Coping with Sustainability, Circularity and Complexity in Optimizing Industrial Symbiosis Networks among Distributed Chemical Processes

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Abstract

For the optimal design and operation of decentralized industrial symbiosis (IS) systems, a multi-criteria decision support tool employing multi-objective optimization (MOO) was developed on a MATLAB® platform. Initial studies had considered exchanging high-purity process carbon dioxide between plants in the IS network (ISN). However, when streams of different concentrations (e.g., spent water) were kept separate, the modelled networks became more difficult to solve. An exploratory examination was undertaken to consider how to model the sharing of contaminated spent water streams between plants in a smaller ISN. The optimization objectives were to minimize fresh material and transportation costs. MOO procedures from the optimization toolboxes and bespoke coding of popular MOO methods were investigated. Multi-criteria decision methods were used to select the ‘most appropriate’ of the non-dominated solutions. The ‘digraph’ function was then used to generate network diagrams displaying source-sink connections and the amount of flow between plants in the ISN. It was found that bespoke-coded scalarized methods, like the ε-constraint method, were more robust than methods relying on the packaged MATLAB MOO functions. Thus, a way was resolved for handling the optimization of more complex ISN models in a numerical computing environment.

**Keywords**: industrial symbiosis, network analysis, multi-objective optimization.

* 1. Introduction

Process systems engineers have turned to methods and tools such as multi-objective optimization (Scotti et al. 2017) and network analysis (Tan et al. 2023) to quantitatively assess and improve the sustainability of systems of chemical plants. Such techniques can be applied to investigate improving the exchange of CO2 of decentralized CO2 reuse systems on petrochemical clusters to reduce emissions (Lee Chan and Janes 2023). However, increasing network complexity in the hope of achieving synergetic benefits is likely to present more problematic analysis.

By filtering current and potential industrial symbiosis (IS) scenarios on the Point Lisas Industrial Estate (PLIE) in Trinidad and Tobago, Lee Chan and Janes (2023) quantified existing instances of sharing by-product process CO2 and found that there are further IS opportunities for reusing valuable high-purity process CO2 to reduce emissions. To build on this, further research aimed at future resource developments of the distributed petrochemical-manufacturing cluster was conducted. Case studies were undertaken to analyze the sharing of waste streams (e.g., contaminated water) and valuable by-product streams (e.g., process CO2) through reuse between different petrochemical plants in the PLIE network. To assist in the initial studies, multi-criteria decision support tools had been developed utilizing multi-objective optimization (MOO) algorithms on a MATLAB® platform. The optimization sought to minimize costs, waste emissions, as well as fresh materials. The graph and network functions in MATLAB could then be used to generate network diagrams that display the connections between the source and sink plants as well as the flow rates between plants in the optimized IS network (ISN). But, modelling exchanges of several materials at different levels of purity would introduce greater complexity to the modelled ISNs. The most reported type of eco-industrial park (EIP) optimization studies is water exchange networks (Tiu and Cruz 2017). Boix et al. (2015) comprehensively reviewed the literature on MOO of water allocation network in EIPs. Rather our motivation was how to perform both MOO and network graphing conveniently in our chosen numerical computing environment, MATLAB.

Therefore, work was undertaken to see what simplifications and improvements to the concepts, methods and tools used to model and optimize more complex multi-material ISN models could realistically be employed. Particularly for non-evolutionary MOO methods, decision analysis is required to select ‘the most appropriate’ solution from a non-dominated solution set or Pareto front (PF). For example, this can be a solution in a smooth PF, where the cost has been rapidly reducing while the other objectives are hardly varying. Hence, to explore the extraction of a ‘compromise’ solution from the PF, some compromise methods (Kundu et al. 2013) and multi-criteria decision-making (MCDM) methods (Kolios et al. 2016) were investigated. The latter methods allow for the decision maker to include additional weightings in extracting the solutions. Therefore, for the MCDM method the number of plant linkages was incorporated into the selection to represent social and IS aspects. As the original aim of a numerical computing environment for combining packaged evolutionary MOO with network graphing and analysis could be achieved with either Scilab or Python and their relevant associated toolboxes, the findings might be transferable to these as well as GNU Octave.

* 1. Methodology

2.1 Model Development

This exercise built on the ‘current case’ in Lee Chan and Janes (2023), but this case study introduced a melamine plant (M) and considered only water reuse among some of the plants. A cut-down version of the petrochemical cluster, consisting of one ammonia plant (A1), one methanol plant using Davy technology (M1) and another Lurgi technology methanol plant (M2) was used. Four types of water qualities: boiler blowdown, wastewater, process water and boilerfeedwater makeup, were modelled. The representative water contaminant was total dissolved solids (TDS). The flow rates of water, in kg/h, to and from the processes were corroborated against sources cited in Lee Chan and Janes (2023). As before, the levelized cost of pipe-borne water transport, in USD/kg, was assessed from the distance between the sources and sinks and the pipeline and pumping requirements. A mixed-integer linear programming (MILP) model of the network was created, but now with four water streams with different levels of TDS. So, an equation that ensures the source purity requirement is achieved, Eq. (1), and two extra objectives to reduce the freshwater requirements and the total levelized cost of water transportation, as represented by Eq. (2) and Eq. (3) respectively, were added to the existing MILP optimization model. In these, is the flow rate of fresh material, is the flow rate of waste material, is the flow rate of medial material, is the TDS in the water and is the levelized transportation cost. Index *i* refers to the source, *j* refers to the sink, *k* indicates the source quality and *p* the destination quality, whilst *q* refers to the material type.

|  |  |
| --- | --- |
|  | (1) |
|  | (2) |
|  | (3) |

The petrochemical cluster model contained 230 constraints, 120 continuous variables and 100 binary variables for algorithmic control purposes.

2.2 Model Optimization and MCDM PF Analysis

The optimization algorithms fell into two groups: packaged evolutionary MOO functions available in the MATLABoptimization toolboxes (MathWorks 2007) as well as bespoke code using scalarized MOO methods. Options within the packaged optimization algorithms were varied and the use of parallel computing was investigated. For each algorithm an attempt was made to generate a non-dominated solution set or PF. Two single objective optimization (SOO) models were created with freshwater minimization and cost reduction as the respective objective functions. The built-in MILP solver, ‘intlinprog’ was used to generate the SOO solutions, which were used as initial points for the optimization and global optimization toolbox solvers. To generate a four-point PF with ‘fgoalattain’ varying weights were used. For comparison, three scalarized MOO methods (viz, weighted sum, weighted metric and ε-constraint) were each coded to generate 25-point PFs. As these bespoke-coded methods required starting and ending points, the SOO solutions were used. The networks were optimized using MATLAB (ver. R2023a).

Two compromise methods (fuzzy LP and global criterion method (GCM) and three MCDM methods (ELECTRE-I, TOPSIS, and PROMETHEE-II) were employed to explore the extraction of a ‘*compromise*’ solution from the PF. Additionally, a social and IS indicator, the eco-connectance (*EC*), was incorporated in the MCDM methods. The dimensionless EC, as represented by Eq. (4), is a modified form of the ‘density’ of the graph (Zhang et al. 2016) and it represents the ratio of byproduct and waste links in the network (*Nw*) compared to maximum possible links in the network, which is a function of the number of plants (*Np*). *EC* was calculated from graph and network algorithm functions in MATLAB. For a simple graph with no self-looping, the closer EC is to one, indicates a more cohesive network.

|  |  |
| --- | --- |
|  | (4) |

* 1. Results

The generated SOO solutions for the MILP model are shown in Table 1. When the initial points were used as starting points in the toolboxes, the ‘gamultiobj’ and ‘paretosearch’ functions produced a PF with only the initial points. The built-in function, ‘fminimax’ produced one point that was the lowest out of all the solutions obtained on the PF.

*Table 1: SOO results for reduced water network*

|  |  |  |
| --- | --- | --- |
| **Objective Function** | **Cost (US$/h)** | **Freshwater consumption (kg/h)** |
| Cost | 102 | 91823 |
| Freshwater consumption | 124 | 90509 |

Without seeding with the SOO points, the ‘gamultiobj’ gave solutions within the SOO solution costs but greater than the SOO freshwater consumption. Both the ‘fminimax’ and ‘fgoalattain’ functions yielded solutions greater than the SOO solutions. A well-defined PF was only obtained with the ‘gamultiobj’ function; however, the run-time was longest. Using parallel computing decreased the runtime for solving the models by 50 % - 80 %. However, even with parallel computing, the ‘gamultiobj’ took five times longer to solve than the other built-in functions.

As shown in Figure 1, the 4-point PF values generated with ‘fgoalattain’ varied roughly by 0.3 % – 1 % from the PFs generated using the scalarized MOO methods. The runtime for the weighed sum and weighted metric methods were about the same, whereas the runtime for the ε-constraint method was 7 times greater. The ‘fgoalattain’ with varying weights method, although with 4 points only on the PF, had a runtime which was 111 times greater than the ε-constraint method with 25 points on the PF.



Figure 1: PF for bespoke and packaged methods

Because the ε-constraint method gave the widest spread of points on the PF, the solutions from this method were used in the extraction of a single solution for the network. For the MCDM methods, a social and IS indicator was factored into the selection slate. Firstly, in scenario S1, equal weightings for the three criteria: freshwater consumption, cost and the number of plant links, were applied. In scenario S2, the cost was weighted twice as much as the other two criteria. Table 2 shows the non-dominated solutions extracted from the PF using the various methods. It was found that the PROMETHEE-II (S2) results were similar to the Fuzzy LP, while the PROMETHEE-II (S1) results were like the GCM results. The solution with the lowest cost for scenarios S1 and S2 is highlighted in Table 2.

*Table 2:  Non-dominated solutions extracted from the PF*

|  |  |  |  |
| --- | --- | --- | --- |
| **Method** | **Freshwater Consumption (kg/h)** | **Cost ($)** | **No. of Plant Links** |
| Fuzzy LP | 90690 | 105 | - |
| GCM | 90509 | 113 | - |
| TOPSIS (S1& S2) | 90509 | 122 | 8 |
| PROMETHEE-II (S1) | 90509 | 115 | 7 |
| PROMETHEE-II (S2) | 90629 | 106 | 4 |
| ELECTRE-I (S2 & S2) | 90509 | 118 | 6 |

The corresponding network graph of interplant exchanges is depicted in Figure 2. Flows of fresh material and flows to waste are not shown. Figure 2 showed that there was reuse of both process and utility water amongst the plants. There was water reuse within all the plants except the melamine plant. The network was analyzed from an IS and sustainability purview and the results obtained are shown in Table 3.



---- Utility water ---- Utility Water

Process water ---- Utility Water

*Figure 2: Network with water flows in t/h*

The PROMETHEE-II (S2) solution has a lower *EC*, which is a function of plant links, since more links probably increases transportation costs. However, the existence of IS in the network, as spent-water exchanges, can be quantified by the *EC*. By computing the hub and authority centrality of the plants, the most important source (M4, from which 96 % of reused water originates) and sink (U, the destination for 51 % of reused water) can be identified. This reinforces other work by Zhang et al. (2016) and Tan et al. (2023) on using network analysis to provide granularity when quantifying IS options.

*Table 3: IS and Sustainability indicators for ‘most appropriate’ compromise solution*

|  |  |  |
| --- | --- | --- |
| **Type of Indicator** | **Indicator** | **Value** |
| IS | Eco-connectance, *EC*\* | 0.2 |
| Environmental | Fraction of waste utilized | 0.5 |
| Social | No. of plant linkages\* | 4 |
| Economic | Cost of freshwater | Million US$0.8/y |
| Circular | Percentage of process water reused | 74 |
| Circular | Percentage of utility water reused | 10 |

\* Calculated after removing self-looping.

Of all the MOO methods evaluated with this network, the ε-constraint method was the most systematic in obtaining a broad PF. The Fuzzy LP was judged the most pragmatic of the methods, which did not require an expansive non-dominated solution set, for determining a single compromise solution. To obtain ‘a most appropriate’ compromise solution according to the decision-maker’s preference, the PROMETHEE-II method was the most practicable of the three MCDM methods explored.

* 1. Conclusions

When increasing complexity of the ISN made the MILP representation more challenging to solve, the bespoke code coped better and outperformed the algorithms in the toolboxes. The results show how MOO coupled with MCDM methods can be successfully used in a numerical computing platform for investigating ISNs. The next step is to incorporate exchanges of discarded water into the larger CO2-reuse model of the PLIE in Lee Chan and Janes (2023) and apply the ε-constraint and PROMETHEE-II methods to realize triple bottom-line benefits (e.g.: reduced CO2 emissions, new revenue streams and skilled jobs) and increased materials circulation.

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