525e Enhancing Life Cycle Inventories Via Reconciliation with the Laws of Thermodynamics

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Many efforts have focused on developing life cycle inventory (LCI) databases of various industrial processes. Nevertheless, collected data are reported in disparate units and obtained from different sources that may be outdated, unreliable, incomplete and/or unverifiable (Ayres, 1995). As a result, such inventories tend to be inconsistent, unrealistic and even physically impossible, i.e. they may violate the laws of conservation of energy and mass as well as the second law of thermodynamics.

Techniques for data reconciliation have been used in Process Systems Engineering for more than two decades. Such techniques have been successful in improving the quality of inconsistent data by enforcing fundamental models and other process information. Using these techniques for reconciling LCI data is non-trivial because unlike chemical process data, LCI data generally show little redundancy and lack multiple measurements for each variable. Additionally, these inventories typically present industrial processes as black boxes, and do not provide information about the composition of resources and relevant reactions. In this paper we will show that despite these limitations, careful use of data reconciliation techniques combined with engineering knowledge about the industrial processes can enhance life cycle inventories by rigorously completing, validating and reconciling existing databases. More importantly, they can enforce the satisfaction of the laws of thermodynamics ensuring that the inventory is physically feasible.

As opposed to the first law of thermodynamics, using the second law for reconciling LCI databases is a more complicated task because this law does not provide an equality constraint. The second law of thermodynamics establishes that the quality of energy inexorably decreases in all real processes, which is quantified as an overall increase of entropy in the universe or more conveniently or as a loss of exergy (Szargut et al., 1988). Exergy losses are caused by driving forces such as temperature differences, chemical reactions and concentration gradients. These losses are necessary for any process to function. Nevertheless, exergy losses also occur due to imperfections and inefficiencies in the process derived from bad design, indiscriminate use of resources, leaks and emissions, etc. Consequently, the degree of exergy losses is a useful indicator of its performance. Because the performance of a process can vary widely from plant to plant, there is not a clean way to use the second law for reconciling LCI databases. However, because there is a minimum loss of exergy that is inevitable, it is possible to ensure satisfaction of the second law in LCI by exceeding this lower limit.

This paper presents an approach for data reconciliation of process inventories to satisfy material balance and the laws of thermodynamics, thus enhancing the quality of LCI databases. This approach adopts the techniques of data reconciliation and exergy analysis to be used in inconsistent process inventories. The proposed approach is applied to the production process of caustic soda based on the LCI data being compiled by the National Renewable Energy Laboratory (www.nrel.gov/lci). Because of the lack of the detailed information about the caustic soda process, four alternatives of the available specific information are suggested via engineering knowledge. These alternatives gradually increase domain specific knowledge and illustrate the strength and challenges of implementing data reconciliation of LCI. Statistical tests for detecting gross errors quantify the quality of the reconciled data. The results show that test statistics for gross error identification and the number of gross error identified become smaller as the number of specific information increases, which means that database for LCI must be validated using the conservative equations.

This presentation will also demonstrate the utility of the second law of thermodynamics validation of the LCI database. Exergy losses for each alternative are calculated and compared with the standard exergy losses that are publicly accessible. The results show that the discrepancies between the exergy losses by the reconciled LCI database and the standard exergy losses becomes smaller as the number of available specific information increases. Such an approach could benefit if companies report values of their process exergy losses and exergetic efficiencies. In the meantime exergy data for industrial processes is used from literature sources such as Szargut et al. (1988).

References

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