

FIPSE-6 Short Presentation 1c

Integration of Sustainability Analysis in Multiple Levels of Chemical Manufacturing

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ABSTRACT

Performing sustainability analysis considering multiple levels of chemical manufacturing is crucial for the future of digital sustainability in process systems engineering (PSE). In such analysis, key performance indicators considering factors other than economics must be quantified so that sustainable decision-making can be pursued. In that context, the GREENSCOPE (Gauging Reaction Effectiveness for the ENvironmental Sustainability of Chemistries with a multi-Objective Process Evaluator) tool was originally developed by the US EPA for sustainability analysis of process designs. This tool has 139 indicators that characterize process efficiency (26), energy (14), economic (33), and environmental (66) aspects. In addition to the extensive library of indicators, GREENSCOPE includes an interface for their visualization using radar plots. This tool can be used during the design phase or during operations for evaluation of stand-alone equipment or process flowsheets. This software tool was also further developed and deployed at West Virginia University (WVU) in collaboration with US EPA to perform design and control for sustainability as well as life cycle inventory estimation of chemicals.

This presentation will address the open problem of integrating sustainability analysis in multiple levels of chemical process manufacturing, focusing on chemical reaction network and process design levels. This problem is challenging as it includes: (i) reaction network mechanism generation considering sustainability and green chemistry principles; and (ii) process design for sustainability with the use of multi-objective optimization methods with several objective functions described by GREENSCOPE indicators. The problem formulation and potential approaches for its solution will be discussed, such as the employment of computational geometry, graph theory and machine learning tools to enable computational tractability of the posed problems for improving PSE for sustainability.

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