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# Using chemical process simulation to design industrial ecosystems

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**Abstract**

Chemical process simulation (CPS) software has been widely used by chemical (process) engineers to design, test, optimise, and integrate process plants. It is expected that industrial ecologists to bring these same problem-solving benefits to the design and operation of industrial ecosystems can use CPS. This paper provides industrial ecology researchers and practitioners with an introduction to CPS and an overview of chemical engineering design principles. The paper highlights recent research showing that CPS can be used to model industrial ecosystems, and discusses the benefits of using CPS to address some of the technical challenges facing companies participating in an industrial ecosystem. CPS can be used to (i) quantitatively evaluate and compare the potential environmental and financial benefits of material and energy linkages; (ii) solve general design, retrofit, or operational problems; (iii) help to identify complex and often counter-intuitive solutions; and (iv) evaluate what-if scenarios. CPS should be a useful addition to the industrial ecology toolbox.


*Keywords:* Industrial ecosystems; Chemical process simulation

## 1. Introduction

Each of the many disciplines that support industrial ecology has added its own tools, adapted and improved by a systems view and ecological principles, to the industrial ecology toolbox. A number of definitions refer to industrial ecology as including the study of the flows of materials and energy in industrial systems. This study is often termed industrial metabolism, a field largely developed by Ayres over the past 30 years. Johansson [1] points out that industrial metabolism has become an important foundation for industrial ecology, in part because it can be applied at different scales of analysis from individual processes and companies to the global environment. Because of the emphasis industrial ecology places on the study of materials and energy flows, tools that facilitate an evaluation of these flows will be particularly useful.

Diwekar and Small [2] note that industrial ecologists use material and energy balances, traditionally used by engineers to analyze industrial unit operations, to understand more complex systems. So, while industrial ecologists are using the mass and energy balance approach upon which the discipline of chemical engineering was built, related chemical engineering tools such as chemical process simulation (CPS), are not yet widely used. In the same way that the aircraft industry uses flight simulators to design and test aircraft, chemical engineers use CPS to design, test, optimise, and integrate process plants. It is expected that CPS can be used by industrial ecologists to bring these same problem-solving benefits to the design and operation of industrial ecosystems, increasing our understanding of potentially complex material and energy relationships. In fact, Ayres [3] discusses systems integration and integrated industrial ecosystems pointing out that "the complex web of exchange relationships among such a set of firms can be called an industrial ecosystem".

CPS is used by chemical engineers (often called process engineers) to model process industries. Process industries are those that involve the physical or chemical transformation of raw materials and energy to products—materials and energy flow in; products, by-products, and unused energy flow out. The chemical, petrochemical, pulp and paper, mining,

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pharmaceutical, power generation, and waste treatment industries are examples of process industries. Much of the manufacturing that takes place at small and medium enterprises, such as corrugated cardboard production, metal finishing, and plastics production, can also be considered as a smaller-scale process industry. Because of their consumption of materials and energy, as well as their prevalence in industrial parks or zones, process industries have an important role to play in facilitating the material and energy cycling in industrial ecosystems.

This paper provides industrial ecology researchers and practitioners with an introduction to CPS and an overview of chemical engineering design principles. The paper also highlights recent research showing that CPS can be used to model industrial ecosystems, and discuss the benefits of using CPS to address some of the technical challenges facing companies participating in an industrial ecosystem.

## 2. Chemical process simulation (CPS)

### 2.1. What is chemical process simulation?

Chemical process simulators are software programs designed to model process plants. CPS is especially important in modeling systems that do not yet exist, or that would be too expensive to 'play' with. Such systems have historically included large scale chemical, process, and manufacturing industries, where materials are measured in thousands of tons, energy use is measured in megawatts, and costs and profits are measured in the hundreds of thousands or even millions of dollars. However, in recent years, CPS has been adapted by smaller, less traditional process industries.

Chemical engineers use CPS to design or retrofit complex process facilities. Using CPS software, chemical engineers can determine the overall effects of potential process changes in one area; predict capital cost expenditures; track/predict emissions; and evaluate optimization and integration options. Furthermore, engineers rely on CPS to answer what-if questions posed by management or operations staff [4]. CPS has advanced to the point that detailed models can replace expensive pilot-scale projects [5].

There are several CPS software packages commonly used in North America. These include ASPEN Plus™, CADSIM Plus™, CHEMCAD™, Gensim™, and Hysys™. Each of these software programs was originally developed with a particular process industry in mind. However, most processes are common (such as heat exchange, or pumping, or mixing) across industries; it is only the nature of the materials being physically or chemically transformed that are unique. Therefore, most of the above software programs have evolved so that they are applicable to many process industries. CADSIM Plus™ has been applied to a group of industries, essentially modeling a limited industrial ecosystem [6,7].

### 2.2. How does CPS work?

The fundamental purpose of CPS is to assist chemical engineers in solving complex mass and energy balances. So, in order to understand how CPS works, it is important to understand how a process mass and energy balance works.

#### 2.2.1. Mass and energy balances

When designing a process plant, or solving operational problems, chemical engineers divide the plant into process units. A process unit is the physical or conceptual apparatus through which the physical and chemical transformations take place. Examples of process units include pumps, which cause a transformation in the pressure of a fluid; evaporators, which physically separate materials, such as water from salt; or reactors, which cause a chemical transformation of their inputs. Every process unit, and every overall process, has one or more inputs, and one or more outputs. These inputs and outputs are also called process streams. They can represent material or energy flows, including losses.

Mass transformations may include reaction, mixing, or separation. So, a mass balance would account for the yield of a product, the flow of sludge and treated water produced by a wastewater treatment system, or the flow of GHG emissions from a boiler. Energy transformations involve heating, cooling, phase changes, or mechanical work, such as turning a shaft. Energy balances determine how much heat is required to generate a given amount of steam, how much electrical energy a pump requires to move a certain flow of liquid from a tank to another process unit, or how many solar panels would be required to meet the energy needs of the average home.

For a steady-state process (no changes over time), the mass balance for *each component* around a process unit, or a group of process units, is:

$$\begin{aligned}&\text{Component}_{\text{Input}} + \text{Component}_{\text{Generated}}\\&\quad = \text{Component}_{\text{Product}} + \text{Component}_{\text{Lost}} + \text{Component}_{\text{Consumed}}\end{aligned}$$

Note that components can be generated and consumed via reactive processes. $\text{Component}_{\text{Product}}$ refers to the amount in the product stream, while $\text{Component}_{\text{Lost}}$ refers to the amount that ends up in waste or by-product streams.

For a steady-state process (no changes over time), the energy balance around a process unit, such as an evaporator, or a group of process units, such as an

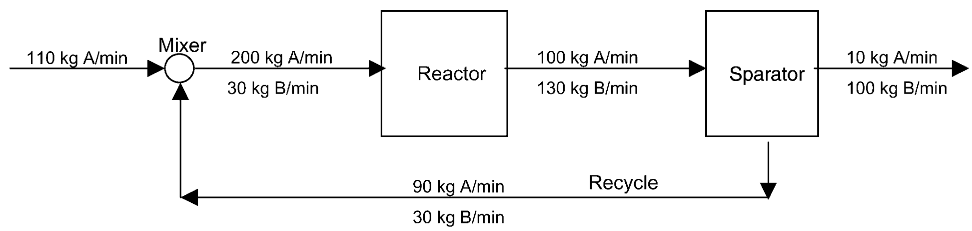


Fig. 1. Simple process flow diagram (PFD) example.

entire chemical plant, is:

$$\text{Energy}_{\text{Input}} + \text{Energy}_{\text{Added}} = \text{Energy}_{\text{Output}} + \text{Energy}_{\text{Lost}}$$

Note that $\text{Energy}_{\text{Input}}$ usually refers to the latent or internal energy in components, for example, the thermal energy a component contains because it is already at a certain temperature when it enters a process unit. $\text{Energy}_{\text{Added}}$ is either thermal (heating or cooling), or mechanical (changing pressure or mixing). $\text{Energy}_{\text{Output}}$ is the energy $\text{Energy}_{\text{Lost}}$ could be energy lost due to friction of moving parts, or energy that is otherwise lost due to inefficiencies, or to heated waste streams, such as flue gas or hot wastewater.

These equations seem deceptively straightforward. Indeed, solving mass and energy balances sometimes requires relatively simple algebraic operations. However, it is expensive to monitor the concentration and flow of every stream in a plant, so often the data must be inferred or estimated. The complexity of mass and energy balances is increased by other factors, such as multiple process units; components that are changing phases, such as water to steam; the presence of purge and recycle streams; chemical reactions; and phase transfer i.e., when ammonia is absorbed from a vapour phase into a solution.

### *2.2.2. Process flow diagrams (PFDs)*

One of the best ways to represent a process is a process flow diagram (PFD). As Fig. 1 shows, the most basic PFD is a drawing with boxes representing process units and lines representing process streams (or conceptual pipes). Often, some of the main material flows or stream compositions will be included as well.

A PFD is a two-dimensional representation of the real, three-dimensional process equipment and piping. In addition to process units, PFDs often show the location of instrumentation such as temperature gauges. Preparation or review of a PFD is usually the first step in completing a mass and energy balance. A completed PFD helps to define the balance problem, and is an excellent means of organizing all of the available

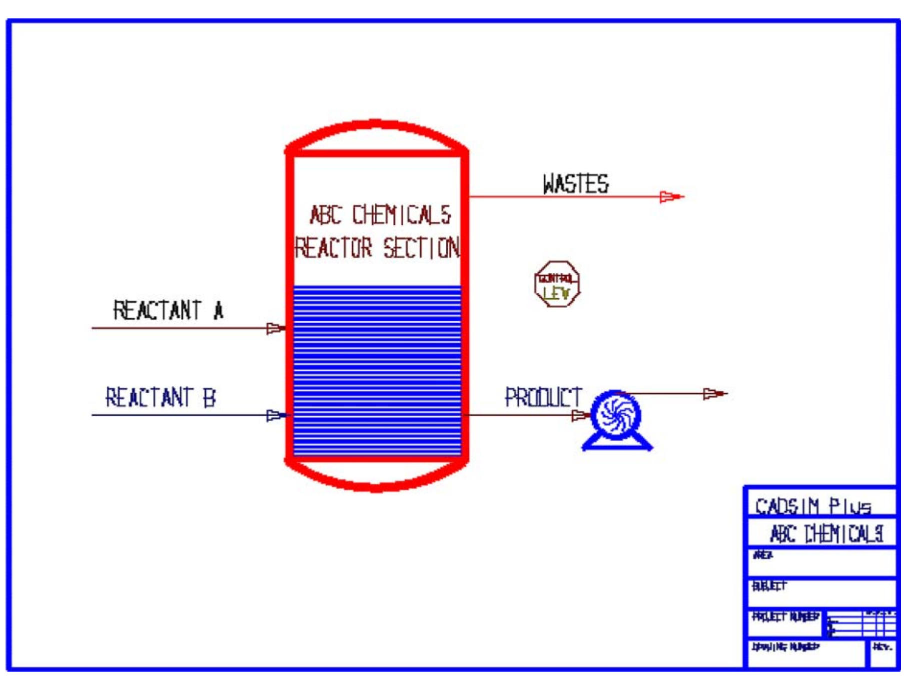


Fig. 2. Example of a simple 'black box' model in a chemical process simulation (CPS) drawing.

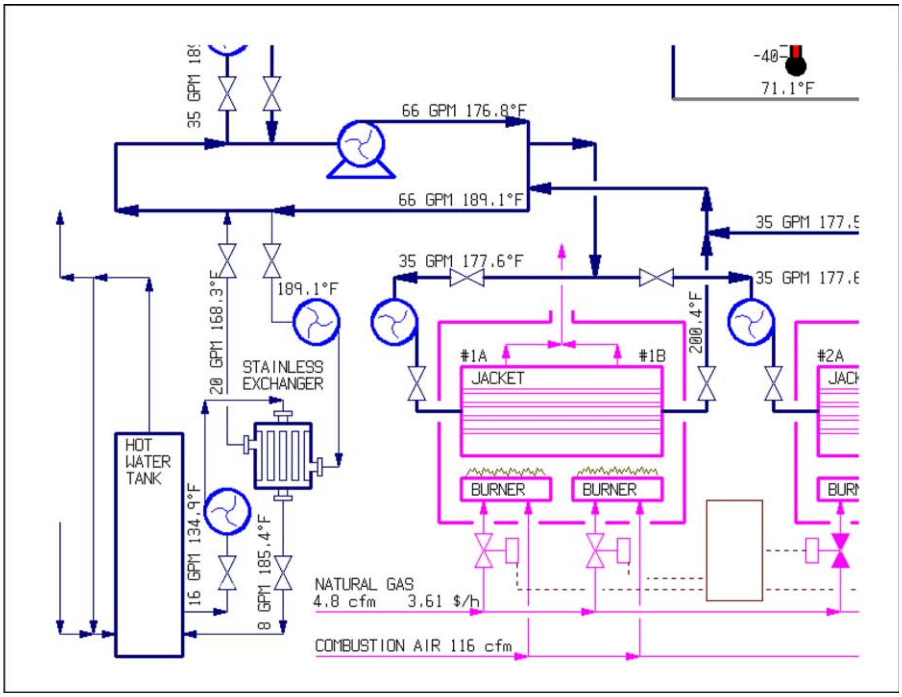


Fig. 3. Example of a complex simulation drawing (used with permission from Aurel Systems Inc.).

process unit and stream information. PFDs are also a useful training and teaching tool, providing an easy way for others to get a quick overview of the process.

Most CPS programs now have a computer aided drafting (CAD) type graphical interface that allows the user to enter process information by 'drawing' the PFD for the process (or sub-process) in question. Simply adding or removing process units or the 'pipes' that connect them can change the model. The PFD for the simulation can be as simple as a 'black box' model, as shown in Fig. 2, or so detailed that control loops are represented, as shown in Fig. 3.

While the PFD is being drawn, the software begins to configure the simulation model. Based on the number of components (the chemicals and other materials used in the process); the number and type of process units; the number of input and output streams for each process unit; and whether temperature and pressure are to be accounted for, the program determines the minimum amount of data that must be entered before the mass and energy balance can be solved. The program then prompts the user for data. The process data can generally be provided in three different ways:

- A direct value i.e., the flow of INPUTA is 15 T/d;
- An equation i.e., the flow of INPUTA is 10% of the flow of INPUTB; or
- An operating condition i.e., the flow of INPUTA is whatever is required to make sure OUTPUTX has a concentration of 56%.

Once the required amount of information has been entered, the program is executed, and the mass and energy balance is calculated. Solving process problems is then an iterative procedure of making changes to the PFD and/or adjusting process data then re-executing the program to obtain the new mass and energy balance values. For example, the user could add a new tank, or change a temperature, and then re-execute the simulation to see how these changes affect the process.

## 3. Applying CPS to industrial ecosystems

CPS has already been used by many industries to model large, complex facilities. For example, CPS was used to complete a steam and energy balance around an entire pulp mill, resulting in the identification of more than 2 million CDN$ annual energy savings [8]. Unfortunately, these types of models, while proving extremely effective at solving design and operational problems at process facilities have been generally quite time-consuming and costly to construct. These issues could be compounded when creating a model of industrial ecosystem, comprising many companies. Can CPS be practically used to model industrial ecosystems?

Recent research indicates that the answer is 'yes'. Using a more holistic approach to engineering design, these models can be created with minimum time and cost. The CPS software CADSIM Plus™ was used to create a 'virtual' industrial ecosystem model, comprising Minas Basin Pulp and Power, which produces recy-

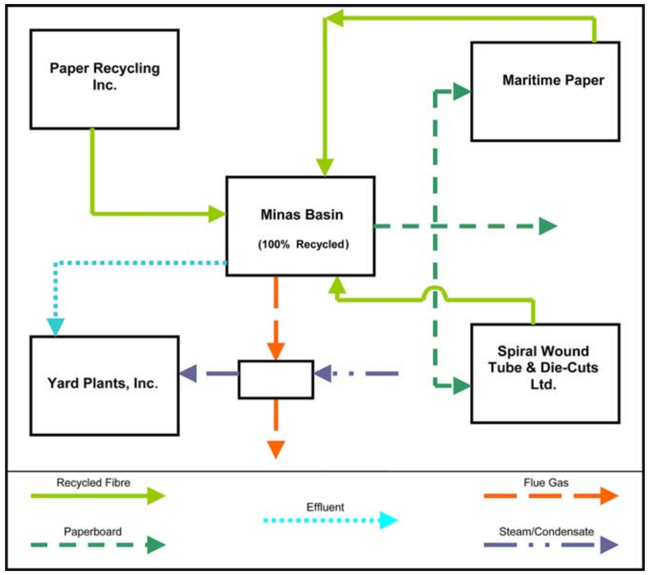


Fig. 4. Simplified PFD for CADSIM Plus Simulation Model of industrial ecosystem.

cled unbleached paperboard; Paper Recycling Inc.[1]; which recovers paper, newsprint, and old corrugated cardboard from the urban forest and redistributes for recycling; Spiral Wound Tubes & Die-Cuts Ltd.[1], which produces paperboard tubes and die-cuts; Maritime Paper Products Ltd., which produces and prints corrugated cardboard sheet and boxes; and Yard Plants Inc.[1], a commercial greenhouse [6,7]. Fig. 4 shows the PFD for this limited industrial ecosystem.

By comparing Fig. 4 with Fig. 3, one can see how the approach to creating a detailed PFD for a portion of a facility was adapted to create a PFD for an industrial ecosystem. In Fig. 3, each process unit in the model represents actual process equipment, such as a Chip Bin, Digester, and Atmospheric Diffuser Storage Tank. In Fig. 4, each process unit represents the *overall* operations of an entire company. The CPS software treats each process unit the same—materials and energy enter the process unit; materials and energy are transformed during the process; and then materials and energy leave the process unit. For both PFDs, the CPS software calculates a material and energy balance around each process unit, as well as a material and energy balance around the entire system.

Fig. 4 also shows some of the potential material and energy linkages among the companies in the limited industrial ecosystem. The linkages include a fiber cycle (recycled cardboard wastes from paper recycling, maritime paper products, and spiral wound tubes and die-cuts are sent to Minas Basin Pulp and Power, which then sends paperboard product to Maritime Paper Products and Spiral Wound Tubes & Die-Cuts); a water linkage (effluent from the Minas Basin Pulp and Power becomes process water for Yard Plants Inc.); and a waste heat recovery cycle (waste heat from the boiler flue gases at Minas Basin Pulp and Power is used to generate some of the steam requirement for Yard Plants Inc.).

A more holistic approach to engineering design was used to create the model. In traditional chemical engineering design, processes were designed in detail, and fairly independently, from the beginning. For example, the design of a pulp mill might be broken into the boilers, pulping, bleaching, washing, and drying process units. The detailed processes are then pieced together like a puzzle to form the overall plant design. In contrast to this segregated approach, Casavant and Côté [6] and Casavant [7] began with the 'big picture', breaking each company down into only two parts—boiler systems and the rest of the process. The same holistic approach was used to model the boiler systems for each company; inner details such as scrubbers, pumps, valves, and control loops were not included.

By starting the design process from the outside, the amount of time required to construct the models is greatly reduced, while still allowing for enough detail to complete a preliminary feasibility assessment by calculating the potential environmental benefits of such linkages. When creating the PFD for the industrial ecosystem shown in Fig. 4, Casavant [7] also set up the model so that several parameters were calculated for each process unit (company) as well as for the overall industrial ecosystem. These parameters included fuel oil consumption, water intake, wastewater generated,

[1] Company name has been genericized as per a confidentiality agreement.

solid waste generated, $SO_2$ emissions, $CO_2$ emissions, and waste heat generated. Then, as potential linkages were explored, either individually or in various combinations, the CPS software can recalculate the system parameters in a matter of seconds. The speed with which CPS software performs complex material and energy balance calculations allows for easy determination of the impacts of various material and energy linkage scenarios. For example, it was determined that using waste heat from Minas Basin Pulp and Power to generate low pressure steam for the greenhouses could reduce the greenhouse fuel consumption by 20% per year. For the fiber cycle involving four of the companies, the CPS software was able to calculate that solid waste to landfill was reduced by 91% compared to the base case scenario, where no linkages existed.

The industrial ecosystem modeled was immature, and the model itself was limited. For example, the linkages modeled were fairly simple. In addition, financial and logistical data must still be incorporated into the model. Furthermore, a higher level of process detail will eventually need to be incorporated into the model to allow for more precise calculations. Nonetheless, the model allowed for the quantitative evaluation of potential linkage scenarios among the companies, and provided enough information to facilitate preliminary decision-making and to highlight potential opportunities worthy of further technical and financial assessment.

## 4. Benefits of using CPS to model industrial ecosystems

### 4.1. Numbers, numbers, and more numbers

The ability to use CPS to model industrial ecosystems brings many benefits to the industrial ecology community. Those designing and operating industrial ecosystems now have a tool to help determine quantitatively the potential environmental and financial benefits gained by the companies in the system. Industrial ecology has been criticized for its lack of data to support its theories. CPS should help researchers and practitioners overcome this hurdle. Furthermore, quantitative evaluation of the environmental and financial benefits will be useful in convincing companies to support the industrial ecosystem model.

### 4.2. General problem-solving

Beyond its ability to generate useful numbers, the addition of CPS to the industrial ecology toolbox means that the same general process problem-solving ability available at the plant level is now available at the industrial ecosystem level. An industrial ecosystem model may be larger, but the way in which CPS is used is the same. As discussed earlier, engineers have been using CPS to calculate complex mass and energy balances needed to evaluate process configurations, track/predict emissions, design or retrofit parts of or an entire plant, optimise operating conditions, and integrate processes. CPS will help researchers and practitioners to approach problem-solving from a systems view, facilitating complicated calculations and allowing the rapid evaluation of different operational scenarios.

### 4.3. Finding complex, counter-intuitive solutions

If all of the solutions to our problems were intuitive and linear, we would already have all our problems solved. Not only are the solutions to our environmental problems likely to be non-linear and in many cases counter-intuitive, but they are increasingly complex, especially when we take a systems view. Research has shown that higher efficiencies and lower environmental impacts are more effectively achieved by optimizing a system of processes than an individual process; however finding the right solution can be challenging.

For example, minimizing an output emission may not always reduce the overall environmental impact. Using their minimizing environmental impact method, which uses an in-house chemical process simulator and accounts for the impact of input and output streams, Stefanis et al. [9] completed a case study for a vinyl chloride monomer (VCM) production process. They optimized the process with and without consideration of the global production chain. They found that optimizing for one type of pollution resulted in the generation of higher values of another type. For example, minimizing air pollution may increase water pollution. In addition, when the optimization was completed for several types of pollution simultaneously, lower overall environmental impacts were achieved in the global system, not the individual system. They also found that there might be a threshold value of abatement above which overall environmental impact begins to increase due to the trade-off in the impact associated with inputs versus outputs.

Furthermore, there may be more than one optimum way to minimize environmental impact of a system of processes. Azapagic and Clift [10] presented a case study of a boron system, covering resource extraction to primary and secondary processing then shipping. Using linear programming methods, they found that there was more than one optimum solution for minimizing environmental impact associated with the system inputs and outputs. As decision-makers struggle to weigh economic, social, and environmental impacts, the presence of more than one optimum solution for minimizing environmental impact may provide them with more options.

Given the complex, non-linear, and counter-intuitive solutions we are searching for, and given the time-consuming and difficult nature of the calculations required to manually calculate the necessary mass and energy balances for a system of interlinked processes, CPS appears to be an effective tool for designing industrial ecosystems. Frosch [11] wrote that creating industrial ecosystems might require "...complex considerations of product and process design, economics and optimization...". These are the tasks for which process simulation was created. In fact, some in the simulation community have already recognized that process modeling can help us work toward a global optimum [5].

### 4.4. Evaluating what-if scenarios

The basic role of a simulation is to mimic the 'real' world. From role-playing simulations that one acts out in anticipation of a job interview, to high tech computer flight simulators that train pilots, simulation has proved to be an invaluable learning tool. Critics of industrial ecology, as well as governments and industries hesitant to promote the concept of industrial ecosystems, often point out that there are few 'real' industrial ecosystems, and then use this as a reason for not supporting the concept. Process simulation is an ideal tool for addressing these concerns. The 'virtual' industrial ecosystem that can be created using process simulation can be used to quantify savings in material and energy use, as well as reductions in emissions. The models can be manipulated to evaluate multiple 'what-if' scenarios. CPS can be used to find answers to many of the questions facing companies evolving in an industrial ecosystem: Is additional energy input needed to facilitate the cycle? Will transportation costs be too high? If Companies X, Y, and Z are interlinked, what happens if X wants to expand its production?

## 5. Conclusions

The concept of material and energy cycling seems straightforward—match up companies that have mutual needs. Unfortunately, the efficient design and optimal operation of even one company presents many challenges. These challenges are only multiplied at the industrial ecosystem level. Research has shown that, while adopting a systems approach can increase environmental and economic benefits, finding the best process solutions can be difficult. Multiple scenarios must be tested to optimise material and energy use among companies in the system. For example, it is possible that increased production of a former waste product by one company may be required in order to meet the demand for this product as a feedstock at an adjacent company. In such a case, it would be necessary to ensure that material use is optimized, and that the overall environmental impact is minimized. Real-life testing is expensive, potentially risky, and unlikely to meet with regulatory approval. Potential participants and investors may be reluctant to commit funds without quantitative proof of the benefits.

CPS has long been used by process industries to solve these types of problems at the plant level. Recently, Casavant and Côté [6] and Casavant [7] found that CPS can also be used to model a group of companies, and, therefore, can be used to model industrial ecosystems. CPS researchers and practitioners can now quantify the potential and environmental and financial benefits for companies in an industrial ecosystem; solve general process design problems; identify complex and counter-intuitive solutions; and evaluate what-if scenarios. Of the eleven goals that Côté and Cohen-Rosenthal [12] list for an industrial ecosystem, CPS will be directly useful in achieving six of them. For example, CPS can be used to design material exchanges and integrated waste treatment to reduce environmental impact; design facilities that maximize energy efficiency; and design facilities that conserve material use. CPS can also be used to test the implications and evaluate the benefits of linkages between companies and their suppliers and customers in the community around the industrial ecosystem. Furthermore, CPS software is now so sophisticated that it can generate emissions reports and be used to train operations staff before they even enter a plant. Therefore, CPS will also be useful in managing information to facilitate the flow of energy and materials. In addition, CPS will also be able to help train and educate management and staff about new strategies, tools, and technologies that will improve the system.

Although Diwekar and Small [2] have focused on a case involving benzene production and the possible economic and environmental options for diphenyl, a by-product of benzene production, they also concur that process simulation and optimization could provide a potentially useful approach to the analysis of industrial ecosystems. While additional studies are needed to illustrate and evaluate the use of CPS to model industrial ecosystems for these particular scenarios, it is apparent that CPS can be an invaluable addition to the industrial ecology toolbox.

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