Bridging the gap between LCA and PSE via a framework for multi-scale sustainable process design

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Recently, a significant amount of process systems engineering (PSE) research has focused on augmenting process design problems with life cycle assessment (LCA) in order to design for both economic and environmental criteria [1, 2]. Despite this widespread use of LCA in PSE research, a knowledge gap exists between the two fields. Advances have been made in both LCA and PSE methods that would prove beneficial when applied in the other field, but thus far the two fields have remained separate. For instance, when LCA is applied to process design problems, the standard inventory method is process analysis, in which the system boundary is drawn around the main process and upstream and downstream processes are added to the boundary until the inclusion of further processes has an insignificant effect on the total inventory [3]. Process analysis can significantly under-represent resource requirements and pollutant production, leading to potentially large errors compared to more comprehensive inventory techniques [4] and creating a risk that apparently optimal designs being in reality highly sub-optimal due to pollutant production and resource consumption that is not captured in the LCI [5, 6]. Hybrid LCA methods that address many of the issues with process analysis have been developed and are currently in use in the LCA community [7, 8, 9]. However, process analysis continues to be used exclusively in PSE applications [10]. In a similar vein, PSE research routinely applies non-linear or mixed-integer non-linear programming to model and design large-scale, complex process networks similar to a life cycle. The type of models used in this context are based on theoretical knowledge of the unit operations that comprise each process and are dependent on thousands or hundreds of thousands of variables [11]. In contrast, the process models used in LCA are fixed vectors of process inputs and outputs that are scaled by the amount of output required [12]. This is due to the inventory calculation methods currently applied in LCA, which are linear algebra and linear programming; both methods require a linear model [13].

We propose closing the knowledge gap between PSE and LCA research with a process design framework that utilizes advances in both fields. The integrated hybrid life cycle inventory (IHLCI) forms the basis for the framework [14]. The IHLCI combines detailed models for the process(es) being designed and key processes in the life cycle with an economic input-output (EIO) model that captures the macro-economic system within which the processes operate. We replace the standard linear process models in the inventory with the more detailed technological models commonly used in PSE design applications, representing life cycle processes as vector functions rather than vectors of fixed inputs and outputs. The vector functions are derived from knowledge of the unit operations within each process and involve design variables at the unit operation and process levels. The IHLCI, unlike other hybrid methods, disaggregates the EIO model into the processes modeled in detail and the rest of the economy; this causes the design variables at the unit operation and process levels to be propagated throughout the inventory such that the life cycle inventory is dependent on decisions made within the process being designed. The inventory calculation and the process design steps are accomplished using the same framework, as the total inventory is determined by the process design. Because the inclusion of design variables leads to the inventory being in general

a non-linear model, non-linear programming instead of linear algebra and linear programming must be used for both the inventory calculation and process design.

Advantages of the proposed framework as well as insight gained from applying the framework will be demonstrated using a case study of a bioethanol production system. The design objectives for the system are production cost, production system emissions and life cycle (production system plus economy) emissions. In order to compare results from the conventional and the proposed approaches, a linear process analysis inventory, linear hybrid inventory and non-linear hybrid inventory are used separately to optimize the system. The proposed design framework captures a significant percentage of life cycle impacts that are not captured by linear process analysis, and finds a better better environmental optima than either of the linear inventory methods. Potential applications and extensions of the proposed framework are discussed.

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