

## Efficient Information and Data Management in Synthesis and Design of Processing Networks - DTU Orbit (09/11/2017)

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Recent developments of Process Systems Engineering (PSE) have focused on different classes of industry-relevant decision-making problems (e.g. planning, scheduling, synthesis and design), under the general framework of Enterprise-Wide Optimization (EWO) (Grossmann, 2005). In EWO, decision-making problems are formulated as superstructure optimization problems, which are solved to identify the optimal decision. In order to formulate large-scale network synthesis problems, large amounts of data are needed to describe i) the superstructure (in terms of list of alternatives and connections between them), ii) each of the process alternatives (in terms of mass balance, waste emissions, operational and capital cost), iii) the optimality criterion (in terms of objective function coefficients such as prices), as well as iv) engineering, commercial and regulatory insights and context related information (such as regulatory limits, and product specs, etc.) (Quaglia et al., 2012). Being those data multisource and multidisciplinary, a consolidation step is required to ensure coherence in problem formulation. The formulation of EWO problems, therefore, requires collecting, consolidating and specifying a large number (typically 1000-100,000) of data (Quaglia et al., submitted). As a result, EWO problem formulation is a time and resource intensive task. Moreover, compilation errors result in faulty problem specifications, and may compromise the quality of the obtained solution. In order to enable industrial use of EWO, therefore, methods and tools for efficient information and data management need to be developed. In this contribution, we present a systematic data architecture, which is integrated in our framework for synthesis and design of processing networks (Quaglia et al., submitted). The data structure is designed to enable automation, systematization and consolidation of the data needed for problem formulation. Those features have been implemented in a software tool for formulation of processing network synthesis and design problems, which guides the user through the steps of problem formulation, integrating automatic data consistency checks and connection to databases of physical properties and process data. Once all data have been specified, the problem is automatically converted into a GAMS readable program, which is executed to solve the optimization problem and identify the optimal processing network, without requiring any further editing from the user. Through the data structure and the formulation software, the workflow for problem formulation is optimized, and time and resources needed to formulate large problems are reduced, while at the same time ensuring internal consistency of the specified data. In this contribution, the framework for synthesis and design of processing network and the data structure are described. The generic and flexible nature of the framework (and of the associated data structure) is demonstrated through the formulation and solution of large scale industrial case studies. The case studies are selected from different industrial segments, such as food processing (soybean processing network), water and wastewater management (refinery wastewater treatment and reuse; municipal water treatment) and biorefinery.

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