



# A systematic framework for enterprise-wide optimization: Synthesis and design of processing networks under uncertainty

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## ABSTRACT

In this paper, a systematic framework for synthesis and design of processing networks under uncertainty is presented. Through the framework, an enterprise-wide optimization problem is formulated and solved under uncertain conditions, to identify the network (composed of raw materials, process technologies and product portfolio) which is feasible and have optimal performances over the entire uncertainty domain. Through the integration of different methods, tools, algorithms and databases, the framework guides the user in dealing with the mathematical complexity of the problems, allowing efficient formulation and solution of large and complex enterprise-wide optimization problem. Tools for the analysis of the uncertainty, of its consequences on the decision-making process and for the identification of strategies to mitigate its impact on network performances are integrated in the framework. A decomposition-based approach is employed to deal with the added complexity of the optimization under uncertainty. A network benchmarking problem is proposed as a benchmark for further development of methods, tools and solution approaches. To highlight the features of the framework, a large industrial case study dealing with soybean processing is formulated and solved.

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## 1. Introduction

The process industry sector is characterized by large capital investments, which are necessary for construction of production sites and facilities. The erection and commissioning of large production sites implies the use of massive amounts of economical, environmental and societal resources. The accuracy of the decision-making and of the design process is therefore of crucial importance, both for the enterprise which is committed to the investment, and for the human society in which the enterprise operates. Several tools have been developed and adopted in order to guide, support and facilitate the decision making process in capital investment projects, such as process management and project portfolio management (Project Management Institute, 2008).

Recent developments in Process Systems Engineering (PSE) have been focusing on formulating and solving processing network problems under the framework of enterprise-wide optimization (Grossmann, 2005). In this approach, the decision-making problem is cast in the form of superstructure optimization, which is formulated and solved as a Mixed Integer Linear or Mixed Integer Non Linear Programming (MIP or MINLP), making use of the integer and binary variables to represent discrete and binary choices.

The main strength of the enterprise-wide optimization approach is in its ability to provide comprehensive and transparent inputs to the decision makers, through a systematic and quantitative analysis. On the other hand, it poses several challenges, due to the size and complexity of the mathematical problem to formulate and solve, as well as to the amount of data which are required (Varma, Reklaitis, Blau, & Pekny, 2007). Often, the nature of the problem requires the formulation of large scale non-linear and non-convex problems (Karuppiyah & Grossmann, 2006) whose solution to global optimality is still an open problem. Finally, the inclusion of data uncertainty in the decision-making problem causes a significant increase in problem size and complexity (Dua & Pistikopoulos, 1998; Karuppiyah & Grossmann, 2008; Paules IV & Floudas, 1992; Sahinidis, 2004). Because of this complexity, formulation and solution of real industrial problems require considerable time and resources investment, as well as deep knowledge of optimization theory and algorithms.

For these reasons, we believe in the importance of developing of a systematic framework for enterprise-wide optimization particularly to motivate and facilitate its use in practice. The integration of state-of-art methods, tools and solution strategies, in a framework for enterprise-wide optimization has in fact the potential of increasing the productivity of the workflow needed to formulate and solve this class of problems; and thereby to enable the use of this powerful tool in industry and public sector, supporting transparent and efficient decision-making process.

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## Nomenclature

### Indexes

$i$	component
$k$	process interval (origin)
$kk$	process interval (destination)
$react$	key reactant
$rr$	reaction
$t$	time (years)
$s$	Monte Carlo sample
$f$	first stage variable
$s$	second stage variable
$det$	solution of the deterministic problem

### Parameters

$MW_i$	molecular weight
$P1_{i,kk}$	raw materials prices
$P2_{i,kk}$	utilities prices
$P3_{i,kk}$	products prices
$P4_i$	wastes disposal price
$SW_{i,kk}$	wastes fraction
$S_{k,kk}$	superstructure (binary)
$SP_{k,kk}$	superstructure of primary outlet (binary)
$\alpha_{j,kk}^L$	coefficient for capital cost estimation
$\beta_{j,kk}^L$	coefficient for capital cost estimation
$dist_{k,kk}$	transportation distance
$\alpha_{i,kk}$	fraction of utility mixed with process stream
$\gamma_{i,kk,rr}$	reaction stoichiometry
$SF_{i,kk}$	split factors
$\theta_{react,kk,rr}$	conversion of key reactant
$\mu_{i,kk}$	specific utility consumption
$dr$	discount rate
$F_{i,kk}^{Max}$	maximum throughput for interval $kk$
$Q_{j,kk}^o$	grid for piecewise linearization of throughput

### Variables

$F_{i,k,kk}$	component $i$ flow from process intervals $k$ to process intervals $kk$
$ff_{i,kk}$	component flow after mixing
$R_{i,kk}$	utility flow
$F_{i,kk}^M$	component flow after mixing
$F_{kk}^{thr}$	throughput in interval $kk$
$F_{i,kk}^{out1}$	component flow leaving process intervals $kk$ through primary outlet
$F_{i,kk}^{out2}$	component flow leaving process intervals $kk$ through secondary outlet
$F_{i,kk}^R$	component flow after reaction
$Ctr_{k,kk}$	component flow after reaction
$y_{kk}$	selection of process intervals (binary)
$w_{j,kk}$	selection of an interval of the piecewise linearization (binary)
$Q_{j,kk}$	disaggregation variable for piecewise linearization of throughput

### Operators

$E_{\theta}(f)$	expected value of function $f$ over the domain of $\theta$
$P_s$	probability of realization of event $s$

### Abbreviations

CAPEX	capital investment
EBIT	earnings before interest and taxes
VSS	value of stochastic solution
UP	uncertainty price

EVPI	expected value of perfect information
UB	upper bound of the objective function
LB	lower bound of the objective function

In line with these considerations, in this manuscript we propose a systematic framework for synthesis and design of processing networks under uncertainty. The framework is based on the integrated business and engineering framework developed earlier (Quaglia, Sarup, Sin, & Gani, 2012a), which is extended to include decision-making under uncertainty.

The structure of the manuscript is as follows. In Section 1 the framework is described, by highlighting the mathematical formulation of the problem and the integration among the different methods and tools. In the Section 2 a Benchmark Network Problem (BNP) is proposed, and its formulation and solution according to the proposed framework is discussed. In the Section 3, the capability of the framework to deal with the size and complexity of an industrial problem is demonstrated, by formulating and solving a large scale case-study which is about synthesis of soybean processing network under uncertainty. Finally, conclusions and future works are presented in the last section.

## 2. The framework

In this section, the framework is presented in terms of its main components. A schematic representation of the framework is given in Fig. 1, where the integration of workflow, dataflow, solution methods and software tools are highlighted.

Step 1 (problem formulation) and 3 (deterministic problem) of the workflow correspond to our framework for synthesis and design of enterprise-wide processing network. A more extensive description of these steps can be found in (Quaglia et al., 2012a).

In the following section, each of the steps is described.

### Step 1. Problem formulation

#### Problem definition

In this step the goal of the analysis is defined by stating the engineering, commercial and financial objectives of the project. On this basis, the objective function is selected and commercial and financial constraints such as maximum capital investment, success criteria among others are collected and systematized in terms of variable bounds.

#### Superstructure definition and data collection

All processing network alternatives including all possible raw materials, products and process technologies are generated and organized in a superstructure, constituted by a network of process intervals. A process interval is defined as a process section, which is able to perform a certain processing task. Commercial and engineering insights, as well as regulations are translated into logical constraints and variable bounds, to exclude infeasible networks from the search space. Relevant data for each of the process intervals are collected and organized in a predefined knowledge structure.

#### Model selection, development and validation

Models for each process interval contained in the superstructure are collected, or generated and validated if not available. Generic process interval models as described in earlier works (Quaglia et al., 2012a; Quaglia, Sarup, Sin, & Gani, 2012b) can be used here. An example of development of generic process interval model is reported in Appendix B. The superstructure, the interval

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