5-4-2019

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ScienceDirect

Procedia CIRP 80 (2019) 602–606

www.elsevier.com/locate/procedia

26th CIRP Life Cycle Engineering (LCE) Conference

Systems Analysis for PET and Olefin Polymers in a Circular Economy

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Abstract

Polyethylene terephthalate (PET #1) and polyolefin plastics such polyethylene (HDPE #2, LDPE #4) and polypropylene (PP #5) are major products from the chemical industry, and they comprise a significant fraction of municipal solid waste that ends up in landfills or as litter and marine debris. The reuse of these polymeric materials can be optimized through systems analysis with a view on materials flow analysis, techno-economics, environmental life cycle assessment, and consequential societal impacts. This contribution will present the overall research approach for this exploratory project within the DOE- and industry-funded REMADE Institute and end with a proposed systems analysis framework.

Keywords: systems analysis, plastics circular economy, sustainability

1. Introduction

Polymers are important materials with useful properties for many manufactured goods including vehicular components, food packaging and in medical applications. To illustrate the importance of these materials, approximately 4% of global petroleum production is incorporated into polymer materials and another 4% of petroleum is used to satisfy energy requirements in polymer processing, in addition to other materials such as natural gas and water [1]. Global production of polymers was 322 million metric tons in 2015 (steel was 1,623 million metric tons in 2015) with the largest producers from Asia, Europe, and the United States [2]. The vast majority of polymers are commodity thermoplastics (90%), which are made up of, polyethylene (both high and low density: HDPE and LDPE) (34.4%), polypropylene (PP) (24.2%), polyvinyl chloride (PVC) (16.5%), with smaller percentages from polystyrene (PS), polyethylene terephthalate (PET), engineered plastics, and high performance polymers. Depending on region around the globe, between 22 and 43% of polymers are landfilled [1], thus wasting a valuable resource, and a significant fraction is lost as litter and marine debris. Of the fraction not landfilled, on average the larger portion is incinerated for energy. However this can sometimes generate hazardous solid waste and mandates expensive air pollution controls to minimize adverse health impacts.

A material balance on plastic flows shows some overall global trends (see Fig. 1) [3]. For the material class of plastic packaging (36% of global plastics production), global discard is 77.5 million metric tons (Mn t), and of that amount 25 Mn t is leakage representing uncontrolled waste management, marine debris, and litter. Collected and managed plastic packaging amounts to 53 Mn t, from which 11 Mn t is recycled,

10.1016/j.procir.2019.01.072

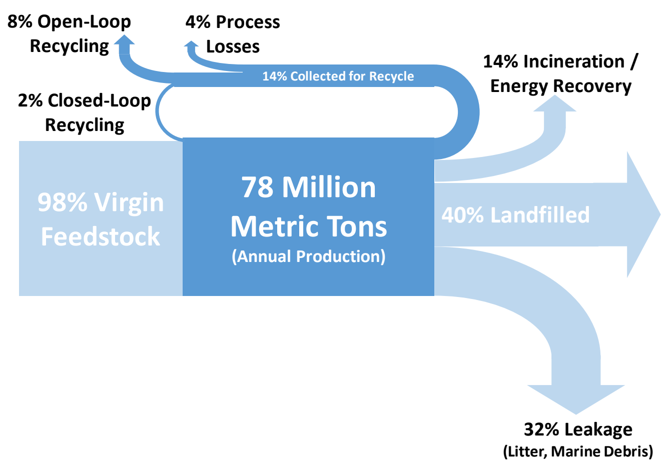

Fig. 1 Global plastics packaging material flows (2016). Adapted from [3]

11 Mn t is incinerated, and 31 Mn t is disposed in a sanitary landfill.

For other plastic material classes such as consumer and institutional products, textiles, electronics transportation, industrial machinery, and buildings, the rates of production and rates of waste generation are not equal because product lifetime distributions are much longer than for packaging [4]. It was estimated that if current production and waste management trends continue, it is estimated that 12,000 Mn t of plastic waste will be either in landfills or dispersed in the environment by 2050 [4].

As an alternative to landfilling, a system of remanufacturing of polymers using mechanical recycling employs a series of steps for waste plastic collection, washing, decontamination, and separation into common materials, plus various unit operations for reprocessing. For example, waste bottles made from polyethylene terephthalate (PET, PETE) can be thermally processed into polyester fibers for clothing or other uses, or can be processed into food-contact or non-food-contact packaging. Polyethylene (PE) is normally reprocessed into plastic lumber and other durable non-food-contact products. In addition, other useful products may be obtained from waste polymers. The American Chemistry Council estimates that as many as 600 plastics-to-oil (PTO) facilities could be established in the U.S. while generating $8.9 billion in annual economic output related to PTO facilities and supporting 39,000 jobs [5]. The oil produced can be substituted for diesel or other fossil fuels in various applications. A recent study demonstrated that alternative fuels produced from pyrolysis of polyolefin plastics in Mexico has the potential to replace 4% of that country's transportation fuel demand with lower greenhouse gas emissions than fossil fuels [6].

Additional research and development activities supporting polymer remanufacturing and chemical recycle are needed to improve economic, energy, and environmental efficiencies of these processes as well as to understand the sustainability implications at various scales, from the unit operation level, process level, facility level, and up to regional, national, and global.

1.1. Research Objectives

While a number of prior studies have addressed the economic risks to organizations that produce and use plastics [1] or have compared energy / environmental benefits of using plastic versus other materials (glass, aluminum, etc.) [7], no prior works have studied the entire plastics circular economy (CE) using sustainability metrics of material use efficiency, energy intensity, production costs for secondary feedstocks, broader impacts to the economy, and life cycle emissions. In this exploratory project we will address knowledge gaps as outlined above, refine the proposed robust systems analysis approach, and identify the data needs and gaps. Our research approach will encompass both U.S. and global perspectives.

2. Work Plan

Our work plan will include the following tasks; **Task 1**. Propose and refine a conceptual model of the evolving plastics circular economy system with U.S. and global perspectives, **Task 2**. Conduct a thorough literature review of the processes involved in the plastics circular economy system along with their economic and environmental metrics, and **Task 3**. Engage in networking and recruitment of industry partners and others to prepare for assessing the sustainability of the current and future plastics circular economy with a focus U.S. Department of Energy-funded Reducing EMbodied-Energy And Decreasing Emissions (REMADE) Institute technical performance metrics (TPMs).

2.1. Task 1: Conceptual Model Development

Although material flow diagrams for plastics have been developed in the past [8], none have been developed with sufficient detail to model all of the technical processes involved in a material's circular economy, or to model potential future processes. In addition, few have incorporated time dependent factors allowing for predictions of waste generation in the future from probability distributions of plastic materials lifetimes [4]. This task will engage in a thorough review of existing circular economy concepts and models in the literature for plastics (e.g. [9-11]), including those hybrid approaches combining material flow analysis (MFA) with life cycle assessment (LCA) [12] and with economic analysis [13]. We will then compile all useful modeling approaches (both U.S. and global perspectives), and develop a plastics circular economy conceptual model that will serve the needs of decision-makers in the present while also allowing for predictions of material flows and associated processes and their impacts in the future.

An important part of this task is defining what is within and what is outside the system boundary. Plastic waste begins when commercial (including construction & demolition waste and automobile waste) and residential end-users discard the material in either trash or recycling bins. Routes of plastic waste are highly dependent on location and can range from municipal trash pickup going straight to the land fill to segregated plastic waste that travels to dedicated separation facilities which separate plastics into #1 and #2 plastics and #3-

7 plastics (or even some separation of these). Most locations fall in between these extremes with single and dual recycling streams being the most common. These materials are sent to material recovery facilities (MRFs) that separate various plastics from paper, glass, and metals. This subtask will determine the most prevalent waste supply chain processes and improvements needed in the future.

There are a number of processing steps to consider in the model for material and energy recycling of waste plastics at the end of life stage. These include processes that fit into both closed-loop as well as open-loop recycling strategies. In both cases, mechanical and chemical recycling processes may be used. Incineration with energy recovery is another important process to include.

2.2. Task 2: Review and Assessment of Plastics Recycling Technologies

Materials recovery facilities (MRFs) receive either single (co-mingled containers and fiber) or dual recycling streams (separate containers and fiber). Many MRFs have an upfront manual sort to remove large items followed by screens to separate three dimensional containers from flat materials and also serves to remove heavy, wet materials. Glass may be removed after this step followed by magnetic and eddy current separation of metals. Air knives and air classifiers separate light materials from heavy. Finally, optical sorters are used to separate various types of plastics, paper grades and colored glass. A variation of this approach is to shred everything at the beginning and use the above methods to separate smaller sized materials. This task will examine the variety of MRF configurations available in the U.S. (and globally) and will be used to adapt INL's existing MRF process model to other common configurations.

In this review of plastics recycling process technologies, equal emphasis will be given to gaining access to commercial- or pilot-scale data as well as availability of process models that predict mass yields and energy consumption of next generation technologies. These data sets and process models are the foundation of a high quality systems analysis for assessing energy consumption, emissions, costs of secondary feedstocks, and even broader socioeconomic impacts at regional, national, or global scales. For example, this model-based approach has been used to assess sustainability of bio-jet fuel production in North Dakota [14].

This task will review the techno-economic analysis (TEA) and LCA literature on mechanical recycling of plastics with an emphasis on the high production volume polymers; PE, PP, and PET/PETE to identify opportunities to update old inventory datasets [15]. We will also investigate the future potential of distributed recycling of polymer feedstocks into 3D printing materials with recyclebots [16-17] and other innovative technologies.

Chemical recycle of waste plastics is important for conversion of difficult to mechanically recycle plastics into monomers, chemicals and fuels. Because there are so many different polymers with varying chemical properties, a large number of chemical recycling technologies have been investigated [18]. This project will review the numerous technologies for thermal, catalytic, and enzymatic conversion of waste polymers [19,20], including data to support TEA and LCA [6,21].

2.3. Task 3. Network of Plastics Circular Economy Experts

Our goal in this task is to establish and sustain an open and collaborative network of experts in the plastics circular economy sector. We seek experts from the global chemical and plastics industry, plastics converters and recycling industries, users of plastics – such as the automotive and consumer goods sectors, and the academic and government research communities. We will recruit these members from the project's network of professional contacts in the areas of LCA, TEA, materials flow analysis, plastics recycling, alternative energy pathways, and sustainability.

3. Preliminary Conceptual Model

This contribution concludes with a discussion of a preliminary conceptual model for the systems analysis of a future plastics CE. A number of prior works have dealt with fundamental questions of what are the features that distinguish a circular economy from a conventional linear economy based on "make, use, waste", including CE's roots and origins in the late 1980s, its definitions, principles, models, and implementation at the micro, meso, and macro scales [22-23]. Another study reviewed more practical issues of CE such as strategies applicable to different parts of the value chain and CE implementation case studies [9]. Others have looked at business models for firms to achieve resource efficiency through circular economy by product service systems (PSS) and concluded that a result-oriented model is most effective, but requires intentional design to reduce environmental impacts [24]. The issue of system boundary was addressed by Korhonen et al. [11] when assessing sustainability of CE projects concluding that they must be viewed as existing within the larger biosphere and extended product supply chains, and also factor in long-term effects to the environment from extending product life-times. In an attempt to address lack of guidance on CE principles, strategies, implementation, and monitoring, the British Standards Institute introduced a new standard "BS 8001:2017-Framework for Implementing the Principles of the Circular Economy in Organizations" [25]. Pauluik [26] reviewed the BS 8001 standards and proposed a more quantitative dashboard including indicators such as material circularity indicator, life cycle greenhouse gas emissions, cumulative energy demand, footprints for water, land, and recourse use, and social life cycle indicators.

Based on prior CE systematization efforts by Graedel et al (2011) [27], Pauluik [26] proposed a general system definition of processes and material flows associated with CE in a product life cycle. In this system definition, the CE processes, stocks, and flows are contained within the wider global socioecological system. The CE processes include the main production processes as well as those for recycling and disposal, but also the non-material parts of the economy, such as energy supply and service providers. This system definition also serves as the basis for material flow analysis, material flow cost analysis, environmental life cycle assessments, and social life cycle assessments.

Based on this prior work, we propose a conceptual model for systems analysis of a plastics CE that should include a number of features; **i.** it should link dynamic material flow analysis with predictions of economic, environmental, and societal impacts, **ii.** it should answer a number of research questions and policies regarding the current and possible future states of a global plastics circular economy, **iii.** it should be used to investigate possible complementarities between plastic mechanical and chemical recycling, and **iv.** the model should provide feedback on effects of uncertainty on predictions of system sustainability to aid in decision-making.

Of particular relevance to the global plastics CE, research questions are in integral feature of the systems analysis. Though preliminary, we pose the following research questions as a starter set for the project team and expert advisory board to propose, discuss, and vet.

- What effects would improvements in polymer recycling technologies have on system performance, and where are such improvements most needed?
- How would the prevalence of chemical versus mechanical recycling affect system performance?
- If renewable (i.e. plant-derived) feedstocks increase vs fossil, what affect would this have on system performance?
- Chemical recycling will create products that can be recycled to the plastics industry and also to other industries (chemicals and fuels). How can the SA model of the plastics CE capture these external costs and benefits?
- How important is population density in plastics CE system performance?

In addition to the research questions, another important feature is the method for obtaining inventory data for the various analyses and assessments. In order to overcome limitations in access to data, our approach will be a bottom-up model-based approach in which all unit operations of the various plastics production, waste sorting, pretreatment, and recycling processes will be modeled with process simulations within Aspen Plus or comparable software tools. To the utmost extent possible, we will validate these models using industry data to be representative of current commercial practices. For process technologies that have yet to be commercialized, of course the process models will be the only recourse for developing environmental inventories and economic analyses. An advantage in this approach is the capability to assemble any waste plastic supply chain that one can imagine and design, and do so without data limitation for systems analyses.

A preliminary conceptual model with the aforementioned features is shown in Fig. 2. A first step will be to establish the sustainability indicators of the current state of the plastics circular economy, comprised of all significant processes in the plastics supply chain involving virgin and recycled materials. Sustainability indicators will include process-level economics such as net present value, internal rate of return, minimum selling price for secondary materials, etc., as well as regional economic effects. Environmental impacts will also be assessed, such as greenhouse gas emissions, cumulative energy demand. Societal impacts will also be included using indicators such as direct jobs, toxic materials use, and occupational safety.

The systems analysis conceptual model can then be used to better understand the system response to changes in a number of state variables or external drivers; for example recycle rates, new policy interventions, technological breakthroughs in materials collection, sorting, or processing, etc. The model can also explore potential trade-offs among indicators of economic, environmental, and societal sustainability to better inform decision-makers.

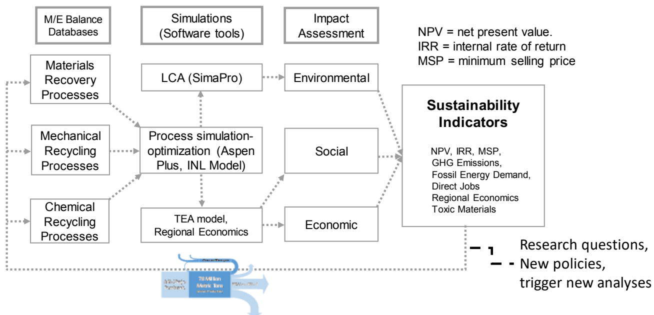

Fig. 2. Preliminary conceptual model for systems analysis of a plastics circular economy. The small blue icon at the bottom represents how future material flows will drive the process modeling and assessment functions.

Acknowledgements

We wish to thank the Richard and Bonnie Robbins Endowment at Michigan Tech.

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