Chapter

MODELING AND SIMULATION OF PROCESS SUSTAINABILITY IN WASTE MANAGEMENT IN SINGAPORE

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ABSTRACT

The implementation of sustainable waste management in Singapore requires effective modeling and simulation methods and tools to evaluate process sustainability and to generate sustainable solutions. This requirement has however presented several challenges due to the current lack of rigorous sustainability measurement methods, effective evaluation systems, and localized inventory data. This chapter presents research to explore some of the challenging issues in sustainability modeling and simulation. It develops a science-based sustainability assessment method to measure, evaluate and compare sustainability footprints of alternative waste management processes. The method provides two techniques for metrics-driven sustainability modeling and agent-based sustainability simulation. Together with a technology inventory to provide the localized and structured information on waste handling technologies and

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operations, the method allows systematic and rigorous assessment of process sustainability in the Singapore's waste management context. An assessment application to a waste-to-material recovery system is presented. Influences of processing technology choices and key operating parameters on environmental impact, economic profitability, social acceptability and other context-specific concerns of the system are measured, simulated and evaluated. The application showed that the two techniques in our method have provided a reliable and practical means for the local recyclers to model and simulate process sustainability. The results have provided them with a better understanding of the factors influencing their sustainable practices and facilitated them to identify and implement process improvements.

1. INTRODUCTION

Waste management practices in Singapore are facing the new sustainability challenges: to maintain their operations technically competitive, economically profitable, environmentally protective, and socially responsible. A series of targets and guidelines have been set for industry to achieve sustainable waste management in Singapore [1, 2]. Implementing sustainability however embodies enormous changes and interactions from the environment, economy, society, technology and regulations [3]. They are frequently related to both quantifiable and qualitative concepts, technological and non-technological decisions. For example, the sustainability performance of a recycling process can be determined by its technological features (e.g. process concept, recycling system design, parameters selection), non-technological conditions (e.g. operating practices, regulations, the local waste strategies), and many other influencing factors. These challenging issues require consistent sustainability information and reliable sustainability assessment to support waste treatment decisions and to evaluate consequences from the selected treatments on the environment, economy and society. Comprehensive sustainability modeling and simulation methods, techniques and tools are therefore needed for a systematic and consistent understanding, evaluation, and improvement of waste management practices in Singapore.

Sustainable waste management broadly implies the development and implementation of innovative waste handling technologies and processes that minimize environmental impacts, conserve natural resources, protect public health and natural ecosystems, and are economically effective. Yet progress for sustainability implementation in practice has been hampered. This is mainly attributed to the current lack of reliable sustainability measurement techniques, effective evaluation systems, and localized inventory data for industry to objectively evaluate and improve sustainability of waste systems. In order to respond to the situation, enormous efforts have been made for sustainability research in waste management. Included are the following research areas:

- Sustainability measurement methodologies and modeling techniques;
- Evaluation systems and analytical tools;
- Data needs in sustainability assessment and acquisition of inventories; and
- Sustainability assessment case studies.

For sustainability measurement and modeling in waste management, the most commonly used methods include life cycle assessment (LCA), material flow analysis (MFA), and sustainability indicators/metrics. A great number of waste LCA models have been developed and used in various waste management applications. Cleary [4] conducted a comparative analysis on twenty LCA models of various waste systems. The analysis found that many models lacked transparent methodological assumptions, which made the LCA results difficult to interpret and compare. Gentil et al [5] also observed large discrepancies in LCA results when different waste LCA models were used. They analyzed different LCA methodologies and technical assumptions, and highlighted several criteria that could have significant impacts on the results. Suggestions were made from their study to strengthen waste LCA modeling. Singh et al [6] reviewed the indicator-based sustainability modeling methodologies, including the formulation strategy, scaling, normalization, weighting and aggregation techniques. According to the dimensions that the indicators addressed, they further classified the sustainability indicators surveyed into twelve categories covering innovation and technology, economy, environment, eco-system, industrial performance, product, energy, social and quality of life, and other aspects.

Although great progress in waste management modeling has been made, few models consider all three dimensions of sustainability in the environmental, economic and social aspects together with applications of the models [7].

The types of sustainability evaluation tools used in waste management can be classified according to the goals that the tools serve, such as for cost-benefit analysis, life cycle analysis, carbon footprint, multi-criteria decision analysis

(MCDA), and the hybrid. Currently, the most mature evaluation systems used in sustainability assessment are LCA-based software tools, such as the GaBi system [8] and the EASEWASTE tool [9]. Others include those based on applied mathematics (e.g. statistical analysis, simulation, and optimization) [10], agent-based systems [11], and decision support systems [12]. For waste decision support, MCDA systems are commonly used. In a recent report, Huang et al [13] reviewed over 300 environmental applications of MCDA. Their analysis indicated that the share of applications of MCDA tools has increased significantly over the past 10 years. It was also shown that MCDA tools would deliver ranking results with small discrepancies. MCDA and other sustainability evaluation systems have provided an effective computing and analyzing means to facilitate the selection of the most appropriate waste treatment solutions.

Besides the modeling methods and computing systems discussed above, data acquisition in sustainability assessment is another critical issue. This may include data collection, validation, processing, and use of data to instantiate sustainability models and to enable computation of sustainability footprints of the assessed waste systems. Although most of the computing tools provide generic life cycle inventories to facilitate efficient use of the software systems, availability and quality of site- or process-specific data and other localized information are still problematic. Ruiz-Mercado et al discussed the data needs and potential data gaps in calculation of sustainability indicators [14]. In a detailed analysis of a waste management system, Villeneuve et al used local data on waste streams and treatment units to assess the system efficiency in terms of recycling rates, energy recovery, emission fluxes and costs [15]. Rather than relying on national statistics of waste generation per capita or generic characteristics of waste treatment technologies, their analysis was based on the specifics of a given waste system to provide decision-makers with quantitative arguments.

Sustainability assessment in waste management practices is rooted underneath the use of comprehensive models with transparent and highly detailed internal and external influences, robust computational tools, and sufficient inventory data. The current assessment methodologies have fulfilled the need to certain degree. There exist great improvement potentials in many assessment areas. Three of them are identified: sustainability modeling, computation tools, and data provision, to which this study intends to contribute.

The method presented in this chapter has an objective to evaluate and improve process sustainability in waste management in Singapore by enabling reliable, practical sustainability modeling, simulation, and data acquisition. It provides two techniques for metrics-driven sustainability modeling and agent-based sustainability simulation. Together with a technology inventory to provide localized and structured information on waste handling technologies and operations, the method allows systematic and rigorous assessment of process sustainability in the Singapore's waste management context. With the metrics-driven modeling technique, the process sustainability characteristics are integrated with the technical objectives of waste management systems to quantify the economic, environmental, social and technological performances in model-based computable metrics. The metric models describe and represent the interactions between the sustainability perspectives and the processing technology choices, key operating parameters, material market conditions, and other influencing factors in waste management. Hence, a simulation tool can further use the metric models to imitate sustainability behaviors of waste management systems with these influencing factors. A software agent is developed as the sustainability simulation tool in this study. The agent consists of four main parts: 1) a software implementation of the sustainability simulation models; 2) a set of Monte Carlo simulation services; 3) a technology inventory with key process data of waste handling technologies and operations, simulation inputs and their restraints; and 4) an overall workflow to coordinate tasks of the agent with other related human/software agents. By continually calculating and comparing process sustainability characterized by the sustainability metrics, the agent simulates process scenarios under uncertain or deterministic conditions to provide a series of reference points for evaluation and improvement of sustainability behaviors of waste management systems.

The chapter is organized as follows. The concept of process sustainability in waste management and the related work are presented in Section 2. Two techniques for metrics-driven sustainability modeling and agent-based sustainability simulation are detailed in Sections 3 and 4 respectively. A case study is discussed in Section 5 to evaluate process sustainability of material recovery options using our techniques developed. A summary of the research findings is given in Section 6 together with a future work plan.

2. PROCESS SUSTAINABILITY IN WASTE MANAGEMENT

2.1. Waste Management in Singapore

Waste management in Singapore involves the collection, transport, treatment, disposal, prevention, reduction, reuse, or recycling of waste, including the recovery of materials and energy from waste. As a small island city-state, Singapore has a high population density (7,126/sq-km for 2010) and a highly industrialized economy (S$59,813/capita GDP for 2010) with very limited natural resources especially a severe scarcity of land (total land area: 712.4 sq-km for 2010) [16]. These characteristics require Singapore to develop innovative, forward-reaching waste management strategies to sustain the economy growth and living standard increasing. Singapore adopts a three-prong strategy to reduce the need for landfill. The three strategies are: waste minimization at source, recycling to reduce the amount of waste disposed of, and incineration to reduce the volume of waste and to recover energy. Specifically, the waste strategy has set the following targets to achieve sustainable waste management in Singapore [1]:

- To increase the overall waste recycling rate from 44% to 60% by 2012;
- To extend the lifespan of Semakau Landfill to 50 years, strive for "zero landfill" and close the waste loop; and
- To reduce the need for new incineration plants to one every 10 to 15 years.

Waste management in Singapore is based on a waste hierarchy for waste minimization (reducing, reusing and recycling), followed by incineration and landfill [17], as shown in Figure 1. The waste management options at the top of the hierarchy are most preferred.

Figure 1 indicates that out of the 6.52 million tons of waste generated in 2010, 58% has been recycled, 40% incinerated, and only 2% for landfill [18]. In order to meet the targeted 60% recycling rate by 2012, new resources recovery facilities have been set to further increase the share of waste minimization and reduce that of waste disposal in Figure 1. Another key thrust is to enhance waste industry capability by promoting innovative technologies to recycle and reduce waste [1] and to maximize recovery of recyclables from waste. To ensure the sustainable development in Singapore, these innovative waste management solutions must provide not only the technological advances but also the superior environmental, economic and social characteristics measured in process sustainability.

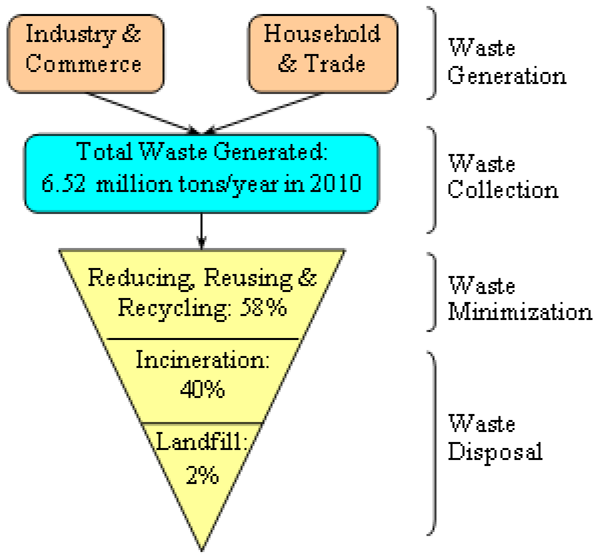

Figure 1. A hierarchy for waste management in Singapore.

2.2. Concept of Process Sustainability

Although generally understood as a waste business goal with a combination of environmental, economic and social objectives, process sustainability is difficult to define and operationalize in waste management practices. There is currently not even agreed consensus on what specific criteria to include in process sustainability, how to measure and compute the concept, what datasets to use, and how to evaluate it in real-world waste processes.

It is however recognized that the sustainability of a waste process should be more generally understood through a wide range of well-known "development drivers for waste management". Wilson [19] defined six such drivers as public health, environmental protection, resource value of waste, closing the loop, institutional and responsibility issues, and public awareness. Escalante [20] suggested five basic functions for conceptualization of a sustainable waste management model: public health protection, value recovery, pollution control, resource conservation, and climate protection.

Table 1. Process sustainability metrics for waste-to-material recovery processes

Sustainability Criteria Category	**Metrics**	**Key Metrics Variable**
Waste Minimization	Process efficiency	Content of materials to be recovered in feedstock, recovered content of materials.
	Resource use efficiency	Selected key process parameters, consumptions of resources in a specific process, best achievable resource consumptions under a given operating conditions.
In-Process Recycling	In-process recycling rate for raw materials	Total consumptions of raw materials, recycled materials in the same process before disposed as waste from the process.
	In-process recycling rate for water	Total consumption of processing water, recycled water in the same process before disposed as wastewater from the process.
Resources Conservation	Recycled/reused/renewable content of material inputs8	Total weight of recycled/reused/ renewable materials consumed, total weight of material inputs.
	Recycled/reused/renewable materials content of outputs	Total weight of recycled/reused/ renewable materials content in outputs, total weight of outputs.
	Renewable proportion of energy consumed in a waste process	Renewable energy consumed, total energy consumed in a waste process.
Environmental Protection	Carbon footprint for GHG emissions	Material/water/energy use, transport, emission factors.
	Energy intensity	Total energy consumption normalized to a unit of output.
	Water intensity	Total water intake normalized to a unit of output.
	Waste intensity by mass balance	In-process recycling rate, recovery rate, concentration of materials to be recovered in feedstock.

Sustainability Criteria Category	Metrics	Key Metrics Variable
Economic Value	Unit cost / Total production cost	Feedstock price, recovered material market value, energy efficiency, production volume, batch size.
	Total process revenue from waste	Recovered material/energy market value, sales quantity.
	Net present value / Internal rate of return	Net cash flow, lifespan of a waste handling facility.
	Payback period	Capital investment, annual operating cost savings.
Society Responsibility	TCLP toxicity level of process residuals	TCLP test data for process residuals.
	Restricted substances intensity of inputs	Weight of restricted substances consumed for a unit of output.
	Hazard potential of chemicals used	Weighted hazard characteristics of chemicals used.

Process sustainability in waste management can be referred as the sustainability at process level. It is process based and contextual. Embraced in this concept are the requirements on economic, environmental and social behaviors of a waste management process. Besides these triple bottom line requirements, process sustainability can also be described and assessed by other designated, context-specific performance criteria, depending on the particular assessment objectives, desired features of the assessed processes, resource requirements and feasibility, etc.

Based on the Singapore's waste hierarchy (Figure 1) and the generally-agreed development drivers for waste management [19], six categories of quantitative criteria are selected to assess the process sustainability in waste management in Singapore. The criteria can capture the effects of waste minimization at source, in-process recycling to reduce waste, conservation of natural resources (material, water and energy), environmental protection, economic value from waste, and social responsibility to protect public health and natural ecosystems. Each of the criteria is measured in a computable metric. Table 1 summarizes exemplary process metrics used in sustainability assessment of waste-to-material recovery processes in this study.

The metrics in Table 1 describe the relationships between a process sustainability criterion and a set of influencing factors (refer to the key metrics variables in Table 1) that can be technical characteristics of a waste technology, operating parameters, material market conditions, and so on. As such, these computable metrics can provide detailed, process-specific sustainability information of a given waste system. The key model variables of the metrics in Table 1 have revealed the major data needs for inventories in order to compute the metrics and simulate process sustainability. Regarding the data needs, metrics modeling and sustainability simulation, Sections 3 and 4 will elaborate our proposed techniques. But first the background and related work in these areas are reviewed as follows.

2.3. Sustainability Measurement with Metrics – Existing Modeling Approaches

There exist a number of approaches to the development and implementation of multi-level sustainability metrics/indicators at the global, country, enterprise, product and process levels. The OECD, IEA and IPCC have led the efforts in establishing the national- and international-level sustainability accounts and indicators. Examples include the OECD's Material Flows and Resource Productivity [21], Energy Efficiency Indicators from the IEA [22], and IPCC's Guidelines for National Greenhouse Gas Inventories Reporting [23].

At the enterprise level, ISO has provided a series of standards for establishing environmental management systems (ISO 14001), corporate greenhouse gas measurement (ISO 14064), and environmental labeling (ISO 14023 and 14025). WRI and WBCSD [24] have been developing a set of GHG Protocols as a life cycle accounting and reporting standard for businesses. GRI [25] has also provided a flexible sustainability reporting framework together with a comprehensive set of indicators and methods. The similar initiative in Europe is the Eco-Management and Audit Scheme [26] that has worked as a voluntary reporting framework for companies to measure and improve their sustainability performance.

At the product and process level, ISO has established methodologies for life cycle assessment (ISO 14040 series) and carbon footprint (ISO/CD 14067) as important indicators to quantify environmental impacts from products and production processes. Other widely adopted, national standards for carbon footprinting and labeling include PAS2050 [27] from the UK, the greenhouse gas inventory protocol [28] from the USEPA, the carbon footprint technical specification [29] from Japan, and many others.

Although the multi-leveled sustainability metrics above have played an important role in defining objectives and monitoring progress towards sustainable development, they need consolidation and harmonization [30]. NIST and OECD have begun efforts to address this issue with a focus on metrics for sustainable manufacturing. The OECD's framework for eco-innovation in industry [31] has been reviewing and consolidating the diverse set of existing metrics, and developing an integrated set of core indicators, metrics, and data collection guides to measure sustainability of industries, their production processes, products and services. Figure 2 shows the published sustainability indicators from OECD [32]. The current 18 indicators are focused on environmental sustainability only. They are classified into three indicator categories: inputs used in industrial processes, operations to turn inputs into products, and products (Figure 2).

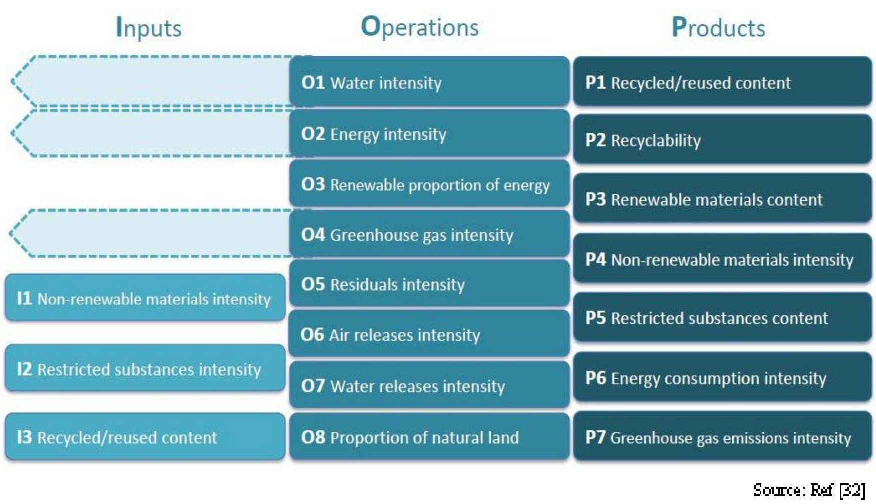

Figure 2. Classification of OECD sustainability indicators.

A selected set of metrics from the indicator categories in Figure 2 are applied to this study to describe some sustainability characteristics of waste-sourced material recovery processes. These include the metrics for water intensity (O1 in Figure 2), energy intensity (O2), renewable proportion of energy consumed (O3), restricted substances intensity of inputs (I2), recycled/ reused content of material inputs (I3), and recycled/reused materials content of products (P1). Specific metrics in the Singapore's waste management context for waste minimization, in-process recycling, resources conservation, environmental protection, economic value, and social responsibility of the waste-to-material recovery processes are also established. Their definition and classification can be found in Table 1.

2.4. Sustainability Simulation – Agent-based Methods

Sustainability simulation is a technique that permits imitation of the sustainability performance with particular conditions in waste operations to analyze and improve sustainability behaviors of waste management systems.

The simulation of process sustainability in waste management can be achieved in many ways. Among others, agent-based systems would provide an effective and practical means to facilitate process sustainability evaluation and comparison. An agent system is well suited for simulating the complex interactions and interdependencies between the underlying model variables (representing recycling system structures, parameters and other influencing factors) and the exhibited sustainability behaviors of waste systems under heterogeneous, even uncertain conditions. It explores the inter-related effects of changes to the waste systems based on an intersection of three scientific fields: the sustainability science, agent-based modeling, and computer simulation. The sustainability science provides methods to characterize the sustainability of a waste system with sustainability models, such as metric models discussed earlier. Agent-based modeling uses the sustainability models as the basis to formulate behavior models, to define simulation scenarios, and to specify relationships between the agents involved in the sustainability behaviors analysis. Computer simulation concerns techniques for simulating the modeled system behaviors on a computer, such as discrete event, equation-based, or Monte Carlo simulation.

Interesting and relevant work have been reported in agent-based sustainability assessment and simulation, such as for urban water systems [33], logistics systems [34], fishery management [35], housing developments [36], ecological economics [37], etc. Although agent-based systems have been successful in the above areas, their applications to process sustainability evaluation of waste management systems have yet been fully explored. This work therefore attempts to fill the knowledge gap by developing an agent-based system for sustainability evaluation and simulation of waste management processes (refer to Section 4 for details).

3. METRICS-DRIVEN SUSTAINABILITY MODELING IN WASTE MANAGEMENT

3.1. Metrics Development Process and Techniques

As understood from Section 2.2, process sustainability in waste management can be viewed from different perspectives. As such, no standard, all-inclusive methodology has yet been available for sustainability metrics development of waste systems. Our metrics modeling technique draws from several methodologies including the LCA framework in ISO 14040 series, the OECD's approach to sustainability indicators development [31], and the USEPA's greenhouse gas inventory protocol [28]. The purpose of the process sustainability metrics is to facilitate the waste industry in Singapore to measure and evaluate their processes for sustainability improvement. Toward this end, six sustainability modeling and assessment activities are conducted:

- Defining goal and scope;
- Selecting sustainability criteria;
- Formulating computable metric models;
- Identifying data needs and collecting, compiling inventory data;
- Calculating metric values for sustainability evaluation; and
- Simulating process scenarios to identify improvement potentials.

The idea behind this metrics development process is that in model-based metrics, quantifiable sustainability properties of a waste process are expressed in quantities with units, values and relationships of the corresponding technical, business systems. As these metric variables are related to the process technological characteristics and other real-world influencing factors, the metric models are functions of process technology choices, waste management operations, market conditions, and so on. The model-based metrics are hence able to unambiguously characterize, measure, and evaluate the process and its sustainability performance, not only for a specified, nominal process state but also for various process scenarios to compare and explore potentials in performance improvement. This metrics-driven sustainability modeling technique is illustrated in Figure 3.

The techniques used in the six activities in our metrics development process in Figure 3 are elaborated. Three are discussed below for goal and scope definition, sustainability criteria selection, and inventory preparation.

Other two for metrics formulation and scenarios simulation will be covered in Sections 3 and 4, while sustainability evaluation will be demonstrated in Sections 5 through case studies.

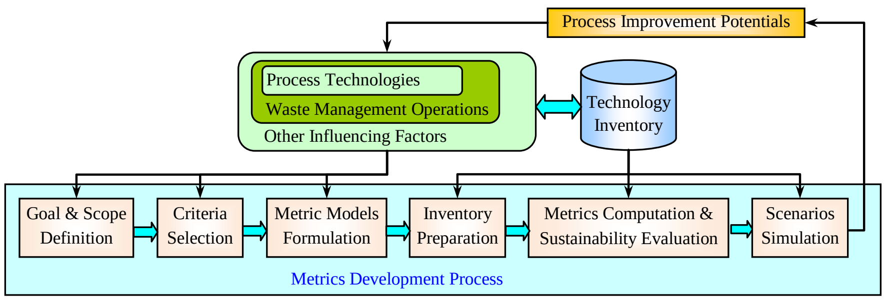

Figure 3. A metrics-driven sustainability modeling method.

The goal and scope definition step in Figure 3 defines the metrics modeling goals and assessment system boundary following the general principles in the LCA framework. It will also set the limits of data to be collected. The key in performing this task is that all definitions must be explicitly specified to minimize hidden assumptions. Boundary setting itself is actually an influential assumption with potentially large effects on both results and the confidence of the decision maker using them [38]. Any flows of resources outside the assessment boundary are inherently precluded from detailed examination. Hence their effects on the sustainability performance of the modeled system would not be directly captured in the metrics, although the interactions and connections between the modeled system and its upstream/downstream systems can be reflected in the metrics through model parameters. Figure 4 depicts an example of boundary setting for metrics modeling of waste-to-material recovery processes. The modeling resolution of the system concerned and its external environment systems is different as the modeling goal has been set for formulating the sustainability characteristics of the material recovery process, rather those of its upstream or downstream processes.

The next step in our metrics development process in Figure 3 is selection of sustainability criteria. It largely depends on the sustainability assessment goals, application needs and contexts, and desired modeling viewpoints as discussed in Section 2.2. Most efforts in sustainability definition are focused on the triple bottom line. Their sustainability criteria are therefore related only to the environmental, economic and social concerns. In the goal and scope definition step in our modeling process, the purpose of this assessment has been defined to facilitate recyclers in Singapore to understand, evaluate and compare process sustainability of their waste systems for performance improvement. Hence, apart from the conventional triple bottom line, our sustainability criteria are selected with taking into additional considerations specific to waste management in Singapore – to strive for zero landfill and close the waste loop (Section 2.1). The criteria cover six context-specific perspectives to define process sustainability as given in Table 1. Under the six criterion categories in Table 1, there are 18 sustainability criteria that can be customized for use in a specific waste process' assessment. All criteria are of quantitative nature and each introduces a computable metric.

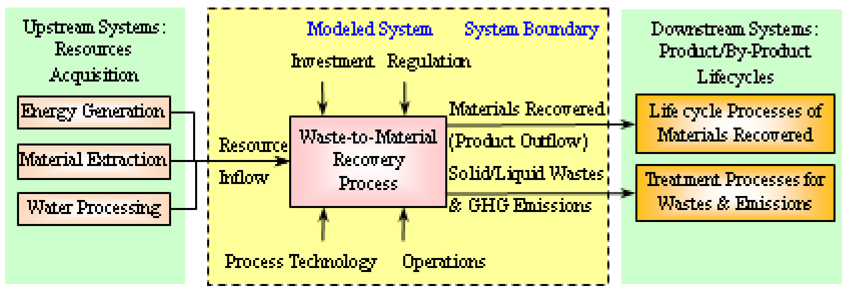

Figure 4. Boundary setting for metrics modeling of waste-to-material recovery processes.

The inventory preparation step in Figure 3 involves identifying data needs and data sources, and collecting, compiling inventory data for process sustainability assessment and scenarios simulation. The inventory data are needed to instantiate the metric models and simulation models. Therefore the starting point for identifying data requirements is to examine model structures, parameters and variables in metric equations. Besides this, many datasets needed are measured directly with laboratory or field tests, modeled with physical, biological or chemical principles and theories, or observed with field guides and experiences. In turn, these activities often help identify additional data needs. Available data sources can be from calculation and computation of existing data, experiments and measurements, interviews and surveys, commercial and open inventory databases, etc. This study also uses local data sources to provide context- and process-specific data. They include reviews of the existing national mechanisms related to the waste industry, national key environmental statistics, waste processing technology reviews, and waste management practices in Singapore. For data collection, to have robust processes is the key to ensure data can be collected and managed systematically and consistently.

Using the boundary, criteria selection and data techniques above, six categories of computable metrics for process sustainability assessment have been selected and listed in Table 1. The key metric variables are also given in the table to facilitate inventory data acquisition. The formulation details of six metrics selected from the six categories in Table 1 are discussed in the following sections. They are carbon footprint for GHG emissions, unit cost, TCLP toxicity level of process residuals, resource use efficiency, in-process recycling rate for chemicals used, and recycled content of material inputs. The application context of the metrics is for the process sustainability evaluation of waste-to-material recovery processes.

3.2. Environmental Sustainability Metrics

There are four process-based metrics under the environmental protection category in Table 1. The carbon footprint metric for GHG emissions from waste-to-material recovery activities is elaborated in this section.

3.2.1. Quantification Methods

There exist several GHG emission quantification methods for industrial processes. The most commonly used ones include:

- Direct measurement of GHG emissions over a period of time for a specified industrial facility or process;
- Site data sampling for calculation of GHG emissions from an industrial site;
- Mass balance methods to compare the total amount of mass entering a process to that leaving the process for emissions estimation; and
- Emission factor methods that use the emission factors derived from the process-specific, or averaged industry-wise, country-wise emission measurements and experiments for emissions calculation.

The choice of an emission quantification method depends on the availability of resources and data needed, the degree of accuracy required, and the way of the estimates to be used. In this study, an emission factors method is selected for estimating carbon footprint in material recovery processes, mainly because of its ease of use and relative low cost for carbon footprint estimation.

Carbon footprint is defined in ISO/CD 14067-1 as a "weighted sum of greenhouse gas emissions and greenhouse gas removals of a process, a system of processes or a product system, expressed in CO2 equivalents (CO2e)". In this study, carbon footprint is used to measure the six types of Kyoto Protocol GHG emissions that a particular waste-to-material recovery process would cause over its lifetime. Carbon footprint is measured in a unit specified by ISO 14067-1 for kg-CO2e/functional-unit. We used one kg of recovered material as the functional unit in this study.

The carbon footprint can be measured according to the USEPA's general emissions equation in *Emissions Factors and AP-42:*

$$E = AD \times EF \times (1 - ER/100) \tag{1}$$

where E = GHG emissions; AD = activity data; EF = emission factor; ER = overall emission reduction efficiency. According to ISO 14064-1, EF is a factor relating activity data to GHG emissions, while AD a quantitative measure of activity that results in a GHG emission.

3.2.2. Emission Sources Analysis of Waste-to-Material Recovery Processes

The CO2e emissions associated with the process activities for materials recovery from waste are identified and categorized into the direct, indirect and optional emissions according to USEPA's Greenhouse Gas Inventory Protocol [28].

Direct emissions in this study encompass those emitted from processing activities for material recovery and from production transport. Indirect emissions include those from the generation of electricity consumed for material recovery. Optional emissions cover the emissions from the production of raw materials used in the recovery processes. Such emissions are the consequences of the activities in the recovery processes, but occurred from sources at the upstream raw material production. The Guidance [28] termed them as optional that can be included in or excluded from the carbon footprint analysis for an assessed process with explicit declarations. From the analysis above, the emission sources of material recovery from waste can be identified. They are: process activities for material recovery; production transportation; energy consumed in the process; and materials/chemicals/water consumed in waste-sourced material recovery.

Applying Eq. (1) to the carbon footprint estimation of material recovery processes, we have developed individual metric models for measuring the direct, indirect and optional CO2e emissions of the processes concerned.

3.2.3. Formulation of GHG Emissions Metric Models

Direct Emission of CO2e from Transport

The direct emission E_i from three GHGs: CO2, CH4, N2O is calculated based on Eq. (1), using $ER = 0$ for baseline scenario assessment. The calculation formula is given by:

$$E_i = EF_i \times \sum_j AD_j^T \tag{2}$$

where E_i is the i^{th} direct emission; i = (CO2, CH4, N2O); EF_i the i^{th} emission factor retrieved from an inventory database; AD_j^T the transport activity data at the process step j.

The individual GHG emissions (CO2, CH4 and N2O emissions) calculated from Eq. (2) are converted to carbon footprint (CO2e emissions) by use of the following formula:

$$CF_{direct} = \sum_i (E_i \times GWP_i) \tag{3}$$

where CF_{direct} represents the direct CO2e emissions composed of CO2, CH4 and N2O emissions (E_i) in transport; E_i is derived from Eq. (2); GWP_i is the i^{th} GWP factor (i = CO2, CH4, N2O).

The Global Warming Potential (GWP) factors (GWP_i) are generic constants in Eq. (3) to describe the radiative forcing impact of one mass-based unit of a given GHG relative to an equivalent unit of CO2 over a given period of time. According to the IPCC standard [39], $GWP_{CO2} = 1$, $GWP_{CH4} = 25$, and $GWP_{N2O} = 298$. They are used in calculation of Eq. (3) in the present study.

Indirect CO2e Emission from the Use of Electricity

Assume the energy used for material recovery is electricity. The emission factor of purchased electricity for each country/region is usually compiled based on a measure of kg CO2e per kWh. Using this factor, the indirect CO2e emission can then be calculated by:

$$CF_{indirect} = EF_e \times \sum_j AD_j^e \tag{4}$$

where $CF_{indirect}$ is the total indirect CO2e emissions from using purchased electricity; EF_e the emission factor of electricity in Singapore; AD_j^e the activity data of electricity consumed at process step j.

Optional CO2e Emission from the Use of Materials/Chemicals

Similar to the indirect emission calculation in Eq. (4), the optional CO2e emissions from the use of materials and chemicals can be accounted by:

$$CF_{optional} = \sum_n (EF_n \times \sum_j AD_j^n) \tag{5}$$

where $CF_{optional}$ is the optional CO2e emissions induced from the use of materials/chemicals in an assessed process; EF_n the emission factor of the n^{th} type of material; AD_j^n the activity data of material n used at the j^{th} process step.

Total Carbon Footprint

From the above equations (2)-(5), the core direct, indirect and optional CO2e emissions can be estimated. The total carbon footprint of an assessed material recovery process is then computed as a summation of these emissions by:

$$CF_{total} = CF_{direct} + CF_{indirect} + Opt(CF_{optional}) \tag{6}$$

where CF_{total} represents the total carbon footprint of a material recovery process; $Opt(\cdot)$ denotes an optional summation operator.

3.2.4. Application Issues of GHG Emission Metrics

In Eqs. (2), (4) and (5), emission factors (*EF*) represent unit rates of emission sources. The acquisition of consistent, location-specific emission factors is a major challenge in the use of the GHG emission metrics in practice. It involves many issues in emission data availability, quality, sharability and accessibility. Although EPA, IPCC, EU and many countries maintain compilations of emission factors, there still are emission factors not readily available, such as those for some chemicals used in waste-to-material recovery processes. In this case, the factors need to be estimated based on chemical reaction equations and the available data in literature, together with additional assumptions. Besides calculation-based methods, emission factors can also be acquired by literature survey and by direct measurement and experiment methods.

Another process-specific model variable in the carbon footprint metrics above is activity data (*AD*). They are quantities of resources consumed for process activities. Specifically for material recovery processes, activity data include consumptions of process materials/chemicals, water and energy, their use efficiency, and production transport distance, etc. In this research, the activity data are mainly collected from a pilot-scale material recovery process under study or from laboratory experiments.

It is known from the metric models in Eqs. (2), (4) and (5) that GHG emissions are dependent of the process parameters through the metrics variables for activity data. Different recovery technologies present different requirements on resources consumption and resources efficiency in material recovery, which leads to different activity data values. Hence they deliver different carbon emissions (CO2e emissions) and different environmental performances. By constructing the GHG emissions metrics as functions of these process technologies, the derived metric model in Eq. (6) would provide an effective tool for evaluating and comparing carbon footprints to explore carbon reduction potentials in material recovery from waste.

3.3. Economic Valuation Metrics

The economic value generated from a waste system is assessed by four metrics in Table 1. Some of the metrics (e.g. net present value and payback period), as general economic performance measures, have had mature and standard definitions and model expressions. They are therefore not covered here. This section introduces the formulation of a process-specific economic metric for unit cost.

3.3.1. Process Cost Modeling Method

To reclaim a given output (*Q*) of material from waste, a recovery facility uses inputs for raw materials (*M*), labor (*L*), energy (*E*) and capital (*K*). The total process cost (*C*) arising from the reclamation process is determined by costs of respective inputs C_i $(i = M, L, E, K)$ and the level of output (*Q*), with a given recovery technology (*T*). Specific to the waste-based material recovery business in Singapore, the feed material cost is a function of the market value *P* of the recovered materials. The total process cost (*C*) is therefore a function of C_i $(i = M, L, E, K)$, *Q*, *T* and *P*. It is expressed as:

$$C = F(C_M, C_L, C_E, C_K, Q, T, P) \tag{7}$$

This study uses unit cost as a key economic metric to measure the process economic value. Unit cost (C^U) is the cost for producing one unit of output material recovered from waste by a given recycling technology. According to Eq. (7), the unit cost of a recovered material can be represented as:

$$C^U = f(C_M{}^U, C_L{}^U, C_E{}^U, C_K{}^U, Q^A, T, P) = \sum_i C_i{}^U + C_O{}^U \quad (8)$$

where $f(\cdot)$ is a function of the unit cost; C_i^U $(i = M, L, E, K)$ the unit cost of the respective production inputs for raw materials (M), labor (L), energy (E) and capital (K); T the given recovery technology reflected by a set of metric parameters in C_i^U and $C_O{}^U$; P the market value of the recovered material; Q^A the quantity of output per year; $C_O{}^U$ the other additional cost elements included in the unit cost function such as costs for maintenance and space rental.

Each unit cost element C_i^U in Eq. (8) can be represented by a cost metric, which quantify economic effects of inputs i $(i = M, L, E, K)$ on the production output of Q given the process technology T and the recovered material's market price P at time t. On the other hand, the cost metrics also capture the influencing technological factors (process concepts, recovery rate, process efficiency, etc.) and production conditions (batch size, processing time) for optimal material recovery from waste. The cost metrics modeling details are explained through the following examples.

3.3.2. Cost Metrics Development

The key technique used in cost metrics modeling is process mapping that establishes relationships between unit cost elements C_i^U and process internal/external factors. These factors may include process parameters, production conditions, economic characteristics, policy influences, etc. The mapping is based on the engineering principles, empirical formulas and testing data, etc. Take the energy cost formulation as an example. We assume a material recovery process relies on electricity as a source of energy. The electricity cost metric, $C_E{}^U$, in Eq. (8) is closely related to the following process details: electricity consumption and energy efficiency at each process step, processing time, batch size, and process failure rate. Therefore the relationship between electricity cost and the set of process parameters above should be established. The economic effects of these influencing factors on the electricity cost per unit of qualified output material (non-defective) are quantified as:

$$C_E^U = S \sum_j 1/\zeta_j E_j T_j / [B(1-\varphi)] \quad (9)$$

where S is the unit cost of electricity supply; ζ_j, E_j, and T_j the energy efficiency, electricity consumption, and processing time at the j^{th} process step respectively; B the batch size of production; and φ the given process failure rate.

The capital investment to a material recovery facility includes the costs for equipment, installation and startup investment. The metric model for calculating the capital cost is sensitive primarily to differences in the sizing of the recovery facility. Given that a base case facility of size Z_b would cost C_b, the total capital cost, C_x, of a facility of size Z_x can then be calculated by

$$C_x = C_b (Z_x / Z_b)^{\alpha}, \quad (10)$$

where α is an investment scale factor.

Assume that the total capital cost C_x in Eq. (10) can be distributed evenly in time over the usable lifetime of the recovery process facility. Using a standard capital recovery factor [40], the levelized capital cost metric model will be derived as:

$$C_K^A = C_x\, r / [1-(1+r)^{-N}], \quad (11)$$

where C_K^A represents the allocated annual capital cost; r the real discount rate; N the recovery facility lifetime in years.

By further distributing C_K^A evenly over the annual production output Q^A and considering the process failure rate φ and the process downtime rate ω, the unit capital cost C_K^U is thus derived by the following metric:

$$C_K^U = C_K^A / [Q^A(1-\varphi)(1-\omega)] \quad (12)$$

Similarly, the relationships between the other identified unit cost elements (i.e. C_M^U, C_L^U and C_O^U) and their influencing process factors can be formulated. For material cost however, as mentioned earlier, the feedstock cost is a function of the selling prices of the recovered materials. In this case, the material cost metric (C_M^U) is a function of both the process inputs and the market conditions. Table 2 summarizes the major influencing factors of cost metrics for material reclamation processes from waste.

Table 2. Influencing factors of the selected cost metrics

Cost Metric	Key Influencing Factor	Other Factor
Material cost (C_M^U)	Material consumption; Recoverables concentration in feedstock; Feedstock purchase price; Market value of recovered materials.	Recovery rate; Process failure rate.
Labor cost (C_L^U)	Processing time per batch of production; Batch size.	Process failure rate; Equipment downtime; Labor Productivity.
Energy cost (C_E^U)	Energy consumption; Energy efficiency; Processing time.	Process failure rate; Batch size.
Equipment cost (C_K^U)	Capital investment; Production volume.	Process failure rate; Equipment downtime; Equipment life span.

3.4. Metrics to Measure Social Responsibility of Processes

The social performances of waste treatment processes are measured with three metrics in this study. Two metrics are detailed in this section: TCLP toxicity level of process residuals and restricted substances intensity of inputs.

TCLP (toxicity characteristic leaching procedure) is one of regulatory requirements commonly used to assess leachability of the hazardous industrial wastes dumped in landfills. It has been well known that many industrial wastes are toxic with leachable heavy metals or other hazardous volatiles. They can impose serious hazards to human health and natural ecosystems. As such, the hazardous chemicals use in industrial processes and wastes treatments must be compliant with the applicable regulations such as TCLP. The TCLP method can be used to determine if process residuals (solid wastes from a waste management process) are characteristically hazardous by examining leaching levels of the wastes to be disposed of. In the current study, TCLP testing is conducted to the process residuals produced after material extraction from hazardous industrial wastes. The following TCLP metric is used in the toxicity level analysis to determine if a residual is safe for disposal after valuables reclaimed.

$$\text{TCLP (measured)} \leq \text{TCLP (regulated-limit)} \quad (13)$$

The use of this metric in the studied processes will be demonstrated in Section 5, which assesses if the measured TCLP values of process residuals meet the local TCLP standard [41] for safe disposal. A good understanding of the toxicity level of the process residuals would lead to better choices of processing techniques and chemicals to reduce the hazards from toxic wastes treatment.

Some waste processing reactions use substances and chemicals restricted by law as a proportion of the production. The OECD sustainability indicator set [32] has provided a metric, known as restricted substances intensity of inputs (I2 in Figure 2), to quantify and monitor the use of restricted substances. We adopt the metric to measure the use of restricted substances in waste processing to reclaim materials from waste. The metric for restricted substances intensity of inputs is defined as:

$$\text{RSI} = \sum_j \sum_i \text{Sub}_{ij} / \text{NormF} \quad (14)$$

where *RSI* depicts the restricted substances intensity of inputs; Sub_{ij} the i^{th} restricted substance consumed at the j^{th} process step; *NormF* the normalization factor. In the present study, we use one unit of output from a waste facility as the normalization factor.

3.5. Formulation of the Contextual Sustainability Metrics

Under the context of sustainable waste management in Singapore, one of the critical targets is to strive for zero landfill and close the waste loop [1]. To serve the needs arising from this, three categories of context-specific sustainability metrics have been selected (Table 1) to effectively measure, monitor and improve the local waste practices. The context-specific metrics categories include: waste minimization at source, in-process recycling, and resources conservation. Apart from the triple bottom line based metrics defined in Sections 3.2 to 3.4, this section establishes the context based sustainability metrics selected from the three categories.

3.5.1. Waste Minimization Metrics

We use two process-specific metrics (process efficiency and resource use efficiency) to evaluate the effect of waste minimization at source brought by waste-based material recovery practices in Singapore.

The resource use efficiency metric is a weighted composite indicator to quantitatively describe the efficiency in the use of raw materials/chemicals, energy and processing water in waste recycling and recovery processes. Our earlier report [42] has covered a detailed discussion on resource use efficiency in material recovery from waste. The following summarize the definition of the metric model for resource use efficiency:

$$\mathrm{Eff} = 1 - \sum_i \sum_j [(u_{ij} - U_{ij}) / u_{ij}]\,(1/N_i)\,W_i \tag{15}$$

where *Eff* is the composite metric for resource use efficiency of a waste processing option; W_i the weight of the i^{th} resource type; i = (material, energy, water); u_{ij} the measured consumption of the j^{th} resource under the i^{th} resource type; j = (material_1, material_2, …, material_n) for the "*material*" resource type and j = (electricity, natural gas, fuel oil, steam, other forms of energy) for the "*energy*" resource type; U_{ij} the expected consumption (best achievables under a given production condition) of the j^{th} resource under the i^{th} resource type; N_i the total number of the resources under the i^{th} resource type.

The resource use efficiency metric model in Eq. (15) will be used in a case study in Section 5 to measure and compare the usage efficiencies of resources in waste treatment by using different material recovery technologies.

3.5.2. In-process Recycling Metrics

The capability of a waste management system to recycle its used chemicals, solutions and processing waters within the same process is measured by two metrics: in-process recycling rate for raw materials and in-process recycling rate for water. The two metrics have similar model structure defined by:

$$R = \sum_i \mathrm{RMat}_i / \sum_i \mathrm{TMat}_i \tag{16}$$

where R is the in-process recycling rate for raw materials or for processing waters; $RMat_i$ the i^{th} type of recycled material or water normalized to a unit of output; $TMat_i$ the i^{th} type of total material or water consumed for producing one unit of output.

3.5.3. Resources Conservation Metrics

Increasing the recycled and reused content of material inputs will reduce the amount of virgin materials required to contribute to resources conservation. Similarly, using renewable energy is another important way to reduce the demand for non-renewable energy. In general, recycled and reused materials and renewable energy sources are also lower in carbon content than their counterparts and therefore contribute less to climate change. The resources conservation effects brought by the use of recycled, reused and renewable materials and energy are measured by the resources conservation metrics. We have adopted the OECD's definitions and formulae [32] for these metrics. Details can be found from OECD references [31, 32].

4. AGENT-BASED SUSTAINABILITY SIMULATION

The sustainability metrics in Section 3 have defined the relationships between the performance measures and waste system parameters, technology choices, external influencing factors, etc. The metrics however need to be implemented in a computing, analyzing and simulation environment to facilitate the actual use of the metrics to support decision making in waste management operations.

An agent-based sustainability simulation system has been developed in this study to fulfill the needs for sustainability evaluation in waste management in Singapore. The agent experiments with waste systems' sustainability performances represented in computable metric models. The performance experimentation is conducted under controlled scenario environments and guided by sustainability simulation models with a prescribed set of goals, such as process profitability evaluation, carbon footprint reduction, cost sensitivity to market price changes, waste minimization potentials analysis, etc. The simulation experiments consist of stimulating a waste system under study with Monte Carlo sampling of the system variables, then observing system sustainability behaviors and its statistics, thus generating estimation to the studied system on its sustainability footprints.

This section highlights our efforts in formulation of sustainability simulation models, development of simulation scenarios, software agent system design and implementation, and Monte Carlo simulation of sustainability performances of waste systems.

4.1. Sustainability Simulation Model

A sustainability simulation model is a formalized and simplified representation of sustainability performance of a waste system. It is built from one or several sustainability metrics, but only the characteristics associated with those sustainability performance goals under study are retained and formalized in the simulation model as model variables. Other metric variables are converted to model parameters in the resulting simulation model. In many cases, a performance simulation model is a combination of several computable metric models, depending on how the metric models have been defined and what the simulation goals are. For example, a process profitability simulation model can be built as a ratio between the total process revenue (*TR*) and the total production cost (*TC*) that are represented by the following metrics:

TR = f1 (Sales quantity, Sales price) (17)

TC = f2 (Production volume, Unit cost) (18)

Considering the metric variables of unit cost in Eq. (8) and Table 2, we have:

TC = f2 (Production volume, Material consumption, Feedstock price, Market value of recovered materials, Processing time, Batch size, …) (19)

Obviously, it is not a good solution to directly use the metrics in Eqs. (17) and (19) to formulate the simulation model for process profitability. Simplification is required based on objectives of this simulation and model structures of the involved metrics. The purpose of the simulation is to examine the process profitability of a waste-to-material recovery facility under: 1) uncertain pricing market for recovered materials; and 2) changing concentrations of recoverables in feedstock (i.e. quality of feedstock). Therefore, the metrics variables related to these two aspects are retained, while others converted. After the re-formulation, the simplified simulation model for process profitability (*PP*) takes the following form:

PP = TR/TC = f (Production volume, Selling price, Recoverables concentration in feedstock) (20)

The uncertain unit cost simulation model has the same set of random and deterministic variables as the expression in Eq. (20). After applying the same simplification principles above, the unit cost (*UC*) simulation model can be represented by:

UC = g (Production volume, Selling price, Recoverables concentration in feedstock) (21)

Similarly, simulation models for other sustainability behaviors of waste systems can be developed. These include carbon footprint under uncertainty, cost sensitivity to market price changes, effect of resource use efficiency on waste minimization at source, and so on. Section 5 demonstrates the applications of some simulation models in case studies.

4.2. Simulation Scenarios

Sustainability simulation is conducted under the controlled computational environments to illustrate how the waste management technologies (e.g. a set of process parameters, processing procedures and techniques), operations and other influencing factors interact with the sustainability performance goals of a waste system. Such environments are defined as simulation scenarios. Two types of scenarios have been developed for deterministic and probabilistic simulations respectively. Details on the development of simulation scenarios for deterministic analysis of sustainability in waste-to-material recovery have been reported in a previous study [42]. The results are summarized in Table 3 for five simulation scenarios with deterministic input parameters. Two material recovery processes: closed-loop process and open-loop process are simulated under the five scenarios to understand sustainability behaviors of the two processes.

Another type of simulation scenarios is designed for sustainability evaluation under uncertain context. One example is process profitability simulation represented in Eq. (20). The random variables for *selling price* and *recoverables concentration in feedstock* in Eq. (20) enter the simulation following certain probability distributions (details in Section 4.3.4). A variety of scenarios have been explored to analyze the process profitability with different levels of production volumes, selling prices and concentrations, and on a chosen set of deterministic parameters. The scenario settings for selected simulation variables and parameters are shown in Table 4. These scenarios are used to explore one of the process sustainability performance goals for *process profitability*.

The scenario settings in Table 4 have been used in case studies in Section 5 to derive process profitability analysis under uncertainty, such as under the current material market trend, whether a recycler shall expand a pilot-scale production to a larger scale still keeping profitability from the material recovery operations; the chance to maintain the unit cost within a given range even the market prices fluctuating; and other what-if analyses for decision making.

Table 3. Simulation scenarios with deterministic input parameters

Process Parameter	Unit	Closed-Loop Process				Open-Loop Process
		Optimal Scenario	Baseline Scenario	Material-Efficient Scenario	Energy-Reduction Scenario	Open-Loop Scenario
Feedstock consumption	kg/kg	1.94	1.98	1.94	1.98	2.00
Acid consumption	kg/kg	1.19	1.62	1.19	1.62	8.16
Additive_1	kg/kg	0.26	0.27	0.26	0.27	0.27
Additive_2	kg/kg	0.26	0.27	0.26	0.27	0.27
Electricity	kwh/kg	17.47	21.84	21.84	17.47	21.84
Water consumption	liter/kg	3	30.6	3	30.6	49.12

Table 4. Scenario settings for *process profitability* simulation

Simulation Parameter/Variable		Scenario A	Scenario B	Scenario C
Key Parameters	Process Efficiency	96%	98%	95%
	In-Process Recycling Rate for Acid	80%	85%	0%
	In-Process Recycling Rate for Water	37%	90%	0%
Key Variables	Selling Price (probobilistic variable)	$14.50-39.50 / kg-material-recovered		
	Concentration (probobilistic variable)	10-55 wt.%		
	Production Volume	0-100 ton/year		

4.3. Agent System Design and Implementation

4.3.1. Multi-agent Environment for Process Sustainability Assessment

The design and implementation of an agent system is discussed in this section. Figure 5 shows a conceptual model to represent the agent in a multi-agent network for process sustainability assessment of waste-to-material recovery systems.

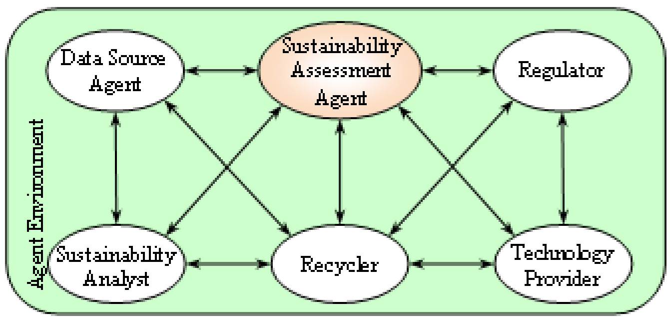

Figure 5. A sustainability assessment agent and its environment.

An overall workflow is designed to coordinate tasks of the agents in the multi-agent environment in Figure 5. Included in the workflow are the simulation procedures to analyze predefined system performance goals. Table 5 highlights such a simulation procedure for the Sustainability Assessment Agent to analyze the probabilistic *process profitability* performance.

As shown in Figure 5, the Sustainability Assessment Agent interacts with other five agents in the environment to fulfill performance goals simulation. Specifically for the *process profitability* analysis, the agent interacts with the Sustainability Analyst and Data Source Agent through the relationships defined between them (refer to Table 5), responses to sustainability assessment request from Sustainability Analyst, uses supporting data and methods from Data Source Agent, and creates assessments to response the needs of the agent network environment. The software development of the sustainability assessment agent is presented below.

4.3.2. Functional Structure of the Software Agent

The Sustainability Assessment Agent is designed to provide deterministic and probabilistic sustainability performance analyses in the multi-agent environment in Figure 5. Its overall software functional structure is depicted in Figure 6.

Table 5. A high-level simulation procedure for probabilistic *process profitability* analysis

Sequence	Action by Sustainability Assessment Agent
1	Perceive a request from Sustainability Analyst for *process profitability* analysis
2	Receive and save simulation inputs
3	Calculate a statistical sample for unit cost at a given production volume
a	Generate a random price sample using a real-market historical price distribution from Data Source Agent
b	Generate a random concentration sample using a triangular distribution from Data Source Agent
c	Compute a random unit cost by instantiating Eq. (21) with the random price and concentration samples generated
d	Simulate the random sampling and unit cost computation over 10,000 replications for a statistical sample of unit cost
4	Estimate a deterministic *process profitability* value from the statistical sample
a	Estimate a true value from the statistical sample of unit cost with a given confidence level
b	Compute a total cost according to Eq. (19)
c	Compute a deterministic process revenue according to Eq. (17)
d	Compute a value for *process profitability* according to Eq. (20)
5	Analyze the *process profitability* by repeating the steps above with different scenario settings (Table 4)

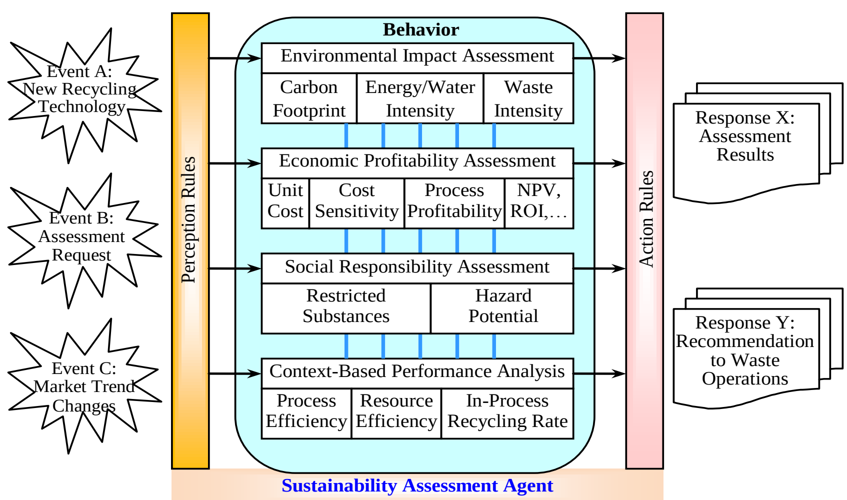

Figure 6. Software functional structure of the sustainability assessment agent.

The software agent is designed to provide four modules of analytical functions for environmental, economic, social and context-based performance assessment as shown in Figure 6. Among these functions, the analyses to carbon footprint, unit cost, cost sensitivity to price changes, and process profitability can be probabilistic or deterministic. All the other functions are deterministic only. For most of the deterministic analyses, the computable sustainability metrics developed in Section 2 are directly used as the simulation models. But for probabilistic analyses, simplified and re-formalized simulation models (details in Section 4.1) with random variables are implemented in the software agent. Currently, some of the analytical functions in Figure 6 are still under development.

Besides providing four functional modules with deterministic and probabilistic analytical capabilities above, the sustainability assessment agent also maintains a technology inventory. The inventory structures and manages the key process data of waste handling technologies and operations, simulation inputs and their restraints, and simulation procedures to support the inventory data needs from the four functional modules. The design of the Economic Profitability Assessment module is detailed in the next section.

4.3.3. Module Design

Take the Economic Profitability Assessment module in Figure 6 as an example. The module is designed to provide five basic computational functions for deterministic analysis:

- Input parameter manipulation: This function edits the input parameters and process scenario definitions in structured information sets and stores them in the technology inventory. Agent algorithms are implemented in this function to ensure the communication and interaction between this agent and other agents in Figure 5.
- Cost Breakdown Structure: The function implements the unit cost metric model in Eq. (8) and other metrics for individual cost elements, such as in Eqs. (9) and (12), in order to provide a cost breakdown structure for the given set of input parameters.
- Unit Cost vs. Production Volume: It analyzes the effect of production volume changes on unit cost, i.e. economies of scale.
- Unit Cost Analysis with Fixed Production Volume: This function draws a profile of cost elements at the user-specified production volume.

- Deterministic Economic Profitability Analysis: It is designed to provide a set of analysis methods for economic performances assessment, such as calculating process profitability, share of cost of materials, process revenue, total production cost, etc.

Figure 7 shows one of the UML use case analyses of this module. The use case diagram illustrates how the five functions above will be used in deterministic economic sustainability analysis.

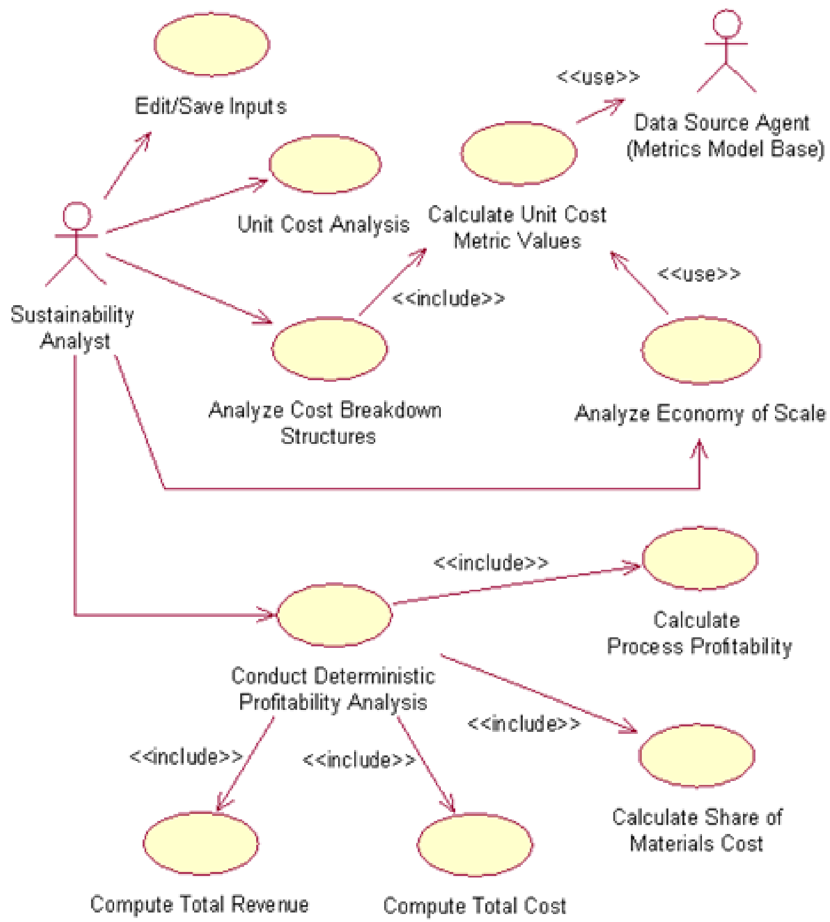

Figure 7. Use case for deterministic economic performance analysis.

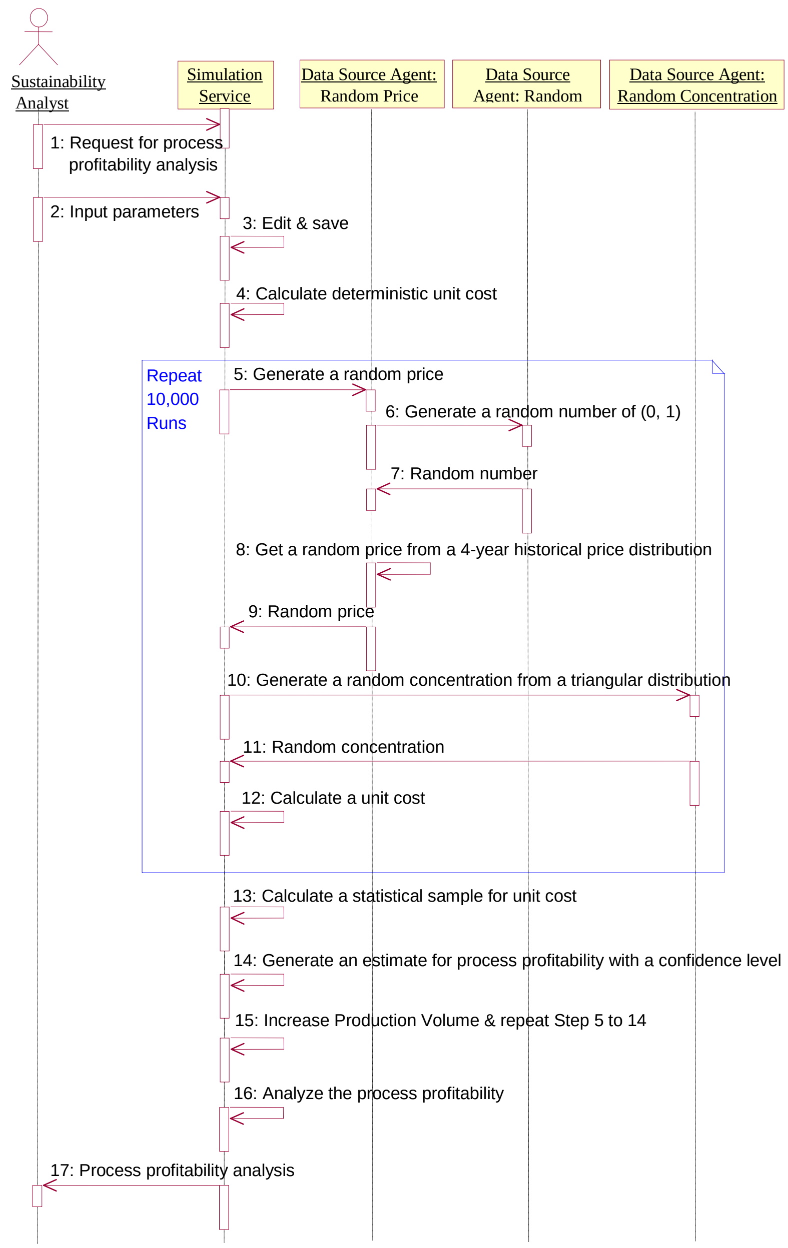

Figure 8. Sequence diagram for probabilistic analysis of *process profitability*.

Apart from the five basic functions above used for deterministic analysis, this module also provides three Monte Carlo simulation services for probabilistic analysis of unit cost, cost sensitivity to price changes, and process profitability. Figure 8 is a UML sequence diagram for design of the time-based execution of simulation procedures associated with the probabilistic analysis for *process profitability*. Basically the module algorithms are designed to follow the simulation procedures specified in Table 5.

4.3.4. Implementation of Agent-based Solutions

The software agent for sustainability assessment in Figure 5 is implemented in C# on the .NET platform. It invokes an external charting package for display of calculation results. MS Visual Studio was used as the integrated development environment for this agent.

Still take the Economic Profitability Assessment module in Figure 6 as an example. As mentioned in the Module Design section, this module provides five basic functions for deterministic analysis and three Monte Carlo simulation services for probabilistic analysis of economic profitability performances of waste management systems. The software implementation for one of the five functions, Deterministic Economic Analysis, is described below as the first example, followed by another implementation example for one of the probabilistic simulation services, Uncertain Unit Cost Analysis.

The Deterministic Economic Analysis function allows an object of Sustainability Analyst to select an economic analysis method built in the agent. For example, if a material cost breakdown analysis is selected for calculating the share of cost of materials (refer to Figure 7), the agent will first retrieve the stored input parameters for a given process scenario setting. It will then calculate the cost for each material type at each recycling process step based on the material cost metric C_M^U. Before being aggregated into the total material cost, the calculated cost for each type of material and for the given process scenario is stored in a 2-dimentional array of $M \times N$ doubles, where M is the maximum number of process scenarios and N the maximum number of material types. By performing the algorithm given in Figure 9, the agent displays a material cost breakdown for the given simulation scenario.

Alternatively, the agent can compare the material cost breakdown across different process scenarios. Figure 10 shows a screen capture for unit cost breakdown and material cost breakdown of five different process scenarios simulated.

```
Set M to be the maximum number of process scenarios simulated
Set N to be the maximum number of types of raw materials used
Create an array A [M, N] to store material cost breakdown computing results
for m=1 to M do
 for n=1 to N do
  Calculate A [m, n] according to the material cost metric C_M^U
 end for
end for
Draw charts for material cost breakdown in A [M, N]
```

Figure 9. An algorithm for material cost breakdown analysis.

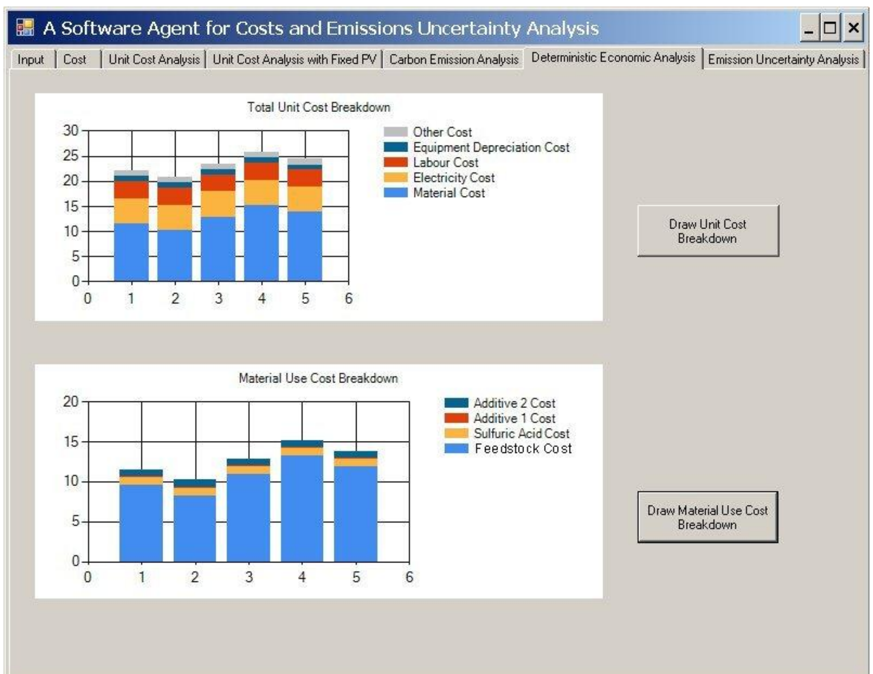

Figure 10. Implementation example for deterministic economic analysis.

Based on the unit cost breakdown in Figure 10, the share of material cost can be computed as a ratio of material cost and unit cost for a specified process scenario. In waste-based material recovery operations in Singapore, the share of material cost always takes the biggest proportion in the total unit cost. Hence the most effective measure to reduce the total unit cost is by improving the material cost, i.e., by improving the chemicals/water consumptions in the recovery processes. The metric for share of material cost would facilitate the material cost analysis towards total unit cost reduction.

The second example is about the implementation of a Monte Carlo simulation service for Uncertain Unit Cost Analysis in the Economic Profitability Assessment module in Figure 6. As indicated in Eq. (8), the material cost for feedstock is a function of the market value of a recovered material. When the selling price of the recovered material is higher, a recycler would expect high revenues from the waste-based material recovery operations, at the same time, higher unit costs due to higher feedstock values [42]. The material selling price is uncertain depending on its market value. We use the 4-year historical market data (2007-2011) retrieved from the London Metal Exchange (LME) as a reference price distribution. Besides this market data based price distribution, our Monte Carlo simulation service also provides a normal price distribution with the mean and standard deviation taken from the 4-year historical price histogram. Both price distributions have been implemented in the Economic Profitability Assessment module for Monte Carlo simulation of uncertain unit cost.

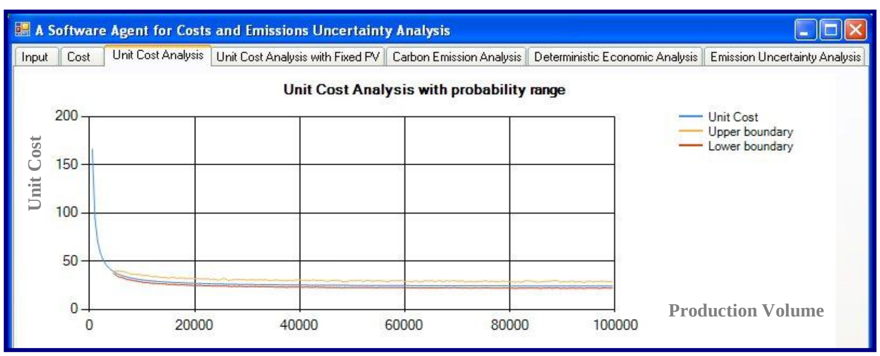

Figure 11. Implementation example for uncertain unit cost analysis.

Another random variable in the unit cost simulation model in Eq. (21) is the recoverables concentration in feedstock. This random variable is considered as a triangular distribution with the lower/upper bound and the most likely value from our concentration experiments. Figure 11 is a screen capture for unit cost changes vs. production volumes (*PV*) in the uncertain context. It is derived from the Monte Carlo simulation using the 4-year historical price histogram and the triangular distribution above as the random input distributions to calculate one unit cost sample for every *PV*. The unit cost sample with all possible values (10,000 replications) is then used to estimate a true value for unit cost with a probability range of ±20% for every *PV*. Changing *PV* over (0, 100000) kg/year, the agent will simulate and display the unit cost change trend with *PV*, as shown in Figure 11.

5. CASE STUDY: EVALUATING PROCESS SUSTAINABILITY OF WASTE-TO-MATERIAL RECOVERY OPTIONS

5.1. Overview of the Waste-to-material Recovery System Studied

Waste-to-material recovery can be any waste management operations that divert the recoverable from a waste stream and result in certain materials with potential economic, environmental, social or any other benefit. The assessed case in this section is a waste-to-metal recovery system. It is designed to reclaim metals from hazardous catalytic wastes. There are two metal reclamation process options available. They are based on the closed-loop and open-loop process concept respectively. Both processes use a common set of unit operations, but with unique process techniques, as summarized in Table 6.

Table 6. Common and unique techniques of the two waste-to-metal recovery processes

Technique		Description
Common	Two-staged acid leaching	Leach metal-containing feedstock with acid solutions in two stages.
	Metal enrichment	Enrich the metal concentration in working solutions.
	Electrowinning	Plate out pure metal from solutions.
Unique	Closed-loop process techniques	In-process recycling of the used acid, plating solutions and dilution waters; Acid separation from solutions by electrodialysis.
	Open-loop process techniques	No in-process recycling implemented and recyclables being disposed of; Replacing acid separation with chemical neutralization of acid.

The major difference between the two technologies lies in how the process recyclables are treated. In the closed-loop process, its unit operations are coupled with in-process recycling techniques, so that the used acid, spent plating solutions and dilution waters from the recovery operations can be recycled and reused within the process itself (Figure 12). The key technique to achieve in-process recycling is electrodialysis that separates the used acid from working solutions for recycling. On the contrary, the open-loop process does not implement these in-process recycling methods and the recyclables become part of a waste stream. Specifically for the used acid, instead of going through the electrodialysis processing, it is chemically neutralized before disposed of. This feature makes the open-loop process to have relatively low energy consumption, but very high chemicals use intensity and more hazardous chemicals usage to neutralize the used acid. The impacts of the process options on the sustainability performances of the studied recovery system are quantified and assessed in the next section. Figure 12 shows the characteristics of the closed-loop metal recovery process discussed above.

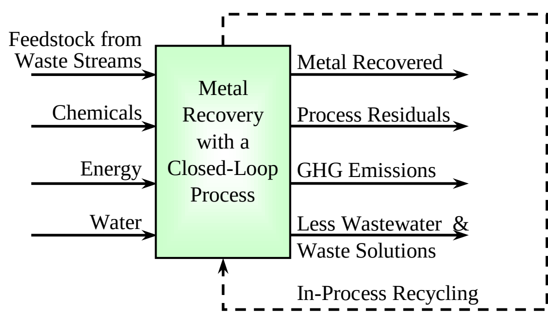

Figure 12. A closed-loop metal recovery process with in-process recycling.

The difference in the process concept (closed-loop or open-loop) and in their corresponding processing methods would determine their raw material consumptions, resource use efficiency, process efficiency, in-process recycling rate, carbon footprint, production cost, thus their process sustainability performances. The following two sections present case studies for deterministic and probabilistic sustainability evaluation of the two metal recovery process options by using the computable sustainability metrics, simulation models, and the software agent system developed in this research. The process scenarios and inventory data defined in Tables 3 and 4 are used in these case studies.

5.2. Deterministic Analysis of Process Sustainability Performances

The deterministic characteristics of process sustainability for the studied metal recovery system are evaluated in this section. These sustainability characteristics include: carbon footprint, unit cost, TCLP toxicity level, and resources use efficiency. A designed pilot-scale recovery system is used to provide technical parameters, activity data and other process-specific information. For deterministic analysis, the computable sustainability metrics developed in Section 3 are directly instantiated with these process data and generic inventory data. The agent system will then calculate process sustainability footprints and evaluate the effects of metal recovery process options and other influencing factors on the sustainability performances of the system assessed.

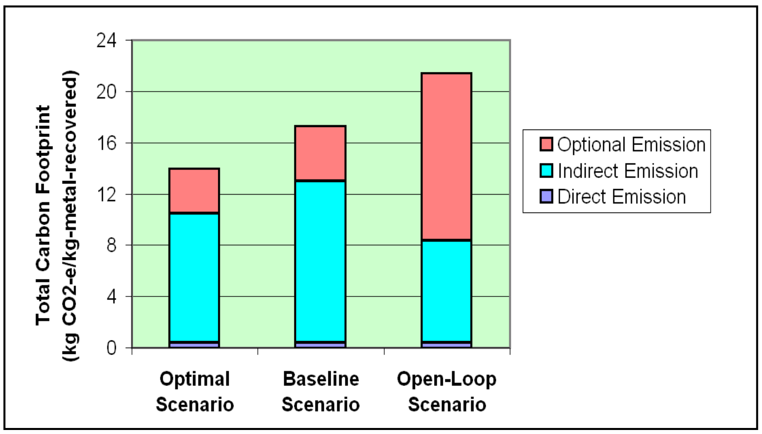

Figure 13. Comparison of carbon footprints of two recovery technologies for three scenarios.

5.2.1. Impact of Processing Technology Choice on Carbon Footprint and Unit Cost

As discussed in the last section, process concepts and their implementation techniques have significant impact on process sustainability. By instantiating the carbon footprint metric in Eq. (6) with the inventory data collected for the closed-loop and open-loop processes in Table 3, the carbon emissions of different metal recovery technologies can be quantified and compared. Figure 13 shows the calculation results of the carbon footprints for the two technologies under three process scenarios in Table 3: the baseline scenario and optimal scenario of the closed-loop process, and the open-loop scenario for the open-loop process.

The results in Figure 13 indicate that the closed-loop recovery technology can deliver lower carbon footprints compared to the impact from the open-loop technology. The total CO2e emissions from the optimal scenario and baseline scenario in the closed-loop process are reduced by 34.65% and 19.22% relative to that from the open-loop scenario. The biggest reduction is from the improved optional emissions (refer to Section 3.2.3 for its definition) as shown in Figure 13. This is mainly due to the effect of in-process recycling implemented in the closed-loop process. By closing the resource-use loop within the recovery process itself, the used dilution waters, chemicals and spent plating solutions are recycled and reused for metal reclamation operations. Therefore the closed-loop process consumes less quantity of virgin chemicals and fresh water, which improves the optional emissions induced from the use of materials. At the same time, in-process recycling also contributes to reservation of natural resources via reduced use of raw materials/chemicals and water.

The implementation of in-process recycling in closed-loop process can not only reduce the total carbon emissions, but also improve the process cost performance. This improvement is measured by the economic metrics developed in Section 3.3 for the unit cost, labor cost, material cost, and so on. To compute the cost metrics, process parameters are collected from the designed pilot-scale facility and from our metal recovery experiments. The market value from LME is used as a reference selling price to calculate the feedstock cost in this study. Table 7 shows the computed unit cost of the three process scenarios and their cost breakdown among the key cost elements (C_i^U and C_O^U) at a production volume of 60 ton/year and a reference selling price of \$20.15/kg (LME market value for the recovered metal on 20-Jan-2012). The currency unit in Table 7 is Singapore dollar, S\$, (US\$ 1 = ~S\$1.30). The three scenarios are the energy-reduction scenario and baseline scenario of the closed-loop process and the open-loop scenario from Table 3.

Unit cost reduction potentials for the energy-reduction and baseline scenarios can be calculated from the data in Table 7. They are measured at 31.31% and 28.10%, respectively, compared to the open-loop option. For the two scenarios of the closed-loop process, the cost reduction is mainly from material savings, due to their implementation of the closed-loop process concept and their use of electrodialysis to separate acid and make it reusable in leaching. In addition, the energy-reduction scenario also presents lower energy cost compared to the baseline scenario, achieved from its reduced electricity consumption. The open-loop scenario has the lowest energy cost in Table 7, because it does not use electrodialysis. Instead, chemical neutralization is used to process the used acid. Acid neutralization requires this process option to consume more chemicals, which offsets its cost savings from low energy consumption and increases its material cost greatly. The overall impact of the open-loop technology on the process economic viability is negative as it increases the total unit cost.

Table 7. Unit cost (S$/kg) and cost breakdown for three process scenarios

Cost Element	Energy-Reduction Scenario	Baseline Scenario	Open-Loop Scenario
Material Cost (C_M^U)	12.24	12.24	22.90
Energy Cost (C_E^U)	4.09	5.11	3.25
Labor Cost (C_L^U)	3.36	3.36	3.36
Equipment Cost (C_K^U)	1.00	1.00	1.00
Others Cost (C_O^U)	1.18	1.18	1.31
Total Unit Cost (C^U)	$21.86	$22.88	$31.83

Although both the unit cost and the breakdown percentage of contributing cost elements vary with the production volume (PV), the material cost always takes the biggest share within the total unit cost as shown in Table 7. For example at the PV of 60 ton/year, materials contribute 53.5% to the total unit cost in the baseline scenario in Table 7. Other dominant cost elements are energy cost (22.3%) and labor cost (14.7%). By examining the cost metric variables of these dominant cost elements, critical influencing factors to unit cost can then be identified. For example, by analyzing the material cost metric, the critical influencing factors have been identified as the materials and chemicals consumption, recoverables concentration in feedstock, feedstock purchase prices and market values of the recovered metal (as shown in Table 2). Effective management and control of these critical influencing factors would have significant impact on the material cost, therefore on the total unit cost of metal recovery processes.

5.2.2. Toxicity Management in the Closed-loop Metal Recovery Process

The feedstock used in this waste-to-metal recovery system is hazardous catalytic waste. The waste treatment in the two studied processes also involves the use of toxic chemicals. As such, toxicity management in these processes is of great and continuous concern of recyclers. In this study, the following measures are implemented with the closed-loop process for toxicity management:

- To avoid the use of toxic chemicals in process reactions as much as possible, such as by using electrodialysis for acid separation and diluent enrichment; and
- To make the recovery reactions as much complete as possible by implementing the multi-staged leaching and in-process recycling techniques.

The purpose is to manage and control the process residuals (solid wastes from metal recovery operations) to meet the local regulatory requirements [41] for safe handling and disposal of industrial wastes in landfills. Towards this end, the TCLP procedure was conducted to determine the leachability of the process residuals from the closed-loop cycles. The TCLP metric in Eq. (13) was then used to evaluate the measured TCLP value against the local standard of the TCLP limit that is set at 5 mg/liter [41] by the environmental regulation in Singapore. The results are plotted in Figure 14.

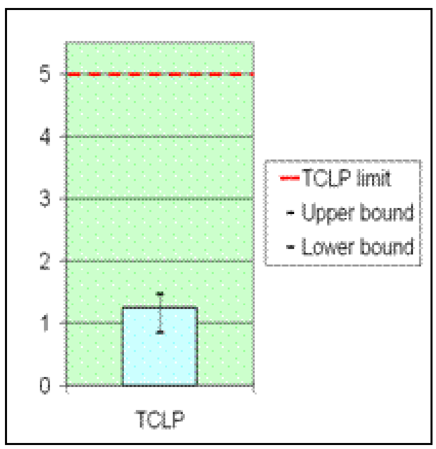

Figure 14. TCLP testing results.

The range of TCLP testing data in Figure 14 is 0.84-1.46 mg/liter for the residuals from the closed-loop metal recovery process. It is known from the test results that the TCLP leaching values of the metal from the process residuals fall well below the TCLP allowable level of 5 mg/liter, which indicates immobilization of the metal in the process residuals. Hence, the residuals from the closed-loop recovery process would not impose any hazardous risks to the environment and society. They are TCLP-compliant for safe and responsible disposal.

5.2.3. Evaluation and Comparison of Process Sustainability for Waste Minimization at Source

Waste minimization at source is one of the three key strategies to reduce the need for landfill in Singapore [1]. Two metrics have been developed to measure the sustainability performances of recycling and recovery processes in terms of their effect of waste minimization at source. They are the process efficiency metric and the resource use efficiency metric (refer to Table 1).

The resource use efficiency metric in Eq. (15) measures the composite efficiency level in the use of energy, raw materials/chemicals, and processing water for alternative metal recovery processes. The resource consumption data of materials, energy and water for the two metal recovery process options are collected and presented in Table 8. Three process scenarios are assessed in Table 8: the open-loop scenario of the open-loop process, the baseline and optimal scenarios of the closed-loop process. The table also specifies the weight factors for each resource type. The optimal scenario is used as the best achievable scenario under the pilot-scale settings of the waste-to-metal recovery system. The resource use efficiencies for these scenarios are calculated by Eq. (15). The results are also reported in Table 8.

Table 8. Process data to evaluate resource use efficiency of process scenarios

Resource Type (*i*)	**Resource (*j*)**	**Resource Consumption**			**Weight Factor (W_i)**	**Number of Resources (N_i)**
		Optimal Scenario (U_{ij})	**Baseline Scenario ($u_{ij}^{Baseline}$)**	**Open-loop Scenario ($u_{ij}^{Open\text{-}loop}$)**		
Material (kg/kg)	Feedstock	1.94	1.98	2.00	0.4	4
	Sulfuric acid	1.19	1.62	8.16		
	Additive_1	0.26	0.27	0.27		
	Additive_2	0.26	0.27	0.27		
Energy (kWh/kg)	Electricity	17.47	21.84	21.84	0.3	1
Water (liter/kg)	DI water	3	30.6	49.12	0.3	1
Resource Efficiency		1	0.633	0.562		

Compared to the open-loop scenario, the baseline scenario of the closed-loop process demonstrated higher resource use efficiency in Table 8. However, the scenario still has further improvement space compared to the material-efficient and energy-reduction scenarios of the closed-loop process. Table 9 compares all the five process scenarios defined in Table 3 for their waste minimization effect in terms of their metric characteristics for process efficiency and resource use efficiency.

Table 9. Comparison of waste minimization performance across process scenarios

Features for Waste Minimization at Sources	**Closed-Loop Process**				**Open-Loop Process**
	Optimal Scenario	**Baseline Scenario**	**Material-Efficient Scenario**	**Energy-Reduction Scenario**	**Open-Loop Scenario**
Process Efficiency Metrics Value (%)	98	96	98	96	95
Resource Use Efficiency Metrics Value	1	0.633	0.940	0.693	0.562

In summary, the above deterministic process sustainability assessments on carbon footprint, unit cost, TCLP toxicity, and waste minimization at source suggest that the closed-loop metal recovery process can deliver better sustainability performances over the open-loop process for the pilot-scale metal recovery system. The baseline scenario, defined according to the existing process settings of the pilot-scale system, can be further improved by implementing the processing techniques and operations revealed from the optimal, material-efficient, and energy-reduction scenarios in this research. The next section focuses on the probabilistic analysis of process economic profitability to reduce the implementation risks in adoption of sustainable waste management technologies and processes.

5.3. Monte Carlo Simulation for Process Profitability Analysis

The process profitability has been described as a ratio between the total process revenue and the total production cost in Section 4.1. Through analyzing unit cost behaviors, the following investigate process profitability of the two metal recovery process options.

In the unit cost simulation model in Eq. (21), there are two random variables: the recovered metal selling price and metal concentration in feedstock. We presume the metal selling prices can be sampled from a 4-year historical price distribution derived from the LME market pricing data, while the metal concentrations sampled from a triangular distribution derived from our feedstock characterization experiments. Using the software agent developed in Section 4 and the Monte Carlo sampling techniques, random values for metal price and concentration are generated from these prescribed distributions. Together with other deterministic parameters, these random values are used to instantiate the unit cost simulation model for one run. After multiple simulation runs, the obtained random outputs from Eq. (21) form a random sample of unit cost. The statistical characteristics of the unit cost sample, such as its mean and standard deviation are used as indicators for evaluating the economic cost performance of the studied metal recovery system.

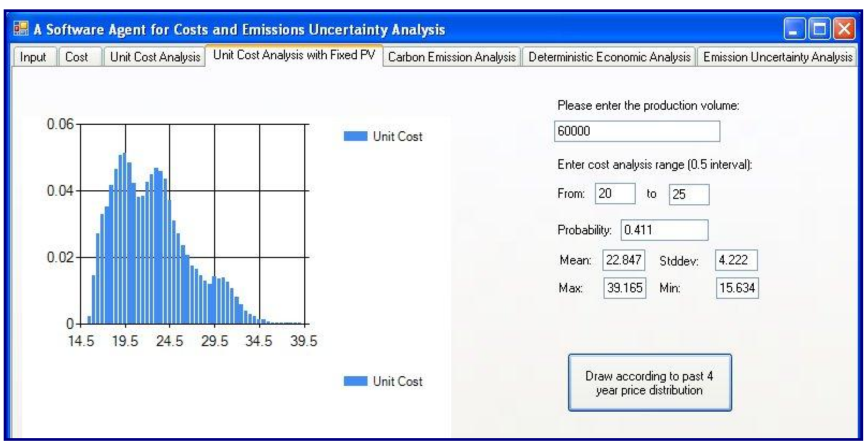

Figure 15. A unit cost sample for the pilot-scale system.

Using the scenario settings in Table 4, Monte Carlo simulations have been conducted for the defined Scenarios A to C in Table 4. Figure 15 shows an uncertain unit cost sample of Scenario A, which is derived from the Monte Carlo simulation using the 4-year historical price distribution and the triangular metal concentration distribution over 10,000 replications. The statistical analysis of the unit cost sample is also shown in the figure. With a given production volume of 60,000 kg/year for the pilot-scale recovery system, the chance to maintain the unit cost within a range of S$(20-25)/kg is 41.1%, no matter how the metal market is fluctuating, as long as it still follows the 4-year historical pricing trend. The mean unit cost and the standard deviation are S$22.85/kg and 4.22 respectively, as shown in Figure 15.

Assume the production scale is expanded from the pilot-scale of 60 ton/year to 100 ton/year. The unit cost is experimented with the Monte Carlo simulation again. Table 10 compares the statistical characteristics of the two unit cost samples of the pilot-scale system and the designed system with the enlarged metal recovery capacity.

Table 10. Comparison of statistical characteristics of two unit cost samples

Recovery System	Production Volume (ton/year)	Mean (S$/kg)	Standard Deviation	Unit Cost Range (Min, Max)
Pilot-Scale	60	22.85	4.22	(15.63, 39.17)
Expanded-Scale	100	22.37	4.21	(15.15, 39.36)

Using the mean in Table 10 as an estimate of the unit cost and the 4-year mean price at the LME [44] as the reference selling price, the process profitability of the two systems under study can then be calculated according to Eq. (20). Table 11 summarizes the calculation results for process profitability of the pilot-scale facility and the expanded-scale system. It is assumed that the sales quantity is equal to the production volume in order to simplify this calculation.

Table 11. Process profitability analysis

	Pilot-Scale	Expanded-Scale
Mean Price [44] (S$/kg)	30.77	30.77
Sales Quantity (ton/year)	60	100
Mean of Unit Cost (S$/kg)	22.85	22.37
Production Volume (ton/year)	60	100
Process Profitability	1.35	1.38

The results for process profitability analysis in Table 11 can be used to support the decision process: whether a recycler shall expand the pilot-scale production to a larger scale, under the given market pricing trend. If so, the recycler would have a probability of 39.7% to experience a unit cost in the range of S$(20-25)/kg and can expect to profit from the expanded metal recovery operations with a slightly higher process profitability level at 1.38 compared to his current pilot-scale operations with a process profitability of 1.35.

CONCLUSION

Two new techniques for metrics-driven sustainability modeling and agent-based sustainability simulation have been developed and used in process sustainability assessment of waste management systems in Singapore. The techniques allow an integration of: 1) science-based characterization of process sustainability in metrics models; 2) agent-based simulation to evaluate and explore sustainability behaviors of waste systems for technology/operation/market changes and what-if scenarios; and 3) technology inventory development to enable objective sustainability evaluation and simulation. This research also provides a practical and reliable software agent for the local waste industry to assess, compare and implement innovative waste-to-material recovery technologies to achieve sustainable waste management targets.

To make sustainability performances visible and improvements measurable, model-based sustainability metrics provide an effective and powerful means. Six categories of model-based, computable sustainability metrics have been presented in this chapter, with a focus on the local sustainable waste management objectives and the triple bottom line considerations. The metrics have been used in evaluating sustainability performances of two metal recovery processes. A number of process scenarios were analyzed and compared. The process change from one scenario to another involves changes in process parameters and other conditions, which can be captured by the data used in calculation of the sustainability metrics. As such, the model-based metrics can reveal which influencing factors are contributing most to which sustainability aspects.

The software agent is developed with a localized technology inventory to allow practical and context-based sustainability assessment using Monte Carlo simulation techniques. The agent simulates the interactions between the sustainability performances and their influencing factors according to the designed simulation scenarios. Both the deterministic and probabilistic simulation scenarios have been developed and used in evaluating process sustainability behaviors characterized by the sustainability metric models and simulation models. The agent system and its Monte Carlo simulation services have demonstrated to be practical and useful as a decision support tool in waste-to-material recovery applications.

A case study for metal recovery from industrial waste has practiced the two techniques for metrics-driven sustainability modeling and agent-based sustainability simulation. Two metal recovery process options are evaluated. The results suggested that the closed-loop process can deliver better sustainability performances than the open-loop process does. This is mainly because the closed-loop process can better use material, water and energy resources by implementing in-process recycling techniques. Compared to the open-loop scenario, the carbon footprint and unit cost with the baseline scenario of the closed-loop system are improved 19.2% and 28.1%, respectively. The closed-loop system also demonstrated the better performances in TCLP compliance and waste minimization at source. It can deliver a sound process profitability withstanding the metal market pricing fluctuations and feedstock quality variations. The case study results have provided the local recyclers with solid data and analyses to support their sustainability decisions and to facilitate them to identify and improve their process sustainability practices.

Future work for this research is identified to include the following:

- To enrich the content of the technology inventory;
- To improve the accuracy of the historical price histogram with full set of market pricing data from the LME and to update the price histogram with the latest available data;
- To further develop the software agent system and simulation models; and
- To promote the two techniques developed in this study to more applications in sustainable waste management in Singapore.

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