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Determining the performance and network properties of petrochemical clusters

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Abstract

The reliance of the petrochemical industry on fossil-based sources will need to be reduced by the introduction of Alternative carbon sources (ACS). Introducing ACS in a petrochemical cluster will require existing processes to be modified or replaced, potentially affecting other chemical processes within the cluster due to existing material and energy interconnections. Therefore, it is important to understand the current level of interconnections, functioning, and performance of the petrochemical cluster before introducing ACS. In this work, a representative cluster model based on the petrochemical cluster of the Port of Rotterdam was developed and considered as a case study. This model was analyzed using complex network analysis and environmental and technical key performance indicators. The selected key performance indicators (KPIs) provide insight into the performance of a petrochemical cluster, while the network properties give an understanding of the exchange of material and energy in an industrial cluster.

Keywords: petrochemical cluster, key performance indicators, complex network properties, material transition, alternative carbon sources

1. Introduction

The petrochemical industry is reliant on fossil-based sources as an energy and carbon source, and therefore it will have to transition to alternative carbon sources to reach the CO_2 reduction goals. The use of new carbon feedstocks (CO_2, biomass, waste) will require the modification or removal of existing chemical processes. Given the high level of interconnections in existing industrial clusters, these changes are likely to impact existing material and energy connections between processes and among companies in petrochemical clusters. Before these impacts can be assessed, it is needed first to evaluate the complexity and interdependency of petrochemical clusters in terms of material and energy connections and quantify their performance so they can be used as a point of departure.

Network analysis is a method used to study complex systems such as industrial clusters. It allows the interdependencies of processes or companies within a cluster to be assessed by quantifying the exchange of material, energy, or knowledge between processes and or companies. Prior studies (Domenech and Davies, 2011; Song et al., 2018) focused on the occurrence of a link between processes and companies, and assumed that each link is equally important. However, processes are diverse, not only in terms of products but also

in terms of production capacities, and the magnitude of their incoming and outgoing materials and energy flows will also vary as a result. Therefore, it is important that the relative importance of the interconnections is identified and included in the analysis.
In addition to understanding the interdependencies of processes within a petrochemical cluster, additional metrics are required to determine the environmental and technical performance of a petrochemical cluster. Key performance indicators (KPIs) that have been used to assess the performance of industrial clusters are, for instance, CO_2 emissions (Yu et al., 2015) and energy consumption (Sokka et al., 2011).

In this work, a new framework for assessing the complex network properties and performance of a petrochemical cluster is presented. The framework was applied to a case study based on the petrochemical cluster in the Port of Rotterdam (PoR).

2. Petrochemical Cluster Model Framework

The methodological framework used to characterize and evaluate the performance of the representative petrochemical cluster (RPC) is presented in Figure 1. The first step is to select the petrochemical processes and utility units that are part of the RPC. For instance, processes producing chemical building blocks (CBBs), intermediate chemicals (ICs), and end-of-value chain chemicals (EVCs) were selected based on the PoR cluster. Additionally, utility production processes that provide the required steam, electricity, and auxiliary chemicals for the chemical processes need to be selected.

In the next step, detailed process models based on publicly available data were built for each selected chemical and utility generation process using Aspen Plus. Each process model was modeled according to the production capacity and process technology of its counterpart in the PoR cluster. These process models provided detailed material and energy balances for each process and utility generation unit. Furthermore, the bare equipment costs and land footprint were determined for each process using Aspen Process Economics Analyzer.

In the third step, the material and energy connections between the processes in the RPC were mapped. This was done by collecting the results of the models and publicly available data on infrastructure and connections of the PoR and using it to match the material and energy requirements within the processes in the RPC. The resulting mapping of exchanges contains all connections between the processes within the cluster and the processes' connections to the outside world. For example, natural gas imported into the cluster, wastewater sent to wastewater treatment plants, and emissions emitted to the environment.

Next, detailed material and energy stream data from the Aspen Plus process models is automatically extracted using an in-house developed Python module. The material and

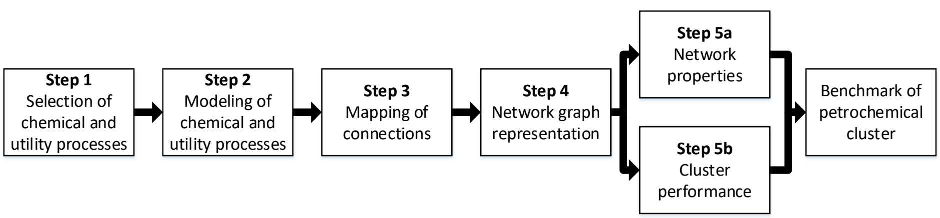

Figure 1: Methodological framework for modeling and assessing a petrochemical cluster

energy data is used to construct a complex network representation in Python using Py3plex (Škrlj et al., 2019). This complex network representation uses graph theory to describe the petrochemical cluster, where the material and energy connections are represented as links, and the chemical and utility generation processes are depicted as nodes. In this work, we developed a multiplex graph of the cluster, where each layer represents a different type of interaction between the nodes. For instance, the first layer represents all the material interactions, and the second layer depicts all the energy exchanges between processes. The only type of interlayer connections are with the counterpart of each node present in the other layers.

Py3plex is based on the complex network analysis Python module NetworkX by Hagberg et al. (2008), thereby allowing the complex network of the graph to be calculated. The number of connections a node has k_i, also known as the degree of node *i,* was determined by:

$$k_i = \sum_{j \in N} a_{ij} \quad (1)$$

where N is the number of nodes, and a_{ij} is zero if there is no direct link between nodes i and j and one if there is. Alternatively, the degree centrality $C_{D,i}$ was calculated by:

$$C_{D,i} = \frac{\sum_{j \in N} a_{ij}}{N-1} \quad (2)$$

The degree centrality only considers whether a connection between processes is present, and the magnitude of the material or energy exchange is not considered in its calculation. It determines the importance of a process in the petrochemical cluster by considering the number of connections it has to other processes in the cluster. To consider the magnitude of the material or energy exchange, the strength of a node s_i was calculated by:

$$s_i = \sum_{j \in N} w_{ij} \quad (3)$$

where w_{ij} is the weight of the link between nodes i and j. For instance, in the context of the transformation of petrochemical clusters, the mass of carbon in a link could be considered to calculate the weight of a link as it allows the most import nodes in terms of carbon flows between processes to be identified.

The final step consisted of determining the environmental and technical performance of a petrochemical cluster. The graph representation and list of connections were used to calculate the key performance indicators carbon efficiency, CO_2 emissions, and total energy usage within the boundaries of the cluster. The carbon efficiency η_{Carbon} of the cluster is calculated by:

$$\eta_{Carbon} = \frac{\sum m_{Carbon,p}^{Product}}{\sum m_{Carbon,f}^{Feed}} \quad (4)$$

where $m_{Carbon,p}^{Product}$ is the mass of carbon present in stream p leaving the petrochemical cluster, while $m_{Carbon,f}^{Feed}$ is the total mass of carbon present in the material feed stream f entering the cluster. The total CO_2 emissions of the petrochemical cluster are determined by the mass of CO_2 present in the streams being emitted to the environment:

$$m_{CO_2} = \sum_{i=1}^{N_{streams}} m_{i,CO_2}^{Environment} \quad (5)$$

Where, $m_{i,CO_2}^{Environment}$ is the mass flow rate of CO_2 in stream i emitted to the environment, and $N_{streams}$ is the total amount of streams emitted to the environment.

As described before, the framework presented was implemented using an RPC based on the PoR cluster, and the results of its implementation are discussed in the next section.

3. Results and Discussion

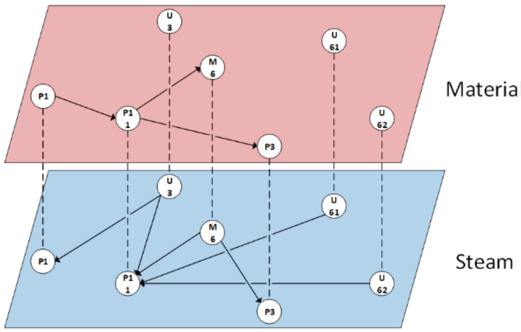

Figure 2: Multiplex graph representation.

Nine utility generation processes and 33 petrochemical processes producing 52 chemicals were selected and modeled in Aspen Plus. Based on these models, a complete mapping of all the material and energy streams of the cluster was created and used to construct a complex network representation of the petrochemical cluster. A two-layer multiplex graph was created containing 49 nodes, where the first layer represented the material exchanges and contained 64 links, while the second layer represented the exchange of energy and contained 48 links. In figure 2, a multiplex graph representation of a small section of the cluster consisting of four chemical processes and three utility generation units is shown.

The degree centrality and strength of the nodes of the material layer are presented in Table 1. It shows that the EDC/VCM plant and the SMR plant are the most interconnected processes of the cluster, followed by the aromatics and olefins plants. The EDC/VCM plant is part of the chlorine sub-cluster, which contains many interconnections. The SMR plant supplies H_2, which is used as auxiliary material in the production of several chemicals, while the aromatics and olefins plant produce the CBBs that are either directly or indirectly used by the other processes within the cluster. Therefore a high level of interconnectivity is expected for these processes. When considering the strength of the nodes, the aromatics plant appears as the most critical process in terms of carbon flows, followed by the ethylbenzene (EB) and olefins plants, respectively.

Table 1: Degree centrality and strength of the most interconnected processes on the material layer

Process	**Degree centrality**	**Process**	**Strength (ktonne of carbon per year)**
Ethylene dichloride/Vinyl chloride monomer (EDC/VCM)	0,19	Aromatics	1757,19
SMR	0,19	Ethylbenzene (EB)	1430,39
Olefins	0,17	Olefins	1110,50
Aromatics	0,17	Propylene oxide/Tert-butyl alcohol (PO/TBA)	978,34
Chlorine	0,13	Propylene oxide/Styrene monomer (PO/SM)	866,78

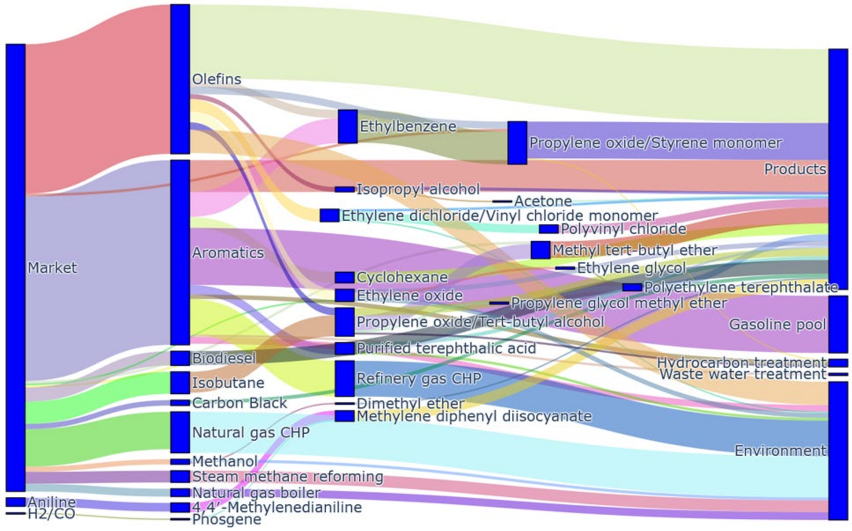

Figure 3: Sankey diagram of all the carbon mass flows in the petrochemical cluster.

In terms of performance, carbon mass flows of the petrochemical cluster are shown in a Sankey diagram in Figure 3. In this diagram, all the chemical processes, the mass flows of carbon between the processes in the cluster, and the carbon flows from and to the outside world are shown. The market represents any material flows being imported into the cluster, while the products represent all material being exported out of the cluster, and the environment represents any CO_2 directly being emitted to the environment. The petrochemical cluster has an overall carbon efficiency of 58.5%. Nearly all the fossil-based carbon feedstock imported into the cluster is sent to the aromatics and olefins plants, with 44.3% and 35. 9% of the carbon feedstock, respectively. These plants transform the carbon feedstock into CBB, and these are distributed across the different value chains that make up the cluster. Therefore, replacing these fossil-based processes with alternative carbon source processes such as CO_2, biomass, or waste will most likely have the most significant impact on the transformation of the petrochemical industry. Additionally, not all chemicals produced by the olefins plant and the aromatics plants are used by the downstream chemical processes in the petrochemical cluster and instead exported out of the cluster. Compared to the strength of the nodes, the importance of the olefins and aromatics is more clearly defined in the Sankey diagram. This is due to the

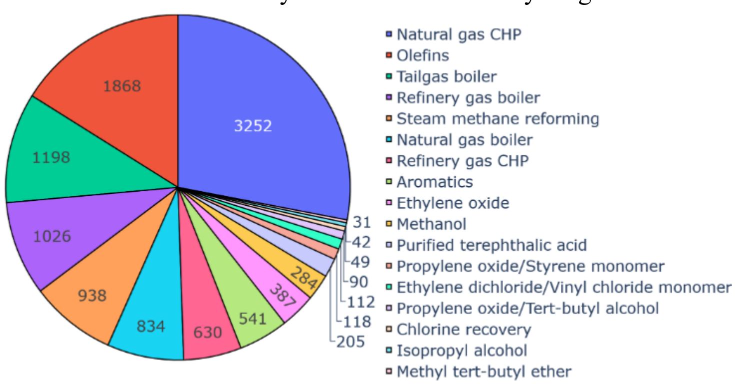

Figure 4: Pie chart of the CO2 emissions of the chemical and utility generation processes in the cluster in ktonne of CO2 per year.

manner the strength of a node is calculated, with only links between processes inside the cluster being considered and not the stream entering or leaving the cluster.

In this case study, the petrochemical cluster emits 11.647 Ktonne of CO_2 every year. The distribution of direct CO_2 emission for all chemical and utility processes emitting at least 25 ktonne per year is shown in Figure 4. A major part of all CO_2 emissions in the cluster is from the utility units that provide the required steam, electricity, and auxiliary chemicals by the chemical processes. The olefins plant has the highest direct CO_2 emissions, as it burns byproducts to provide the heat required for the process. However, new alternative carbon source processes could result in a shift of CO_2 from inside the cluster to outside the cluster. Therefore, an LCA cradle-to-gate approach should be implemented. This will be investigated in further research.

4. Conclusions

The transformation of a petrochemical cluster to more sustainable carbon sources can impact the exchange of material and energy between processes and the performance of the cluster. Thus, network properties and performance indicators are required to assess the current petrochemical cluster and future configurations. In this work, a framework was presented for modeling a petrochemical cluster from the bottom up based on the cluster in the Port of Rotterdam. This model was analyzed using complex network analysis and environmental and technical key performance indicators. In future work, the network properties and performance of a modified cluster, including alternative carbon source processes, will be compared with the benchmark developed in this work, allowing the potential impacts of the transformation of petrochemical cluster to be identified.

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