq. (2)) is sufficient for most models/data. Whilst it is possible to evaluate each of these terms using direct numerical integration, a more efficient method is to approximate the functions $f(x_i)$ and $f(x_{i,j})$ with analytic functions.

$$y \approx f_0 + \sum_{i=1}^{N} f_i(x_i) + \sum_{i=1}^{N}\sum_{j=i+1}^{N} f_{ij}(x_{i,}x_j) \quad (2)$$

2.3 Mathematical programming methods for network modelling

The aim of HDMR surrogate method is to reduce the computational complexities of lower level models but maintain their accuracies, which facilitates the formulations of network level problems with combining plant level surrogate models, as shown in Fig. 1. However, it must be noted that the HDMR surrogate method is only available in the condition of existing systems, where unit operating conditions, process structures and plant designs are known. At industrial network level, the network structure is unknown and must be determined to optimally exchanging resources between the plants. This requires the use of mathematical programming methods to formulate a network superstructure that includes all the potential resource connections. A detailed modelling method for building network superstructures has been proposed by Pan et al. [34], and will be developed for modelling material networks, water networks and energy networks in this research.

2.4 Optimisation methods

Although benefits of the conventional optimisation methods have been appreciated, their applications are still limited in EIP problems, as large scale nonlinear programming models are usually required based on these methods, leading to computational difficulties associated with a large number of nonlinear formulations (nonconvex terms), variables and constraints. In this paper, the most challenge task is to propose a series of optimisation approaches to address the problems with respect to numerous EIP aspects, such as efficiently sharing resources (including information, materials, water, energy, infrastructure, and natural resources), reducing waste and pollution, and minimizing environmental impact while simultaneously increasing business success. To achieve this objective, the whole EIP system has been divided into four levels (unit level, process level, plant level and industrial network level), which is not allowed to grow to a size that makes the resulting optimisation problem intractable, and an efficient optimisation approaches is proposed for each level optimisation.

The key characteristics of modelling industrial problems are nonlinearity and combinatorial complexity. The MILP-based iterative method proposed by Pan et al. [24, 26, 29, 34-36] is developed to overcome both the combinatorial issues related to the large number of possible activities and the non-linear nature of process production in EIP problems. This developed optimisation approach presents an iterative procedure for solving complex MINLP problems, including variable initialization, model linearization, solving MILP problems, solution analysis, and initial variable updating. As shown in Fig. 2, an objective value (better than the initial objective value of the MINLP problem) is estimated first. The initial values of variables are given from the problem initial status. Based on these initial values, the MINLP model is linearized with the use of first order Taylor series expansions, heuristic rules and variable initialization, and then an MILP model is obtained. The MILP problem can be solved to minimise the variable differences between MILP and MINLP problems by using CPLEX solver in the software tool, General Algebraic Modelling System (GAMS), a high-level modelling system for mathematical programming and optimisation. The initial values of the MINLP problem variables are updated iteratively with the values from the MILP solution until the variables of MINLP problem are similar to those given by the MILP solution. The objective of the iterative procedure is to find the MILP problem solution which also can be used as the solution in the MINLP problem.

In other word, Fig. 1 presents the general procedure of the proposed approaches for multi-level modelling and optimisation of an EIP, where four levels from EIP's bottom to top are described; then simulation software tools, literature models and practical data provide sufficient input parameters for building HDMR surrogate models at unit level, process level and plant level respectively, the networks at the top EIP level are structured based on the proposed mathematical methodology with plant surrogate models for model simplification; once each level operating model is obtained, it can be optimised with the developed optimisation approaches. Since generalized modelling and optimisation approaches have been proposed, two cases at process level and industrial network level will be tested with the detailed methods in the next two sections.

3. Methodology demonstration 1: an algae gasification process in dual fluidized bed gasifiers (process level)

The algae gasification process proposed by Azadi et al. [31] has been applied to dual fluidized bed gasifiers to convert algae to syngas and hydrogen for the realization of algal energy in the near-term future. In this case, the algae gasification process is simulated using Aspen Plus^{TM} process simulation package, and five key process-input parameters (i.e. algae oil content, feed water flowrate, gasifier temperature, and steam-to-biomass and air-to-fuel ratios) are taken into account to build the process surrogate models related to the lower heating value (LHV) of syngas, cold gas efficiency (CGE), and H_2 yield. Moreover, the operation of this process can be optimised further to obtain the highest raw material conversion (CGE), thus minimising the process waste and improving the suitability of the process.

3.1 Process simulation (Aspen Plus^{TM})

Fig. 3 presents the detailed flowsheet of the algae gasification process built in Aspen Plus^{TM}. The process feed, dry algae (ALGAE: 1 kg/s, 20 ^{o}C and 1 bar), is separated into solids (SOLIDS) and volatile matter (VM) in a pyrolyzer (PYROL) at first. VM is then reacted with two steam fluids (HTSTEAM and 23) in a reformer (REFORMER: 800 ^{o}C and 1 bar), which produces RGIBBSOU including H_2, CO, CO_2, CH_4, H_2O, H_2S, NH_3 and P. The combination of SOLIDS with RGIBBSOU is separated in a cyclone (CYCLONE: 800 ^{o}C and 1 bar) to obtain gas (GAS) and char (CHAR). GAS stream can be split into two parts after a splitter (B1), where one part of GAS (3: 0.831 of GAS split fraction), the high temperature syngas (SYNGAS), is used to heat the air (AIR) in the first exchanger (HX1: 750 ^{o}C of cold stream outlet temperature) and the water (WATER) in the second exchanger (HX2: 120 ^{o}C of hot stream outlet temperature) sequentially, while another part of GAS (AUXFUEL: 0.169 of GAS split fraction) and the hot air (HOTAIR) from HX1 are fed into a combustor (COMBUST: 950 ^{o}C, 1 bar, and allowable products include CO_2, O_2, N_2, H_2O, NO_2, SO_2, P) for CHAR combustion. Hot fuel gas (HOTFLG) separated from the combustion stream (COMBOUT) will be cooled down in the third exchanger (HX3: 800 ^{o}C of cold stream outlet temperature) and the fourth exchanger (HX4: 120 ^{o}C of hot stream outlet temperature) which increase the temperatures of steam (LTSTEAM) and water stream (MOISTURE).

The simulation addressed in this work is similar to the algae gasification process presented in Reference [30, 31], which includes using the Peng–Robinson equation of state for thermal calculations and Gibbs energy minimization, and equilibrium-based reactors for the reformer and combustor, and more details can be found in [31]. Simulation results are obtained with varying the five input parameters mentioned in the beginning of this section. The ranges of these parameters are shown in Table 1.

3.2 Process modelling and optimisation (HDMR surrogate methodology)

To analyse the process performance, three objective values are considered separately, including the LHV of syngas, cold gas efficiency (CGE) defined as the ratio between the sum of the energy content of all of the products to that of the feed, and H_2 yield. The HDMR method introduced in Section 2.2 has been programmed in an advanced software tool (MoDS$^{®}$), and is utilized to build the surrogate models for describing the process operations accurately [37]. Moreover, Eq. (2) is reformatted in Eq. (3) for a better model expression.

$$y = C + \sum_{i=1}^{N}\sum_{k=1}^{K} A_{i,k} \times x_i^k + \sum_{i=1}^{N}\sum_{j=i+1}^{N}\sum_{k=1}^{K}\sum_{n=1}^{K} B_{i,j,k,n} \times x_i^k \times x_j^n \tag{3}$$

In the above surrogate expansion, C is a constant term, $A_{i,k}$ and $B_{i,j,k,n}$ are the first and second order coefficients, x_i and x_j represent input parameters, and y is function value. Table 2 presents the detailed surrogate models obtained by using MoDS$^{®}$. Thus, the algae gasification process can be expressed as a black-box model with the above surrogate formulations (Fig. 4). Table 2 and Fig. 4 show the efficiency of a HDMR surrogate model, namely using a very simple formulation to represent a complex process in which a great of its internal functions are unknown. Using the HDMR surrogate model we aim to find the process operation condition which maximise the LHV of syngas, or CGE, or H2 yield, which also can be achieved with the use of optimisation solvers provided in MoDS$^{®}$. Table 3 shows the optimal solutions in three scenarios (maximisations of LHV, CGE and H_2 yield), where the small errors between surrogate results and original simulation data (2.82%, 3.15% and 1%)

demonstrate the accuracy and efficiency of the proposed surrogate modelling approach. This HDMR surrogate method is not only used for optimising process operation but also for process uncertainty analysis and its global sensitivity analysis. The uncertainty analysis and global sensitivity analysis of the same algae gasification process have been presented in our previous work [30, 31] with the use of the proposed HDMR surrogate method.

It is must be noted that, the modelling and optimisation approach based on the HDMR surrogate methodology mentioned in Section 2.2 can be used to solve the problems of an existing system (e.g. unit, or process, or plant) efficiently. However, if the configuration of a system is unknown, such as considering a design problem for material exchanges at EIP network level, the mathematical programming and optimisation methods proposed in Sections 2.2 and 2.3 are required for building the superstructure of the addressed network and finding the optimal connections between all the network elements. This will be presented in the next section.

4. Methodology demonstration 2: a material network design for Jurong Island EIP (industrial network level)

This section presents a new model for minimizing network cost and CO_2 emission of material exchanging at Jurong Island in Singapore. It considers material network problems incorporating raw material purchasing, freight transportation selection (including trucks, short-sea vessels and pipelines), and the CO_2 emissions associated with the selected transportation options. A case study is carried out to demonstrate the efficiency of the proposed approach, which addresses 14 companies producing 13 products as the raw materials for 21 companies, and aims to achieve the economic and environmental benefits simultaneously with the optimal material transportations between the above companies. The following work includes a problem statement of the material network at Jurong Island in

Singapore, data collection for the study, model for optimising the material network, and the optimal results and discussion.

4.1 Problem statement

An important part of Singapore’s industry, Jurong Island, spread over an area of approximately 32 square kilometres. More than 100 companies are resident on Jurong Island, which produce a wide range of products including petroleum products, fine chemicals and pharmaceuticals, as described in Fig. 5 [38]. Jurong Island meets all investor requirements (basic infrastructure, logistics, services and access to the feedstock), which makes the industrial symbiosis realizable. Companies can buy and sell feedstock and products in an integration system. To achieve such integration of materials, a new material transportation model will be built, leading to a cost efficient and environment-friendly structure.

First of all, the following information must be collected to derive the proposed approach for material network problems:

(1) Superstructure of the material network (i.e. all potential material connections between all companies).

(2) Company locations in the material network (i.e. distances between all potential connecting companies).

(3) Feedstock information of each company (i.e. demands of raw materials per year, and their prices).

(4) Product information of each company (i.e. plant capacities per year, and product types).

(5) Parameters for calculating transportation costs related to different transportation tools (i.e. trucks, short-sea vessels and pipelines).

(6) Parameters for calculating CO_2 emission related to different transportation tools (i.e. trucks, short-sea vessels and pipelines).

(7) Parameters for calculating installation costs of pipelines (it is assumed that trucks and

short-sea vessels can be hired, and their costs have been combined in their transportation cost in the item (4) mentioned above).

For the minimization of network cost and CO_2 emission, the optimisation methodology of material exchanging is to determine:

(1) Structure of the material network (optimal material connections between the network companies).

(2) Suitable strategies for material purchasing from local market and international market.

(3) Suitable freight transportation selections (trucks, short-sea vessels and pipelines).

(4) New pipeline installation.

(5) Total transportation cost in a certain project life time.

(6) Total CO_2 emissions associated with transportation in a certain project life time.

4.2 Data collection

Data collection is the major challenge in the study. Some actual data have been provided by the local government sectors, which describes company locations at Jurong Island. However, most of information required in Section 4.1 is unknown without the collaboration from the government due to their confidentiality concerns. In order to obtain all necessary information for the network modelling addressed in this work, several approaches have been utilized, including public internet searching and literature reviewing. Even though the obtained information is incomplete from Singapore at the moment, the proposed work will be as accurate as we would like it to be once all the real data are given by users. The relevant data collection work is described in details as follows.

(i) Company information

Plant capacities and product prices for 35 companies are available from internet. E.g. in Shell Eastern Petroleum Pte Ltd at Jurong Island, the capacity of alcohol ethoxylates is 40 kt/yr [39], and its price is 1750 \$/mt [40]. Based on the product information from the above companies, raw material information (such as raw material types and their amounts) of these companies is estimated by reviewing their main chemical processes. Fig. 6 presents an illustration of searching raw materials for Shell OMEGA Process from reference [41], which provides the main feedstock information and process configuration to produce ethylene glycols (MEG).

(ii) Superstructure of the material network

The information of 35 companies have been collected, including plant capacities, raw material demands, material prices, and the distances between upstream and downstream plants, based on the internet searching. Table 4 shows the abbreviations for all sources and demands in the material network. Moreover, Tables 5 and 6 describe the distances between all the potentially connectable companies, and the detailed source and demand information in the addressed network. Consequently, the superstructure of the material network is obtained by connecting all the potential upstream and downstream plants given in Tables 5 and 6, as shown in Fig. 7.

(iii) Transportation costs and CO_2 emissions of material exchanges

Transportation operations are one of central aspects in material network problems. Chemical materials are usually transported by trucks, ship vessels and pipelines. Lots of review literature can be found in this area [42]. Some general parameters proposed in References [43] and [44] can be utilized to calculate the transportation costs and CO_2 emissions with using different transportation tools (Table 7). It is also assumed that trucks and ships can be hired from third-party logistics providers, and pipelines must be installed first if they are chosen for the transportation.

4.3 Model for optimising the material network

Since all the necessary information is obtained with data collection, it is possible to model the material network with the consideration of material purchasing, transportation routes, transportation tool selection, infrastructure installation, transportation costs and CO_2 emissions associated with the selected transportation tools. To build such a network model, it is assumed that the companies located in different islands must require short-sea shipping, or short-sea pipelines, or both for material transportation, and the material exchanges between the companies in the same island should use trucks, or land pipelines or both. Furthermore, if the local market cannot provide enough materials to the demand plants, these materials must be purchased in the international market. Thus, several binary variables are proposed to describe the selection of transportation tools (trucks, short-sea ships, pipelines, and international ships), as presented as follows:

$$rt_{r,d} = \begin{cases} 1, if\ source\ r\ is\ transported\ to\ demand\ d\ with\ trucks \\ 0, otherwise \end{cases}, \forall r \in R, d \in D$$

$$lpt_{r,d} = \begin{cases} 1, if\ \ source\ r\ is\ transported\ to\ demand\ d\ with\ land\ pipelines \\ 0, otherwise \end{cases}, \forall r \in R, d \in D$$

$$it_{r,d} = \begin{cases} 1, if\ \ source\ r\ is\ transported\ to\ demand\ d\ with\ international\ shipping \\ 0, otherwise \end{cases}, \forall r \in R, d \in D$$

$$wt_{rs,js} = \begin{cases} 1, if\ \ source\ rs\ is\ transported\ to\ demand\ ds\ with\ short-sea\ ships \\ 0, otherwise \end{cases}, \forall rs \in R_s, ds \in D_s$$

$$wpt_{rs,ds} = \begin{cases} 1, if\ \ source\ rs\ is\ transported\ to\ demand\ ds\ with\ short-sea\ pipelines \\ 0, otherwise \end{cases} \quad \forall rs \in R_s, ds \in D_s$$

$$wit_{rs,ds} = \begin{cases} 1, if\ \ source\ rs\ is\ transported\ to\ demand\ ds\ with\ international\ shipping \\ 0, otherwise \end{cases} \quad \forall rs \in R_s, ds \in D_s$$

In the above variables, R is the set of all sources can transport their materials with land transportation, D is the set of all demands can receive materials with land transportation, R_s is the set of all sources need to transport their materials with sea transportation, and D_s is the set of all demands must receive materials with sea transportation. $rt_{r,d}$, $wt_{rs,ds}$, $lpt_{r,d}$ and $wpt_{rs,ds}$ are used to describe the material purchasing in the local market, while $it_{r,d}$ and $wit_{rs,ds}$ are propose for buying materials from the international market.

Eqs. (4)-(9) express the transportation activities at the material network, where the amounts of materials transported from sources to demands must be restricted with the relevant selections, e.g. if trucks are chosen for transporting source r to demand d ($rt_{r,d}$ = 1), its transporting amount ($mrt_{r,d}$) can be a positive value; otherwise ($rt_{r,d}$ = 0), no materials is transported (namely $mrt_{r,d}$ = 0). The amounts of materials transported with short-sea ships ($mwt_{rs,ds}$), land pipelines ($mlpt_{r,d}$), water pipelines ($mwpt_{rs,ds}$) and international shipping ($mit_{r,d}$ and $mwit_{rs,ds}$) are formulated in the same way. M is a sufficiently large positive number.

$$mrt_{r,d} \leq M \times rt_{r,d},\ \forall r \in R, d \in D, \tag{4}$$

$$mwt_{rs,ds} \leq M \times wt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{5}$$

$$mlpt_{r,d} \leq M \times lpt_{r,d},\ \forall r \in R, d \in D, \tag{6}$$

$$mwpt_{rs,ds} \leq M \times wpt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{7}$$

$$mit_{r,d} \leq M \times it_{r,d},\ \forall r \in R, d \in D, \tag{8}$$

$$mwit_{rs,ds} \leq M \times wit_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{9}$$

The total demand of material (dj_d and djs_{ds}) is the sum of its amounts transported with trucks ($mrt_{r,d}$), short-sea ships ($mwt_{rs,ds}$), pipelines ($mlpt_{r,d}$ and $mwpt_{rs,ds}$) and international shipping ($mit_{r,d}$ and $mwit_{rs,ds}$), as described in Eqs. (10) and (11).

$$dj_d = \sum_{\forall r \in R} \left(mrt_{r,d} + mlpt_{r,d} + mit_{r,d} \right), \qquad \forall\, d \in D, \tag{10}$$

$$djs_{ds} = \sum_{\forall rs \in R_s} \left(mwt_{rs,ds} + mwpt_{rs,ds} + mwit_{rs,ds} \right), \qquad \forall\, ds \in D_s\,, \tag{11}$$

The source constraints are presented in Eqs. (12) to (15), where the total amount of material (ri_r or ris_{rs}) transported from source r / rs cannot be larger than its production (pri_r or $pris_{rs}$).

$$ri_r = \sum_{\forall d \in D} \left(mrt_{r,d} + mlpt_{r,d}\right), \qquad \forall\, r \in R, \tag{12}$$

$$ris_{rs} = \sum_{\forall ds \in D_s} \left(mwt_{rs,ds} + mwpt_{rs,ds}\right), \qquad \forall\ rs \in R_s\,, \tag{13}$$

$$ri_r \leq pri_r, \qquad \forall\, r \in R, \tag{14}$$

$$ris_{rs} \leq pris_{rs}, \qquad \forall\ rs \in R_s\,, \tag{15}$$

The transportation costs and CO_2 related to using trucks, short-sea ships and pipelines are calculated based on the References [43] and [44]. In Eqs. (16) and (17), $rtc_{r,d}$ is the truck cost for transporting source r to demand d, ct is truck transportation cost per material amount and distance, $drt_{r,d}$ is the distance between source r and demand d, $crt_{r,d}$ is the truck CO_2 emission for transporting source r to demand d, and cet is truck CO_2 emission for transporting per material amount per distance.

$$rtc_{r,d} = ct \times mrt_{r,d} \times drt_{r,d},\ \forall r \in R, d \in D, \tag{16}$$

$$crt_{r,d} = cet \times mrt_{r,d} \times drt_{r,d},\ \forall r \in R, d \in D, \tag{17}$$

Eqs. (18) and (19) are the formulations of transportation cost ($wtc_{rs,ds}$) and CO_2 emission ($cwt_{rs,ds}$) for short-sea ships, where $csst$ is short-sea shipping transportation cost per material amount and distance, $dwt_{rs,ds}$ is the distance between source rs and demand ds, and $cset$ is short-sea shipping CO_2 emission for transporting per material amount per distance.

$$wtc_{rs,ds} = csst \times mwt_{rs,ds} \times dwt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{18}$$

$$cwt_{rs,ds} = cset \times mwt_{rs,ds} \times dwt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{19}$$

Moreover, pipeline transportation is considered in Eqs. (20)-(25), including transportation costs ($lptc_{r,d}$ and $wptc_{rs,ds}$), CO_2 emissions ($clpt_{r,d}$ and $cwpt_{rs,ds}$), and installation costs ($ilptc_{r,d}$ and $iwptc_{rs,ds}$). $clpt$ and $cwpt$ are transportation cost per material amount and distance for land

and short-sea pipelines. *celp* and *cewp* are CO_2 emission per material amount and distance for land and short-sea pipelines. i*clpt* and i*cwpt* are installation cost per distance for installing land and short-sea pipelines.

$$lptc_{r,d} = clpt \times mlpt_{r,d} \times drt_{r,d},\ \forall r \in R, d \in D, \tag{20}$$

$$wptc_{rs,ds} = cwpt \times mwpt_{rs,ds} \times dwt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{21}$$

$$clpt_{r,d} = celp \times mlpt_{r,d} \times drt_{r,d},\ \forall r \in R, d \in D, \tag{22}$$

$$cwpt_{rs,ds} = cewp \times mwpt_{rs,ds} \times dwt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{23}$$

$$ilptc_{r,d} = iclpt \times lpt_{r,d} \times drt_{r,d},\ \forall r \in R, d \in D, \tag{24}$$

$$iwptc_{rs,ds} = icwpt \times wpt_{rs,ds} \times dwt_{rs,ds},\ \forall rs \in R_s, ds \in D_s, \tag{25}$$

The total material purchasing cost (*tpc*) is the sum of the costs buying materials in the local market (using trucks, short-sea ships, land pipelines and short-sea pipelines for transportation) and international market (using international shipping). ip_r and ips_{rs} are the prices of sources *r* and *rs* sold in the local market. It also is assumed that the cost of purchasing material in the international market is 1.05 times of its local market price as international shipping cost and CO_2 emission converted into tax have been combined in the international cost, as shown in Eq. (26).

$$\begin{aligned} tpc = &\sum_{\forall r \in R} \sum_{\forall d \in D} \left[ip_r \times \left(mrt_{r,d} + mlpt_{r,d} + 1.05 \times mit_{r,d} \right) \right] \\ &+ \sum_{\forall rs \in R_s} \sum_{\forall ds \in D_s} \left[ips_{rs} \times \left(mwt_{rs,ds} + mwpt_{rs,ds} + 1.05 \times mwit_{rs,ds} \right) \right] \end{aligned} \tag{26}$$

Since the CO_2 emission caused by international shipping has been considered in the total material purchasing cost, the total CO_2 emission of the material network (*tce*) will include the emissions from truck transporting ($crt_{r,d}$), short-sea shipping ($cwt_{rs,ds}$), and pipeline operating ($clpt_{r,d}$ and $cwpt_{rs,ds}$).

$$tce = \sum_{\forall r \in R} \sum_{\forall d \in D} \left(crt_{r,d} + clpt_{r,d} \right) + \sum_{\forall rs \in R_S} \sum_{\forall ds \in D_S} \left(cwt_{rs,ds} + cwpt_{rs,ds} \right) \qquad (27)$$

To consider the network cost and CO_2 emission in one objective, carbon tax (*ctax*, e.g. 50 \$/t-CO_2 used in Reference [2]) is utilized to express the penalty caused by CO_2 emission in the network. Thus, the total cost of the material network in a certain lifetime (*obj*) can be formulated as the sum of transportation cost, the penalty caused by transportation CO_2 emission, and the cost of pipeline installation. In Eq. (28), *ify* is the interest factor of the project lifetime, and *acf* is the annual cost factor.

$$obj = ify \times \left[tpc + ctax \times tce + \left(\sum_{\forall r \in R} \sum_{\forall d \in D} ilptc_{r,d} + \sum_{\forall rs \in R_S} \sum_{\forall ds \in D_S} iwptc_{rs,ds} \right) \times acf \right] \qquad (28)$$

Consequently, the model for minimizing network cost and CO_2 emission for material exchanging in an industrial park consists of the objective function given in Eq. (28) and model constraints given from Eqs. (4)-(27).

4.4 Results and discussion

The material network problem is solved with CPLEX solver in GAMS based on the collected information in Tables 4-7. The objective is to minimize the total network cost and CO_2 emission (expressed in Eq. (28)). There are five scenarios (assuming project lifetimes with 0% rate of interest) considered in this section, namely 1 year, 10 years, 20 years, 50 years and 100 years of lifetimes. The comparison of the optimal solutions in these lifetimes is shown in Table 8.

In Table 8, it can be found that, the same material purchasing strategy is proposed in all solutions, where most of materials are from the local market, and the rest mounts of materials exceeding the local market provision are bought from international market. Fig. 8 presents the optimal network structure for such material purchasing strategies. Table 8 also shows that, for a short-term consideration, especially in one year lifetime, trucks and ships are used for local material transportation as pipeline installation is more expensive in this situation. However, with the increase of project lifetime, more pipelines are installed to reduce the annual network cost and CO_2 emission. When a very long-term plan is addressed, e.g. 100 years, land pipelines are recommended for internal land transportation, and ships are still utilized for short-sea freight due to the very high investment of installing offshore pipelines (85320 \$/km of land pipeline installation vs. 620000 \$/km of offshore pipeline installation, as shown in Table 7). In the condition of the optimal solution for 100 year lifetime, the total network transportation cost is 7.11 M\$ (0.071 M\$/yr of annual cost), which is only 10% of the total network transportation cost in the solution of one year lifetime (76.6 M\$ of total cost, and 0.766 M\$/yr of annual cost). Moreover, the CO_2 emission also decreases significantly (90% of reduction) when the optimal solution of 100 year lifetime is proposed, leading to releasing less CO_2 associated with material transportation (reducing 900 t/year of CO_2 emission). More details about material transportations for the plan of 100 year lifetime can be found in Tables 9.

5. Challenges and applications in future EIP research

Since the proposed modelling and optimisation approaches have been demonstrated in two different level EIP problems (process level and industrial network level), it is possible to address more aspects for further EIP research, such as data collection, the combination of material exchanges, energy systems and waste-water treatment networks to achieve industrial symbiosis based on the guidelines of industrial ecology, and the feasibility of implementing surrogate models in this complex network design problem.

5.1 Data collection

The first step of EIP research is data collection, which requires the collaboration from local government sectors and companies to provide the necessary information for designing an EIP, such as the raw materials, products, by-products and waste materials of companies, and their inflows and outflows. This can be used to determine possible synergies for the addresses EIP, and the pathways between suppliers and customers. However, as mentioned in Section 4.2, data collection is the main barrier in the research. The companies in the network are usually unwilling to provide the aforementioned data due to the potential confidentiality issues. The only way of collecting data at the current stage is to utilize internet search techniques. Some companies might publish their production information online, like process flow diagram [41], raw material requirements [41], and plant capacities [39]. But these are unavailable most of the time. Thus, many literature processes are regarded as the alternatives to the real processes, which does not restrict the proposed approach to be implemented in real situations as long as the accurate data are given by the companies.

5.2 Industrial symbiosis in the addressed EIP

This paper presents the detailed model construction process and the development of optimisation approaches for a complex four-level EIP system. The sustainability has been achieved on two cases at process level and material transportation network level, respectively. In Section 3, the optimal process can produce syngas under the highest raw material conversion (CGE) thus minimising the process waste. The optimal solution obtained in Section 4 has minimised the CO_2 emission associate with material transportation. More sustainable issues can be considered when other EIP level problems are modelled and optimised. Based on the current data collection, CO_2 is found to be the major waste or by-product released from the material network designed in Section 4. Moreover, as stated by Dong et al. [4] and Lu et al. [6], chemical industry and energy providers are the largest sectors for life cycle carbon footprint in an industrial park. Thus, the treatment of CO_2 released from chemical plants and power plants is the key issue in the addressed EIP system. Although the optimal solution obtained in Section 4 has minimised the CO_2 emission associate with material transportation, which is still a few amount compared with the industrial CO_2 release. To reduce such a huge amount of CO_2 emission, some researchers proposed to use CO_2 and ammonia to produce urea [45]. Installing a new urea plant will require more electricity powers, utilities and fresh water, which need to efficiently retrofit the existing power network and water network to satisfy the new demands. Moreover, several CO_2 capture plants must be installed to collect the CO_2 released from chemical plants and power plants, also leading to the modifications of the existing networks [27]. It is also mentioned by Roberts [46] that, the system that utilises the emission and waste flows of industry and consumption, is the domain of industrial ecology. Based on this guideline of industrial ecology, Fig. 9 presents a design framework of EIP optimisation. In future work, water and energy networks well as material network between chemical and power plants will be studied simultaneously; power plants provide electricity and heat to all plants; the clean water from water treatment also can be reused; and emission and waste flows are utilised in the whole system for environmentally-friendly consideration.

5.3 Implementation of the proposed approaches in the EIP design

The EIP framework shown in Fig. 9 is a complex network system including a great number of plants and potential connections for material, water and energy exchanges. To solve such a large scale EIP problem, the proposed multi-level modelling and optimisation approaches (see Fig. 1) are utilized. It can be found in Fig. 1 that, the EIP system has three network problems (material, water and energy networks) at the top level, a number of plant operation problems at the second level, and a large number of process and unit optimisation problems in the last two levels. The upper level models are composed of the models from the adjacent lower level with linking functions. Using surrogate models to represent these linking functions can overcome the computational difficulties caused by high dimensionality EIP problems (from units, to processes, plants and industrial networks), which has been demonstrated in a process-level problem in Section 3.

Based on the above discussion, an optimisation strategy is proposed to solve the EIP problem raised in Section 5.2.

(1) The lower level problems are solved or simulated to generate data for building their surrogate models. At unit level, literature models or commercial software tools can be used to predict unit performances [23, 25, 28], which will provide the calculation or simulation results to create unit surrogate models. Moreover, some commercial software packages, such as Aspen Plus^{TM} and GateCycle^{TM} [27], offer "good enough" models for simulating process and plant operations in chemical and power plant industries. Thus, it is also possible to obtain process and plant surrogate models based on the relevant simulation data.

(2) The detailed plant models are then replaced with their surrogate models in the industrial network design problems. This reduces the complexities of network design problems significantly, as plant surrogate models are much simpler than the detailed models and maintains a high accuracy.

(3) The industrial network design problems are solved with the optimisation approaches proposed in Section 2.3 to optimise the network structures, and the inflows and outflows of each plant.

(4) The determined variables of the upper level problems are set to be the input parameters to the lower level problems, which are solved accordingly. For example, plant production is optimised under the restrictions of plant inflows and outflows determined in the network design problems, and then these optimised plant data are passed to each process problem to find the best process operation; finally, the obtained

process data are utilized in unit models to achieve better unit performances.

Fig. 10 is used to describe above optimisation strategy in details. Consequently, the multi-level modelling and optimisation in EIP problems are realised with the proposed strategy throughout the whole EIP system, from units to processes, plants and industrial networks. First, surrogate modelling methods provide simply but accurate models for unit, process and plant problems. Second, it is easier to solve the network design problems with plant surrogate models due to the significant reduction of model complexity. Third, the optimisation approaches proposed in Section 2.3 can solve the problems at each EIP level, some of which have been demonstrated in Section 4 and References [24, 26, 27, 29, 34-36].

6. Conclusion

EIPs have been widely studied in the recent decades. The main difficulty of this research is caused by coupled networks and their complexities. This leads to most of researchers only considering a single type of EIP networks (water network, or energy network, or material network) with simple assumptions of resource variability to reduce the problem complexity. However, to optimise an EIP, all types of resource should be considered simultaneously within the whole network. Complete understanding of the complexity of these issues requires a substantial amount of supporting realistic models relative to each potential member of the EIP.

This paper presents the general modelling and optimisation methods for industrial parks (namely novel multi-level modelling and optimisation methodologies). The industrial park addressed is an integration system consisting of the EIP problems at four levels: three network problems (material, water and energy networks) at the top level, a number of plant operation problems at the second level, and a large number of process and unit optimisation problems at the last two levels. Each problem at each EIP level can be formulated as a model (Sections 2.2 and 2.3), and solved using the optimisation approaches proposed in Section 2.4. In Sections 3 and 4, one process and one material transportation network are optimised, showing that our approaches can achieve maximum raw material conversion for the process, and minimise transportation costs and carbon emission in the material transportation network. The models presented for this process and material transportation network are the two sub-models in the EIP system. More sub-models, such as detailed unit and process operation, chemical and power plants, material networks (utilisation of waste and by-product), water networks and energy networks, will be built and integrated in the next phase in our research, as stated in Section 5.2. Then, the methodology introduced in Section 5.3 will be used to integrate all the EIP sub-models, transfer the information from the top level problems to lower level problems, and achieve the optimisation and sustainability of the whole system.

In future work, it will be necessary to consider manipulating material and energy flows from larger systems (like urban systems) to industrial parks. According to the urban system addressed by Chen and Chen [5], an industrial park is a part of the urban system. The industrial park studied in this paper included energy production sector (Ene), water and soil sector (W&S), industry, trade and service sector (ITS), domestic sector (Dom), local environment (Loc), and distal environment (Dis). Based on the proposed modelling approaches, each compartment in the urban system can be described by a surrogate model which presents highly approximate input-output behaviour (resource and energy flows) of the compartment. Finally, the urban system model is composed of the compartment surrogate models with linking functions. Using surrogate models to represent these linking functions can overcome the computational difficulties caused by high dimensionality urban problems. At last, economic, social, legal and environmental requirements will be considered as the boundary conditions for the urban problem which can be optimised with the use of our advanced optimisation method to achieve its economic and environmental benefits. The characteristics of the optimal system are expected to be low carbon emission, high by-product reuse, and low energy and material consumption.

Nomenclature

Indices

d	demand that can receive materials with land transportation
ds	demand that must receive materials with sea transportation
i	input parameters of an HDMR surrogate model (Eqs. (1) and (2))
j	input parameters of an HDMR surrogate model (Eqs. (1) and (2))
r	source that can transport their materials with land transportation
rs	source that need to transport their materials with sea transportation

Sets

D	set of all demands that can receive materials with land transportation
D_s	set of all demands that must receive materials with sea transportation
R	set of all sources that can transport their materials with land transportation
R_s	set of all sources that need to transport their materials with sea transportation

Parameters

acf	annual cost factor
$A_{i,k}$	the first order coefficients in a reformatted surrogate model (Eq. (3))
$B_{i,j,k,n}$	the second order coefficients in a reformatted surrogate model (Eq. (3))
C	constant term of a reformatted surrogate model (Eq. (3))
$celp$	CO_2 emission per material amount and distance for land pipelines
cet	truck CO_2 emission for transporting per material amount per distance
$cewp$	CO_2 emission per material amount and distance for short-sea pipelines
$clpt$	transportation cost per material amount and distance for land pipelines
$cset$	short-sea shipping CO_2 emission for transporting per material amount per distance
$csst$	short-sea shipping transportation cost per material amount and distance
ct	truck transportation cost per material amount and distance
$ctax$	carbon tax
$cwpt$	transportation cost per material amount and distance for short-sea pipelines
dj_d	total amount of material transported to demand d
djs_{ds}	total amount of material transported to demand ds
$drt_{r,d}$	distance between source r and demand d
$dwt_{rs,ds}$	sea distance between source rs and demand ds
f_0	mean value of $f(x)$ in an HDMR surrogate model (Eqs. (1) and (2))
$\mathrm{i}clpt$	installation cost per distance for installing land pipelines
$\mathrm{i}cwpt$	installation cost per distance for installing short-sea pipelines
ify	interest factor of the project lifetime
ip_r	prices of source r sold in the local market
ips_{rs}	prices of source rs sold in the local market
k	exponent of x_i in a reformatted surrogate model (Eq. (3))
K	maximum exponent of input parameters in a reformatted surrogate model (Eq.

	(3))
M	a sufficiently large positive number
N	number of input parameters of an HDMR surrogate model (Eqs. (1) and (2))
n	exponent of x_j in a reformatted surrogate model (Eq. (3))
pri_r	production of source r
$pris_{rs}$	production of source rs
x_i	input parameters of a reformatted surrogate model (Eq. (3))
x_j	input parameters of a reformatted surrogate model (Eq. (3))
y	function value of a reformatted surrogate model (Eq. (3))

Variables

Continuous

$clpt_{r,d}$	transportation CO_2 emission for transporting source r to demand d with land pipelines
$crt_{r,d}$	transportation CO_2 emission for transporting source r to demand d with trucks
$cwpt_{rs,ds}$	transportation CO_2 emission for transporting source rs to demand ds with short-sea pipelines
$cwt_{rs,ds}$	transportation CO_2 emission for transporting source r to demand d with short-sea ships
$ilptc_{r,d}$	installation cost of land pipelines for transporting source r to demand d
$iwptc_{rs,ds}$	installation cost of short-sea pipelines for transporting source rs to demand ds
$lptc_{r,d}$	transportation cost for transporting source r to demand d with land pipelines
$mit_{r,d}$	amount of transporting source r to demand d with international shipping
$mlpt_{r,d}$	amount of transporting source r to demand d with land pipelines
$mrt_{r,d}$	amount of transporting source r to demand d with trucks
$mwit_{rs,ds}$	amount of transporting source rs to demand ds with international shipping
$mwpt_{rs,ds}$	amount of transporting source rs to demand ds with short-sea pipelines
$mwt_{rs,ds}$	amount of transporting source rs to demand ds with short-sea ships
obj	total cost of the material network in a certain project lifetime
ri_r	total amount of material transported from source r
ris_{rs}	total amount of material transported from source rs
$rtc_{r,d}$	transportation cost for transporting source r to demand d with trucks
tce	total material transportation CO_2 emission in a material network
tpc	total material purchasing cost in a material network
$wptc_{rs,ds}$	transportation cost for transporting source rs to demand ds with short-sea pipelines
$wtc_{rs,ds}$	transportation cost for transporting source rs to demand ds with short-sea ships

Binary

$it_{r,d}$	1 if source r is transported to demand d with international shipping; otherwise, it is 0
$lpt_{r,d}$	1 if source r is transported to demand d with land pipelines; otherwise, it is 0
$rt_{r,d}$	1 if source r is transported to demand d with trucks; otherwise, it is 0
$wit_{rs,ds}$	1 if source rs is transported to demand ds with international shipping; otherwise, it is 0

$wpt_{rs,ds}$	1 if source *rs* is transported to demand *ds* with short-sea pipelines; otherwise, it is 0
$wt_{rs,ds}$	1 if source *rs* is transported to demand *ds* with short-sea ships; otherwise, it is 0

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List of tables

Table 1 Ranges of input parameters for surrogate modelling of the algae gasification process

Parameters	Lower bound	Upper bound
$\boldsymbol{x_1}$**:** Algae oil content (%)	0.00	40.0
$\boldsymbol{x_2}$**:** Gasifier temperature (^{o}C)	700	900
$\boldsymbol{x_3}$**:** Steam to biomass ratio (kg/kg$_{algae}$)	0.40	0.80
$\boldsymbol{x_4}$**:** Fuel-air equivalence ratio (kg/kg$_{algae}$)	0.10	0.25
$\boldsymbol{x_5}$**:** Feed water (kg/s)	0.25	1.00

Table 2 Detailed surrogate models of the algae gasification process

Coefficients	$y = C + A_{1,1}x_1 + A_{2,1}x_2 + A_{3,1}x_3 + A_{4,1}x_4 + A_{5,1}x_5 + A_{1,2}x_1^2 + A_{2,2}x_2^2 + A_{3,2}x_3^2 + A_{4,2}x_4^2 + A_{5,2}x_5^2 + B_{1,2,1,1}x_1x_2 + B_{1,3,1,1}x_1x_3 + B_{1,4,1,1}x_1x_4 + B_{1,5,1,1}x_1x_5 + B_{2,3,1,1}x_2x_3 + B_{2,4,1,1}x_2x_4 + B_{2,5,1,1}x_2x_5 + B_{3,4,1,1}x_3x_4 + B_{3,5,1,1}x_3x_5 + B_{4,5,1,1}x_4x_5$		See Eq. (3)
	LHV (MJ)	H_2 (kg/s)	CGE (%)
C	20.73	0.0532	1.08
$A_{1,1}$	0.18	0.00057	0.0011
$A_{2,1}$	-0.00019	0.00003	-0.00027
$A_{3,1}$	-4.84	0.0452	-0.215
$A_{4,1}$	-16.02	0.03	0.167
$A_{5,1}$	-3.42	0.05	-0.068
$A_{1,2}$	0	0	-0.00002
$A_{2,2}$	0	0	1.59
$A_{3,2}$	0	0	-0.0175
$A_{4,2}$	0	0	-2.07
$A_{5,2}$	0	0	-0.071
$B_{1,2,1,1}$	0	0	0
$B_{1,3,1,1}$	0.0383	0.00042	0.0026
$B_{1,4,1,1}$	-0.245	-0.00091	-0.0114
$B_{1,5,1,1}$	0.0242	0.00033	0.0018
$B_{2,3,1,1}$	0.00114	-0.00004	0.00005
$B_{2,4,1,1}$	0.00486	-0.00004	0.00020
$B_{2,5,1,1}$	-0.00165	-0.00005	-0.00007
$B_{3,4,1,1}$	8.724	0.0233	0.375
$B_{3,5,1,1}$	-0.07	-0.0263	-0.00641
$B_{4,5,1,1}$	10.95	0.0354	0.46
R^2	0.98	0.95	0.9

R^2: coefficient of determination

Table 3 Optimal solutions in three scenarios (maximisation of LHV, CGE and H_2 yield) based on the obtained surrogate models for the algae gasification process

	Surrogate models						Simulation results	Error (%)
	x_1	x_2	x_3	x_4	x_5	Objective value		
Max LHV (MJ)	40.00	900	0.4	0.1	0.25	24.364	23.695	2.82
Max H_2 (kg/s)	40.00	700	0.8	0.25	1	0.1406	0.1363	3.15
Max CGE (%)	28.83	900	0.4	0.1	0.25	0.9206	0.9300	1.00

$\boldsymbol{x_1}$**:** algae oil content (%); $\boldsymbol{x_2}$**:** gasifier temperature (^{o}C); $\boldsymbol{x_3}$**:** steam to biomass ratio (kg/kg$_{algae}$); $\boldsymbol{x_4}$**:** fuel-air equivalence ratio (kg/kg$_{algae}$); $\boldsymbol{x_5}$**:** feed water (kg/s)

Table 4 Abbreviations for all sources and demands in the material network at Jurong Island

Source plants		
Companies	Products	No.
Celanese Singapore Pte Ltd	Acetic acid	r1
Ellba Eastern Pte Ltd	Propylene Oxide	r2
ExxonMobil Chemical Asia Pacific Pte Ltd	Ethylene	r3
	Benzene	r4
Invista Singapore Pte Ltd	Adipic Acid	r5
Lucite International Singapore Pte Ltd	Methyl methacrylate Monomer	r6
Mitsui Phenols Singapore Pte Ltd	Phenol	r7
	Bisphenol A	r8
Petrochemical Corporation Of Singapore Pte Ltd	Ethylene	r9
	Propylene	r10
	Butadiene	r11
Shell Chemicals Seraya Pte Ltd	Propylene Oxide	r12
Singapore Acrylic Pte Ltd	Acrylic Acid	r13
Singapore Methyl Methylacrylate Pte Ltd	Methyl methacrylate Monomer	r14
Sumitomo Chemical Singapore Pte Ltd	Methyl Methacrylate Monomer	r15
Jurong Aromatics Corporation Pte Ltd	Benzene	r16
Eastman Chemical Singapore Pte Ltd	Oxo-Alcohols	r17
Shell Eastern Petroleum Pte Ltd	Ethylene oxide	r18

Demand plants		
Companies	Products	No.
Asahi Kasei Plastics Singapore Pte Ld	Polyphenylene Ether	d1
Celanese Singapore Pte Ltd	Vinyl Acetate Monomer	d2
Chevron Phillips Singapore Chemicals (Pte) Ltd	Linear Polyethylene	d3
DIC Alkyphenol Singapore Pte Ltd	Para-tertiary Butylphenol	d4
DuPont Company (Singapore) Pte Ltd	PA66	d5
Eastman Chemical Singapore Pte Ltd	Oxo-Alcohols	d6
Ellba Eastern Pte Ltd	Styrene Monomer	d7
	Propylene Oxide	d8
Huntsman Singapore Pte Ltd	Polyetheramines	d9
Lucite International Singapore Pte Ltd	Methyl methacrylate Monomer	d10
Mitsui Phenols Singapore Pte Ltd	Phenol & Cumene	d11
	Acetone & Cumene	d12
Shell Chemicals Seraya Pte Ltd	Styrene Monomer	d13
	Propylene Oxide	d14
Singapore Acrylic Pte Ltd	Acrylic Acid	d15
Singapore Glacial Acrylic pte ltd	Glacial Acrylic Acid	d16
Teijin Polycarbonate Singapore Pte Ltd	Polycarbonate Resin	d17
	Butyl & Ethyl & Methyl acrylates	d18
Asahi Kasei Synthetic Rubber Singapore Pte Ltd	SSBR	d19
CCD (Singapore) Pte Ltd	Vinyl Acetate Monomer	d20
Rohm and Haas Chemicals Singapore Pte Ltd	MBS	d21
Sumitomo Chemical Asia Pte Ltd	SSBR	d22
Shell Eastern Petroleum Pte Ltd	Alcohol ethoxylates	d23
	Polyether polyols &Propylene glycols	d24
Huntsman Singapore Pte Ltd	Polyetheramines	d25
Shell MEG	MEG	d26

Table 5 Distances between the potential connectable companies (km)

	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10	d11	d12	d13	d14	d15	d16	d17	d18	d19	d20	d21	d22	d23	d24	d25	d26
r1																				6						
r2									1.5															4		
r3		4	5.3							3.8										1.5						
r4							8				5		8													
r5					2																					
r6																					3.5					
r7	1			1.5																						
r8																	0.5									
r9		4	1.5							4										6.3						
r10						3.2		2.2				3.1		2.2	3	3										
r11																			8			3				
r12									1.5															4		
r13																		0.5								
r14																					3.5					
r15																					3.5					
r16							10.4				5.3		10.4													
r17																							8			
r18																									7	4

Table 6 Source and demand information in the material network

Sources

	r1	r2	r3	r4	r5	r6	r7	r8	r9	r10	r11	r12	r13	r14	r15	r16	r17	r18
Amount (kt/yr)	500	250	1900	580	115	120	300	210	1010	1000	55	181	73	200	223	438	65	150
Price ($/t)	555	1750	1254	1364	1700	2010	1510	2072	1254	1124	2161	1750	1988	2010	2010	1023	1605	3190

Demands

	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10	d11	d12	d13	d14	d15	d16	d17	d18
Amount (kt/yr)	35.3	68.4	400	10	38.8	87.5	412.5	181	28.2	33.6	411.5	205.8	292.5	131.1	42.6	35	202	39.2

	d19	d20	d21	d22	d23	d24	d25	d26
Amount (kt/yr)	10.3	283.8	12	8.3	9.9	285.7	27.8	574.8

Table 7 Parameters for calculating costs and CO_2 emissions of trucks, ship vessels and pipelines [40, 41]

		Transportation cost ($/t×km)	CO_2 emission (g CO_2/t×km)	Installation cost ($/km)
Trucks		0.1000	138	
Ships		0.0150	31	
Pipelines	Land	0.0017	10	85320
	Sea	0.0017	10	620000

Table 8 Comparison of the optimal solutions under different life times

Optimal solutions	Transportation cost (10^3 × $/yr)				Raw material purchasing cost (10^9 × $/yr)		Pipeline installation cost (10^6 × $)		CO_2 emission associated with transportation per year (t/yr)					Total costs related to transportations (transportation + pipeline installation) in different life times (10^6 × $)				
	Trucks	Short-sea ships	Pipelines		Local market	International market	Land	Sea	Trucks	Short -sea ships	Pipelines		Total	1 year	10 years	20 years	50 years	100 years
			Land	Sea							Land	Sea						
Solution 1 (1 year)	743.81	22.23	0	0	3.48	1.54	0	0	1026.5	45.9	0	0	1072.4	**0.77**	7.66	15.32	38.30	76.60
Solution 2 (10 years)	97.52	22.23	10.99	0	3.48	1.54	1.47	0	134.6	45.9	64.6	0	245.1	1.60	**2.77**	4.08	8.00	14.54
Solution 3 (20 years)	16.43	22.23	12.37	0	3.48	1.54	2.79	0	22.7	45.9	72.7	0	141.4	2.84	3.30	**3.81**	5.34	7.89
Solution 4 (50 years)	3.99	22.23	12.58	0	3.48	1.54	3.39	0	5.5	45.9	74.0	0	125.4	3.43	3.78	4.16	**5.33**	7.27
Solution 5 (100 years)	0	22.23	12.64	0	3.48	1.54	3.62	0	0	45.9	74.3	0	120.3	3.66	3.97	4.32	5.37	**7.11**

Table 9 Optimal transportation solution in 100-year life time

	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10	d11	d12	d13	d14	d15	d16	d17	d18	d19	d20	d21	d22	d23	d24	d25	d26
r1																				283.8 (LP)						
r2																								132.9 (S)		
r3										33.6 (LP)																
r4																										
r5					38.8 (LP)																					
r6																										
r7	35.3 (LP)			10 (LP)																						
r8																	202 (LP)									
r9		68.4 (LP)	400 (LP)																							
r10						87.5 (LP)		181 (LP)				205.8 (LP)		131.1 (LP)	42.6 (LP)	35 (LP)										
r11																			10.3 (LP)			8.3 (LP)				
r12									28.2 (LP)															152.8 (S)		
r13																		39.2 (LP)								
r14																					12 (LP)					
r15																										
r16							26.5 (LP), 386 (I)				411.5 (LP)		292.5 (I)													
r17																							9.9 (S)			
r18																									27.8 (I)	65 (S), 509.8 (I)

Number (K): the amount of material (kt/yr) is transported with transportation K; **T**: truck transportation; **S**: short-sea transportation; **LP:** land pipeline transportation; **I**: international purchasing. E.g. **35.3 (T):** 35.3 kt/yr of material is transported with trucks; **9.9 (S):** 9.9 kt/yr of material is transported with ships; **400 (LP):** 400 kt/yr of material is transported with land pipelines; **27.8 (I):** 27.8 kt/yr of material is purchased from international market.

List of figures

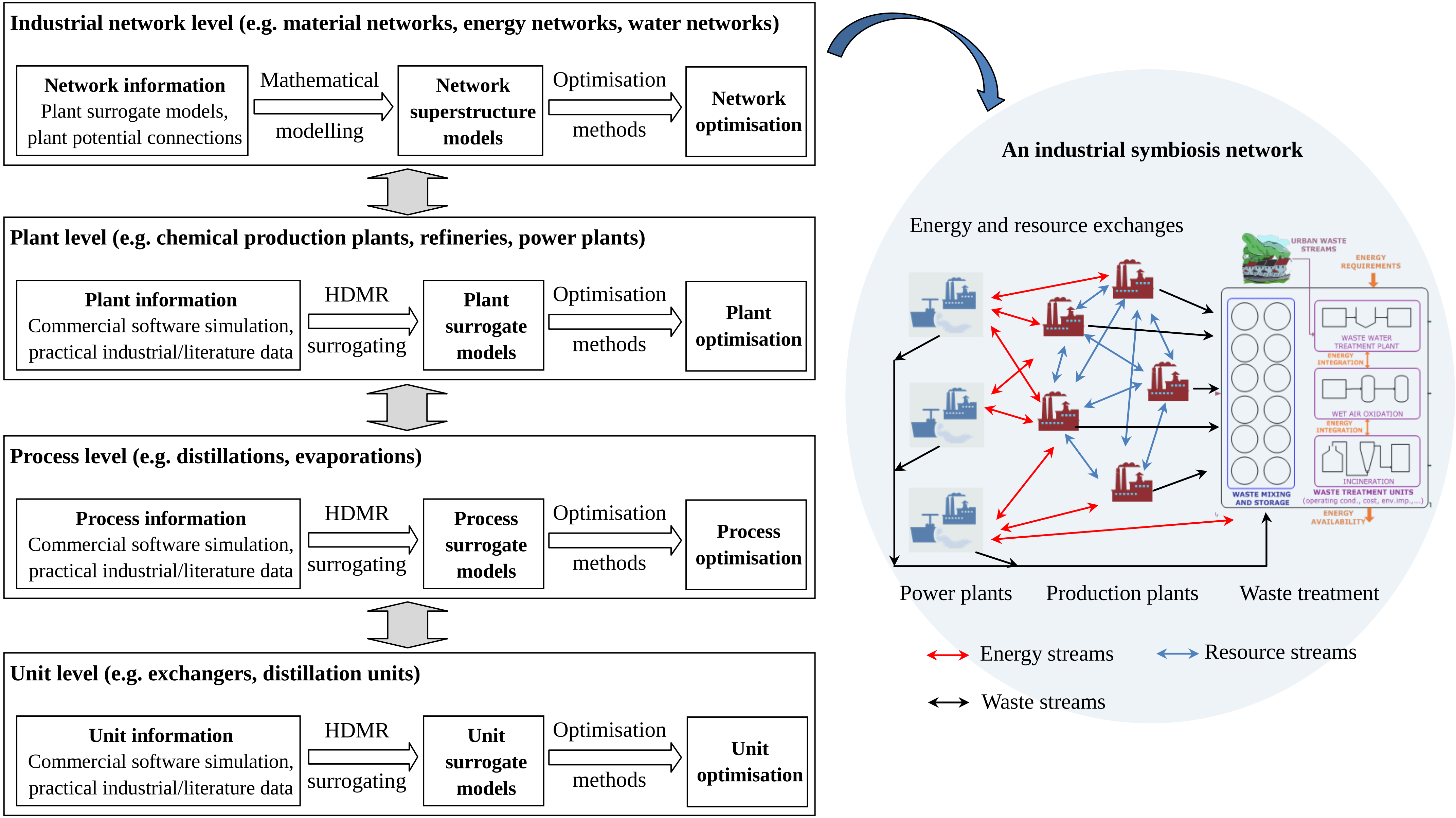


Fig. 1 An illustration of hierarchy model and overall symbiosis network of an EIP

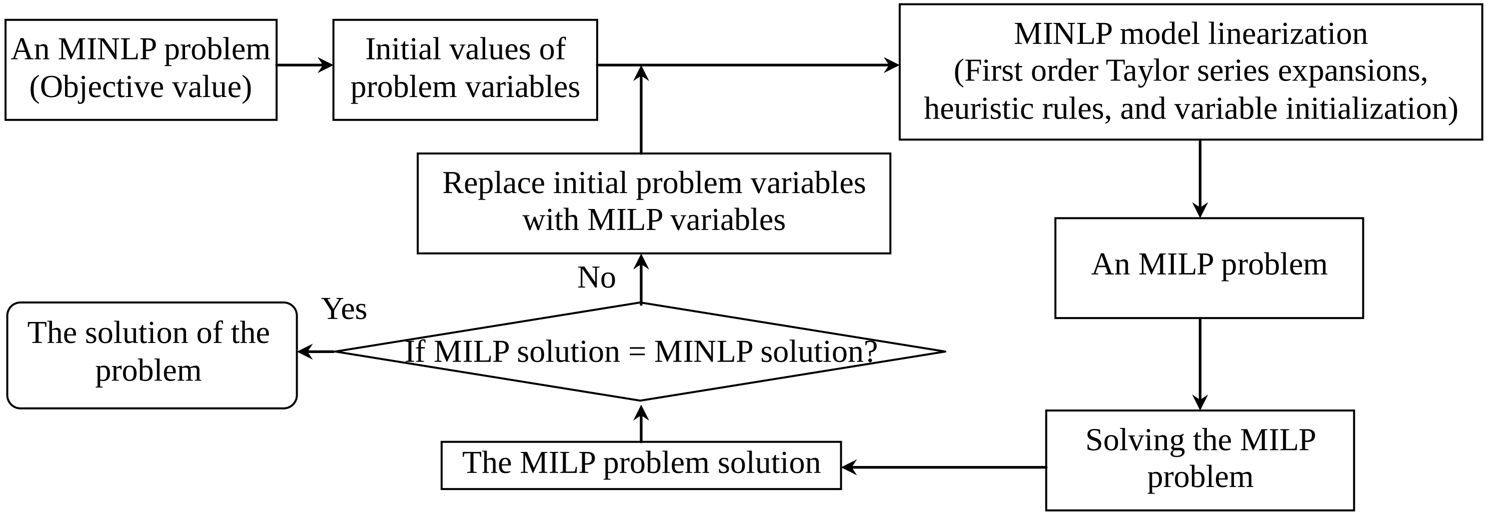


Fig. 2 Procedure of MILP-based iterative optimization approach

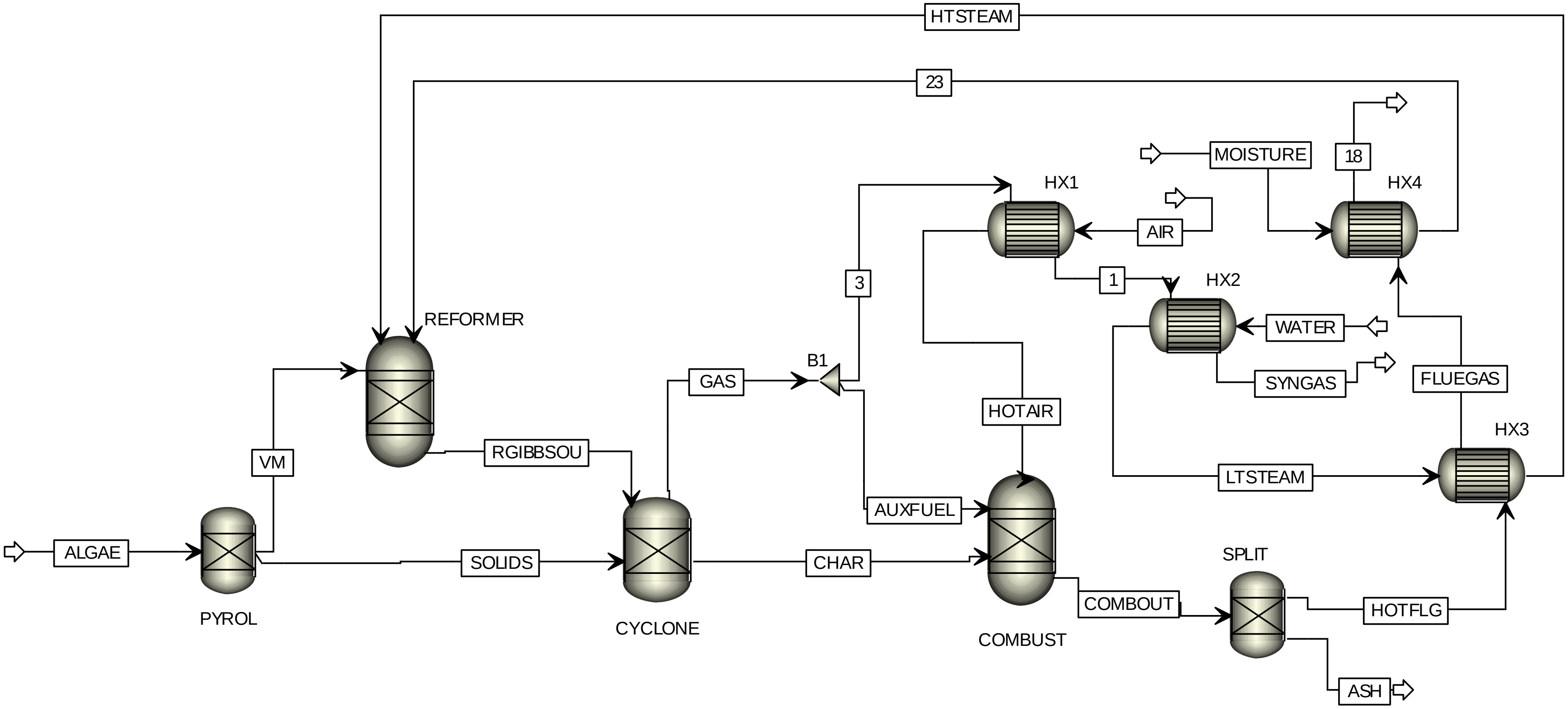


Fig. 3 Flowsheet of the algae gasification process built in Aspen Plus$^{\text{TM}}$

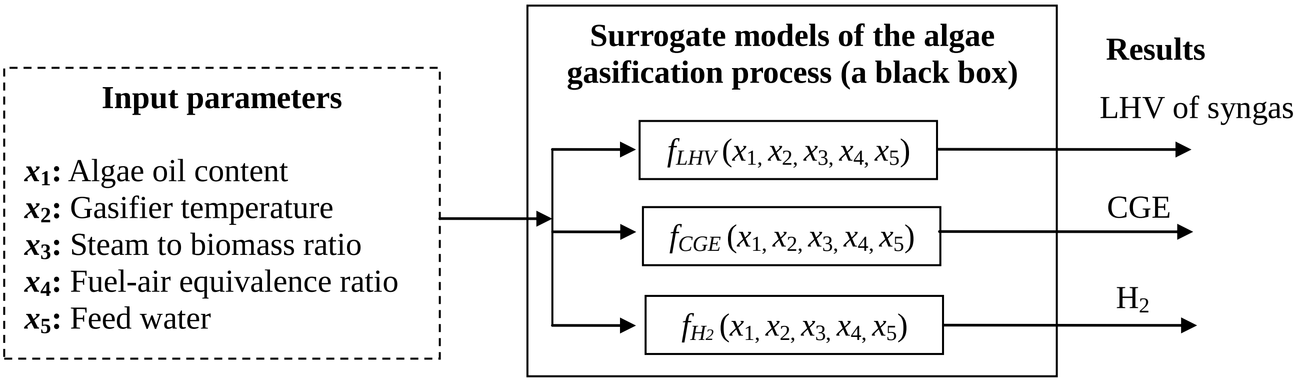


Fig. 4 An illustration of describing the algae gasification process as a black-box model with surrogate formulations

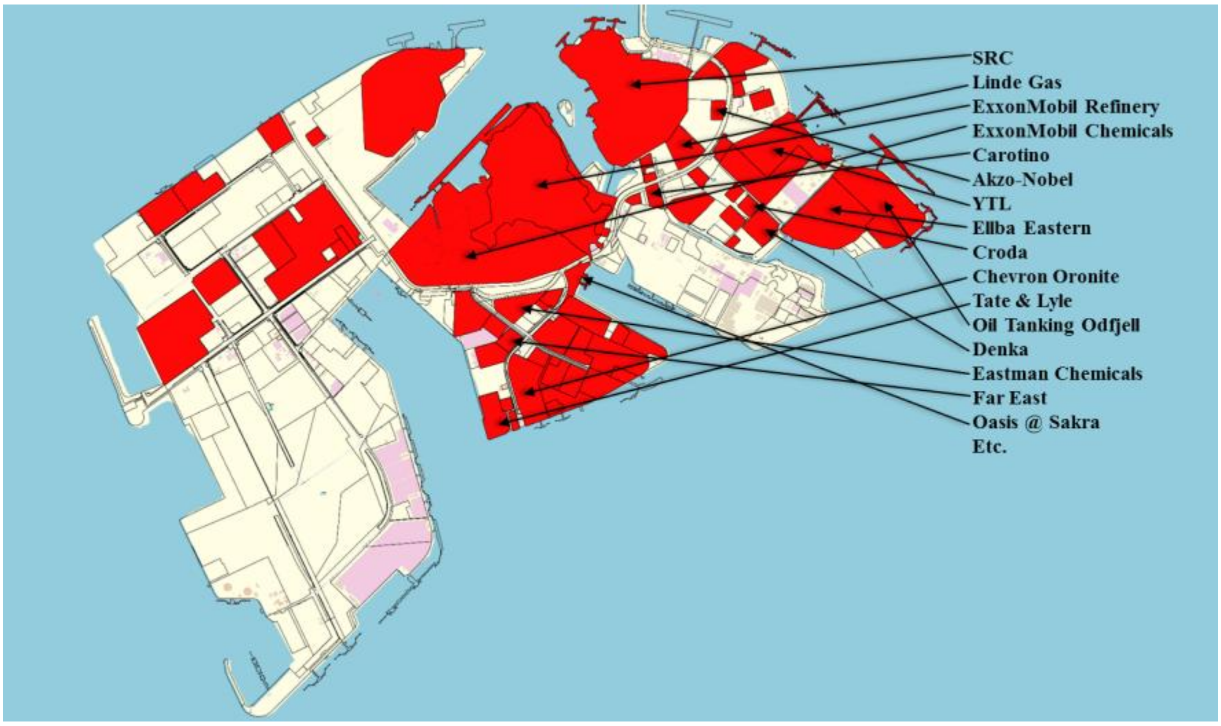
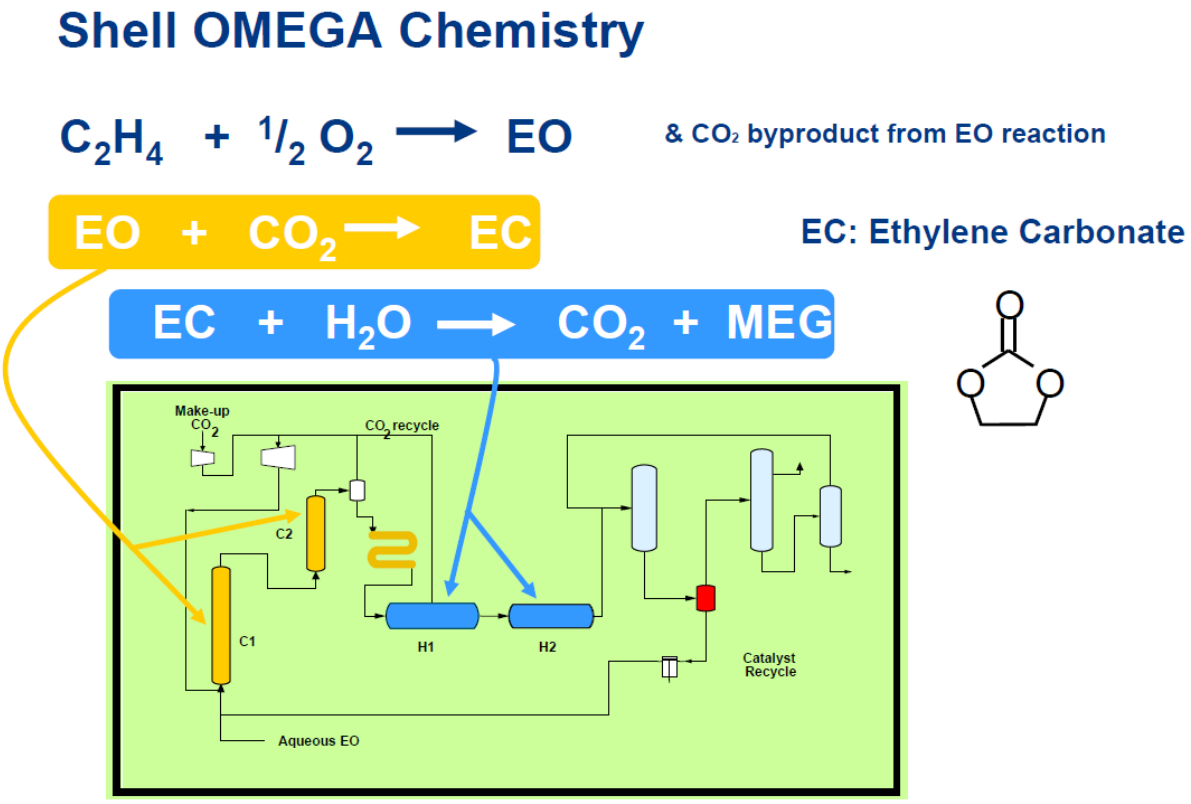


Fig. 5 Map of Jurong Island in Singapore [38]



Shell OMEGA Chemistry

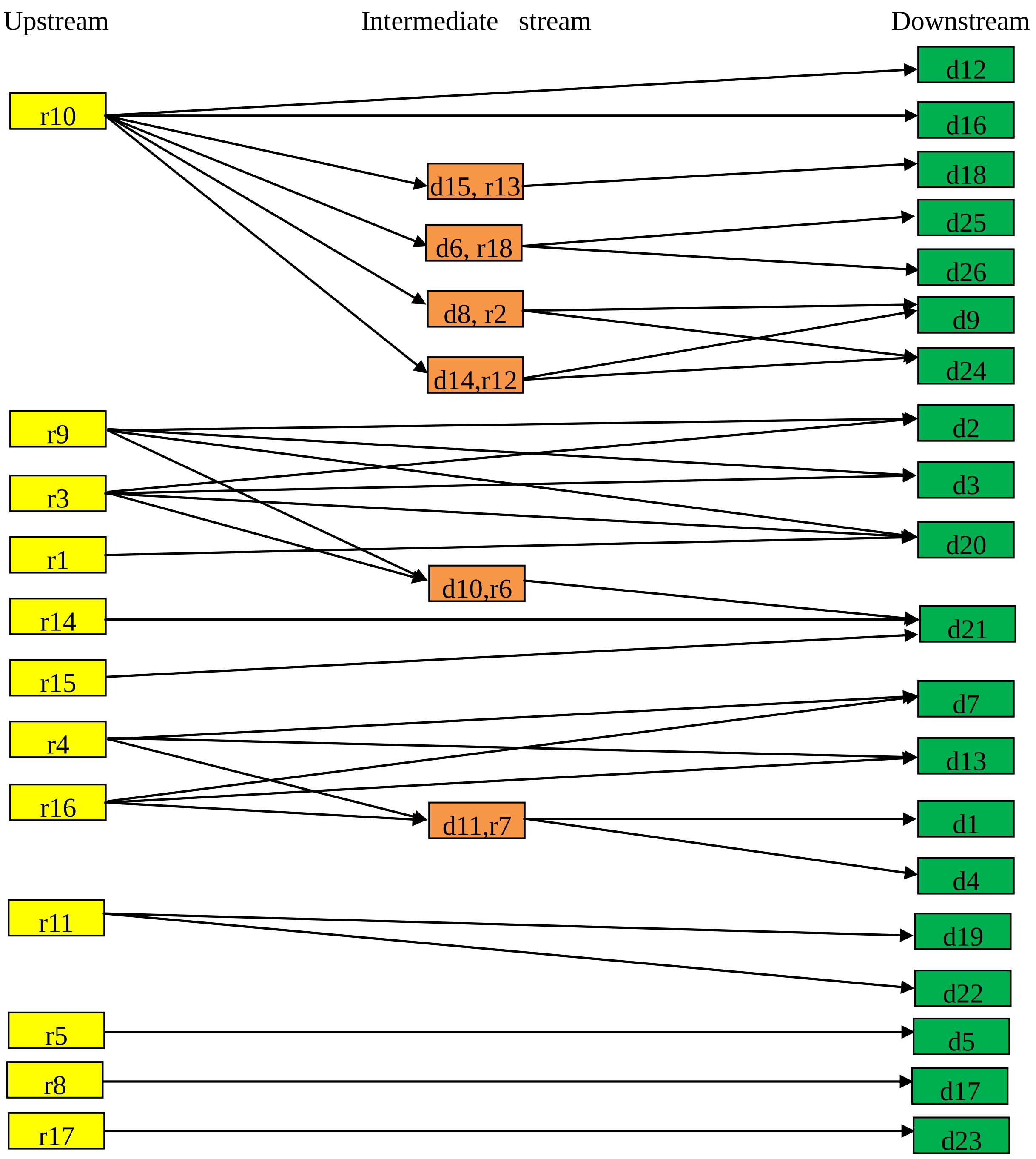
$C_2H_4 + {}^1/_2\,O_2 \longrightarrow EO$ & CO_2 byproduct from EO reaction

$EO + CO_2 \longrightarrow EC$

EC: Ethylene Carbonate

$EC + H_2O \longrightarrow CO_2 + MEG$

Fig. 6 An illustration of searching raw materials for Shell OMEGA Process from reference [41]



r: source plant producing materials; d: demand plant receiving materials

Fig. 7 Superstructure of the material network in Section 4

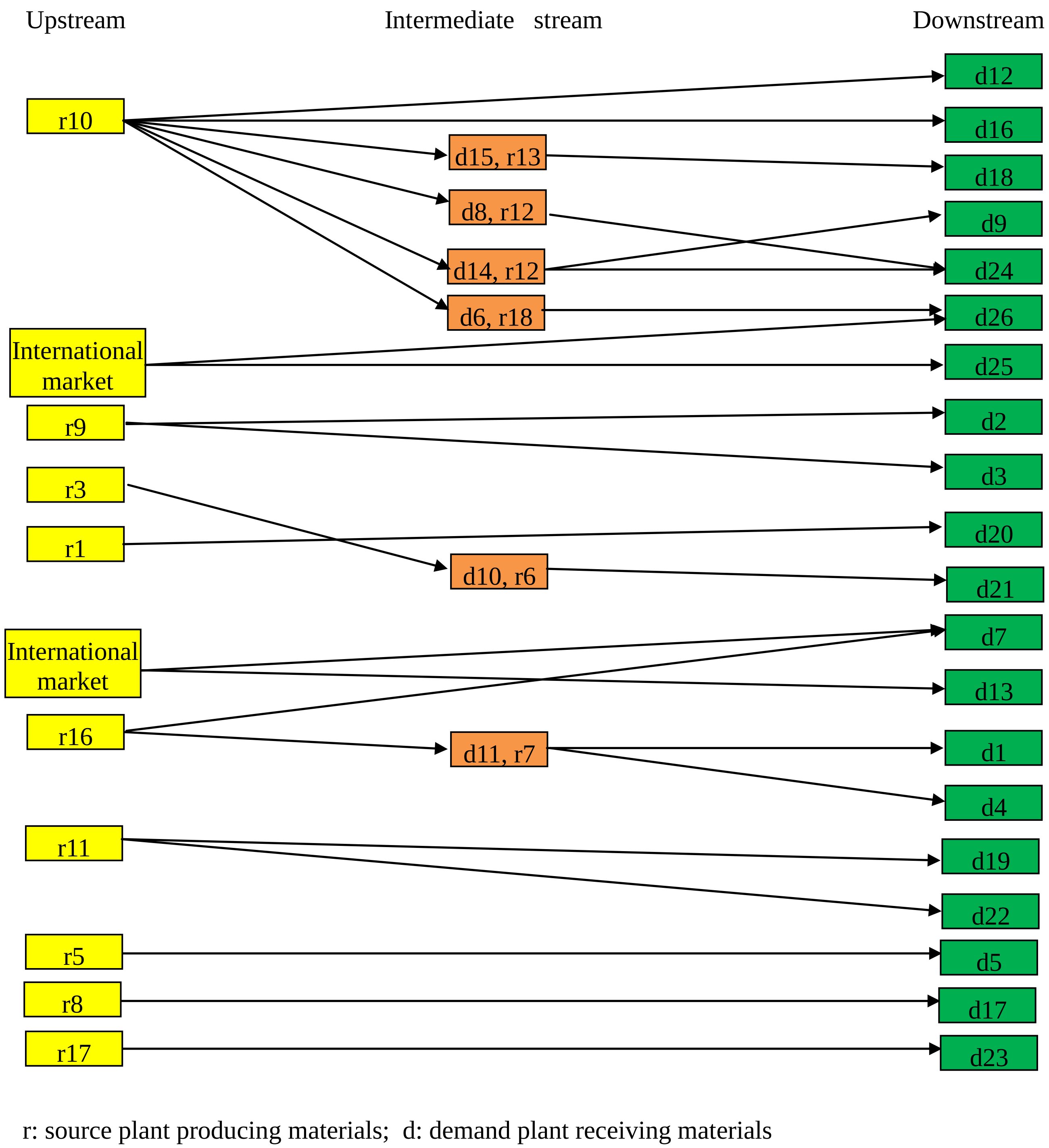


Fig. 8 Optimal structure of the material network in Section 4

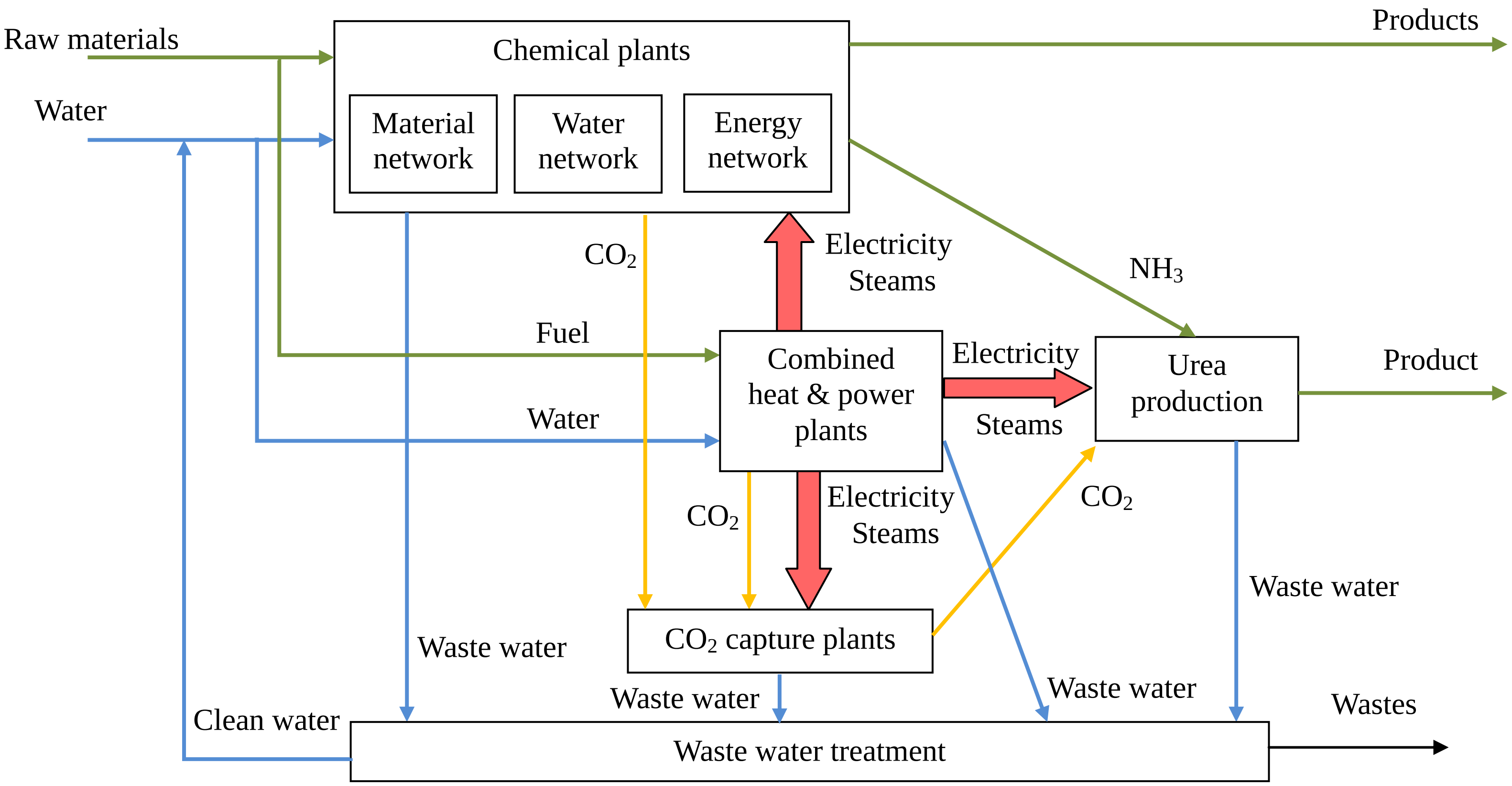


Fig. 9 A design framework of EIP optimisation in future study

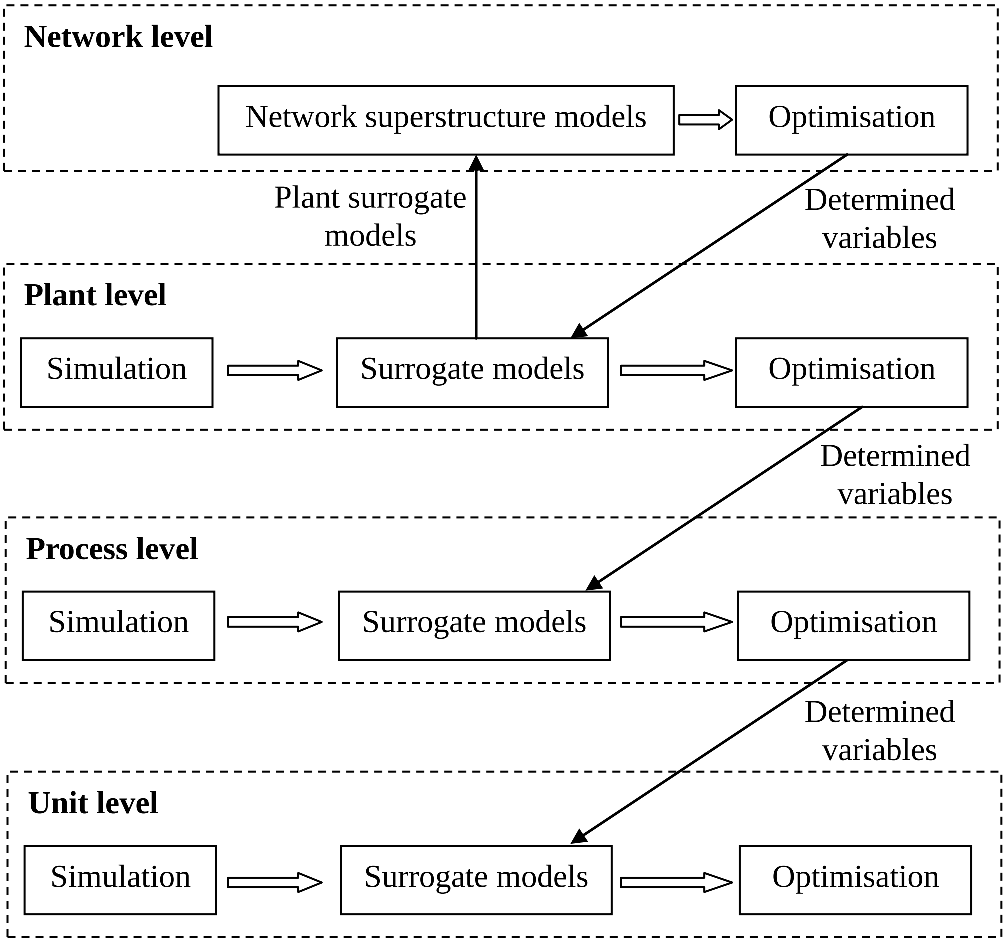


Fig. 10 An illustration of the optimisation strategy proposed for the EIP problem in Section 5.2