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An integrated knowledge-based framework for synthesis and design of enterprise-wide processing networks

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Abstract

Today chemical processing industries manufacture a wide range of products and provide services that touch billions of people's lives across the globe in many different ways. Making this requires an effective management of innovation in product and process development. On the other hand, the synthesis and design of processing networks is a complex and multidisciplinary problem, which involves many strategic and tactical decisions at business (considering financial criteria, market competition, supply chain network, etc) and engineering levels (considering synthesis, design and optimization of production technology, its feasibility, sustainability, R&D needs, etc), all of which have a deep impact on the profitability of knowledge based industries. In this talk, an integrated business and engineering framework for synthesis and design of processing network within enterprise wide context is presented. A systematic approach is used to manage the complexity and solving simultaneously both the business and the engineering dimension of the problem. This allows generation and comparison of a large number of alternatives at their optimal point. The result is the identification of the optimal raw material, product portfolio and process technology selection for a given market scenario, their sustainability metrics and risk of investment under market uncertainties enabling risk-aware decision making. The framework is highlighted with successful applications for soybean oil processing (food technology), biorefinery network (renewable chemicals) and wastewater treatment network (petrochemical industry).

Scope and objective

Today chemical processing industries manufacture a wide range of products and provide services that are essential for maintaining wellbeing and sustaining modern lifestyle of mankind.

These products and services touch billions of people living across the globe in many different ways: from products used in home care, personal care, to products that provides energy essential for transportation to fertilizers, herbicide for agriculture to textile for fashion and much more. A conservative estimate put the number of products that processing industries are manufacturing ca 30,000 and increasing (Conte & Gani, 2010). These trends is set to continue in future where we are likely to see more and more diversity and functionality of products and services.

Clearly the chemical processing industries has been tremendously successful and innovative in the past. Equally important for processing industries, is the development of process technologies required to manufacture the products starting from raw materials and other resources such as utilities. Hence the challenge is not only identifying the needs for products but also developing appropriate and cost-effective processing technologies. The current paradigm for product and process development in fact involves a number of steps which are outlined in Table 1. Briefly these steps can also be summarized as follows: (i) customer needs, (ii) Idea generation, (iii) process selection, (iv) manufacturing. Bottom line of process and product development efforts is that it is resource-intensive enterprise, which needs to be managed optimally.

Table 1. Product and process development paradigm in processing industries

• Need Identification • Product Design and Selection • Conceptual Process Synthesis and Design • Raw Materials Selection • Supply Chain Definition	Piloting Detailed Engineering Engineering, Procurement & Construction Production Plan & Schedule Operations, Marketing, sales & distribution

Implementation of product and process development paradigm in processing industries is in general organized in a functional structure, with separate departments working in a coordinated and integrated manner on enterprise-wide projects. The harmonic synchronization and integration between different functions is for large companies a necessary condition for obtaining the complete business potential of its activity (Williams and Samset, 2010).

An important example of enterprise-wide problems is the synthesis and design of processing networks. This involves a combination of strategic decisions (such as the selection of the product portfolio, of the raw materials and of the process technology) and of tactical decisions (the determination of the optimal processing conditions, of the optimal material flow through the processing network etc).

In industrial practice, this problem is often described as “do the right project, do the project right” and is tackled by the coordinated work of business and process engineering departments. Business department deals with the layer of strategic decisions and screening of alternatives to select the right project to execute on the basis of strategic considerations, employing financial and economical tools or indicators such as Balanced Scorecard and project NPV. On the other hand, process engineering deals with the layer of tactical decisions, related to design and optimization of the selected alternative with the help of tools such as process simulators.

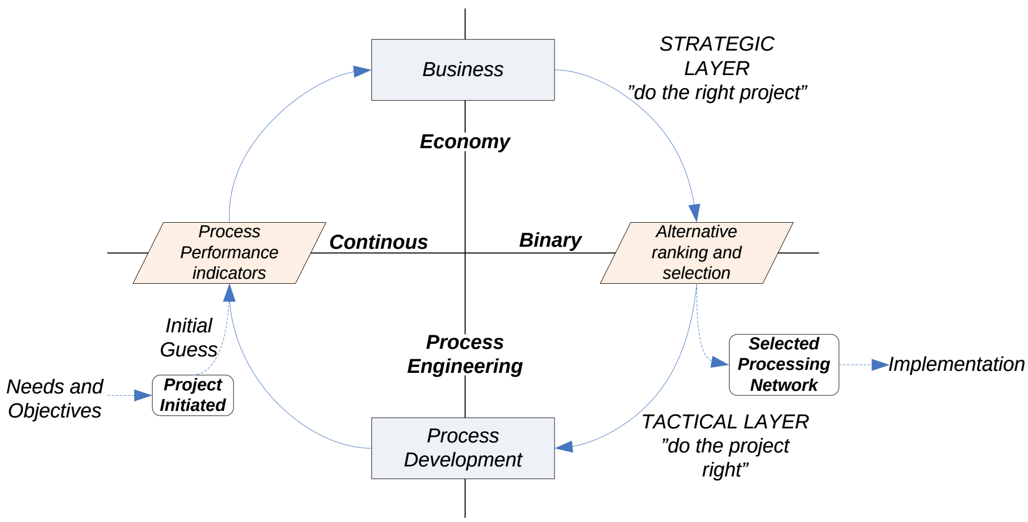

Figure 1: Recursive workflow for business and engineering decisions - "do the right project, do the project right" decomposition (Quaglia et al., 2011)

The decomposition of the problem into two layers (strategic and tactical) and solving them separately one at a time has some drawbacks. First of all, two layers of decomposition are not independent but interdependent, since the calculation of the economical indicator for the strategic decisions at business level requires the knowledge of the performance indicator for a given process, which are the end results of the design and optimization at engineering level. As a consequence the two layers need to be solved iteratively.

Moreover, this procedure outlined in Figure 1, is arguably not optimal for applications which require several successive solutions of the problem over the project lifetime, for example because of variation of parameters value (i.e. prices in volatile markets) or of process knowledge and modeling (i.e. new technology). For the same reason, the number of alternatives which can be evaluated is also limited, since otherwise it is time and resource intensive. Finally, analysis techniques such as sensitivity analysis and scenario planning are in general applied to each of the layers separately, and therefore cannot capture the interdependencies between them.

The scope and objective of this talk is precisely to overcome the above mentioned challenges. This is to be achieved by the development of systematic methods and computer aided tools designed to manage the complexity of the problem supporting the simultaneous integrated solution of both problem layers. Such a computer-aided framework promises to benefit the industry by making extensive, transparent and updated information available to the decision makers at cost effective manner meaning less time and resources would be used to generate many alternatives and solutions relative to traditional sequential approach.

Hence in this talk, a framework for enterprise-wide synthesis and design of processing network, integrating business and engineering dimensions is presented. The increased complexity of the problem resulted from considering the synthesis and design of processing networks as open problems is represented using a novel approach, which is based on a modified formulation of the transhipment problem integrated with a superstructure to consider non fixed topologies. The optimisation problem is cast as a Mixed Integer Non Linear Program (MINLP), and solved to determine simultaneously the optimal value of both the strategic decisions (represented by binary variables) and of the tactical decisions (continuous variables). Excel is used for compiling the necessary input data for the solution of MINLP problem, while GAMS is used for implementing and solving the problem.

Discussion

Integrated business and engineering framework

The framework employs simulation based engineering as enabling technology to generate many ideas, rapidly screen, evaluate and select for their feasibility and other assessment metrics set by business departments for final decision making.

The integrated business and engineering framework for synthesis and design of processing networks is composed of 5 steps including data collection, model development and solution and result analysis. A schematic representation of the workflow and different interactions between engineering and business decisions are given in Figure 2 (Quaglia et al., 2011).

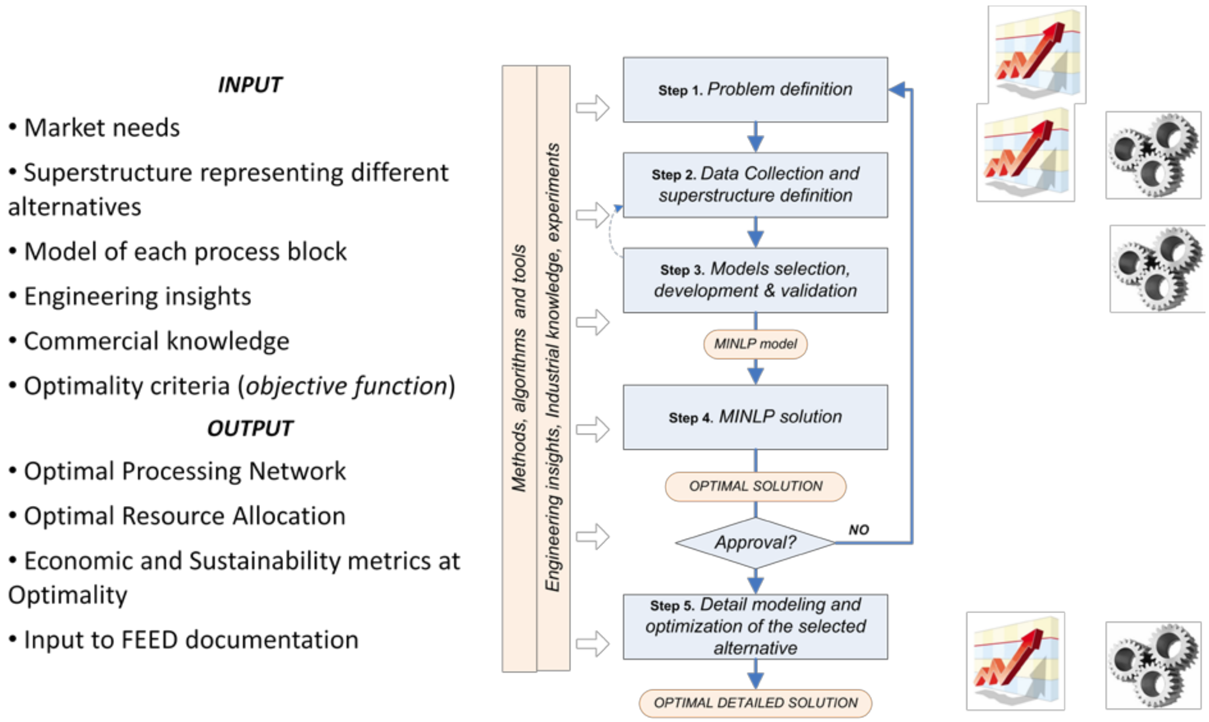

Figure 2. Computer-aided framework for integrated business and engineering dimensions for design of enterprise wide-processing networks (Quaglia et al., 2011)

In step 1, the problem is defined by identifying the scope, the future scenario subject for analysis and selecting the objective function and all the additional performance and sustainability metrics. Data for to this step is constituted mostly by business and strategic considerations, and therefore are provided by business departments.

In step 2, all the available industrial, commercial and regulatory information relevant to the problem are collected and organized accordingly to a predefined knowledge structure. The potential raw materials and products are identified, and the different processing alternatives are represented in the form of a superstructure, consisting of a network of process intervals (PI) and of a list of logical constraints to exclude infeasible and redundant alternatives.

Food safety and Environmental Health and Safety (EHS) regulations are translated into a list of logical and operational constraints, to exclude hazardous and non-compliant alternatives from the search space.

Since the knowledge base that is integrated at this step is multidisciplinary and multisource, particular emphasis is given to data reconciliation and consistency, as well as to systematic knowledge representation into an efficient database structure. This step takes input mostly from engineering but also from corporate business knowledge and expertise.

In step 3, all models needed for the problem formulation are collected or generated. These include the models of each of the process intervals read as process technology alternative, which constitute the superstructure, as well as all cost/value and sustainability models needed to calculate the objective function from the design variables and the performance metrics defined in step 1. All models are validated against experimental data or industrial knowledge available. This step is mainly executed with data from engineering department.

The objective function, the superstructure and all the logical, operational and process constraints defined in the previous steps are collected to formulate the MINLP problem:

$$\max f(x, y)$$

$$s.t. \, g(x, y) \geq 0$$

$$h(x, y) = 0$$

$$x \in X$$

$$y \in \{0; 1\}^n$$

Where f is an objective function which represents the economic potential, x represents the vector of continuous variables, y is the vector of binary variables. X is a continuous feasible region of continuous variables defined by their lower and upper bounds, g and h are the vectors of inequality and equality constraints respectively.

In step 4, In this step the MINLP problem formulated in step 3 is solved. The solution gives the optimal value of the optimization variables (where the binary represent the optimal strategic decisions and the continuous variable the optimal tactical decisions), together with the objective function and the performance indicators calculated at the optimal solution. On the base of these results, the identified solution is evaluated to decide whether to proceed to its implementation.

In step 5, refers to detailed modeling and optimization of the selected alternative using any appropriate process simulator.

Software Infrastructure

The framework is complemented by a software infrastructure based on excel as GUI for data input and GAMS for the resolution of the formulated MINLP problem. Data exchange between the 2 software is based on binary files through the use of GDXXRW tool (GAMS Development Corporation, 2011). The DICOPT solver is used to solve the MINLP problem (Geoffrion, 1972, Viswanathan and Grossmann, 1990). Detailed modeling and optimization of the selected alternatives can be performed using ICAS (Morales-Rodriguez and Gani, 2007) or any appropriate process simulator. A schematic representation of the software infrastructure and of the data flow for the execution of the framework is shown in Figure 3.

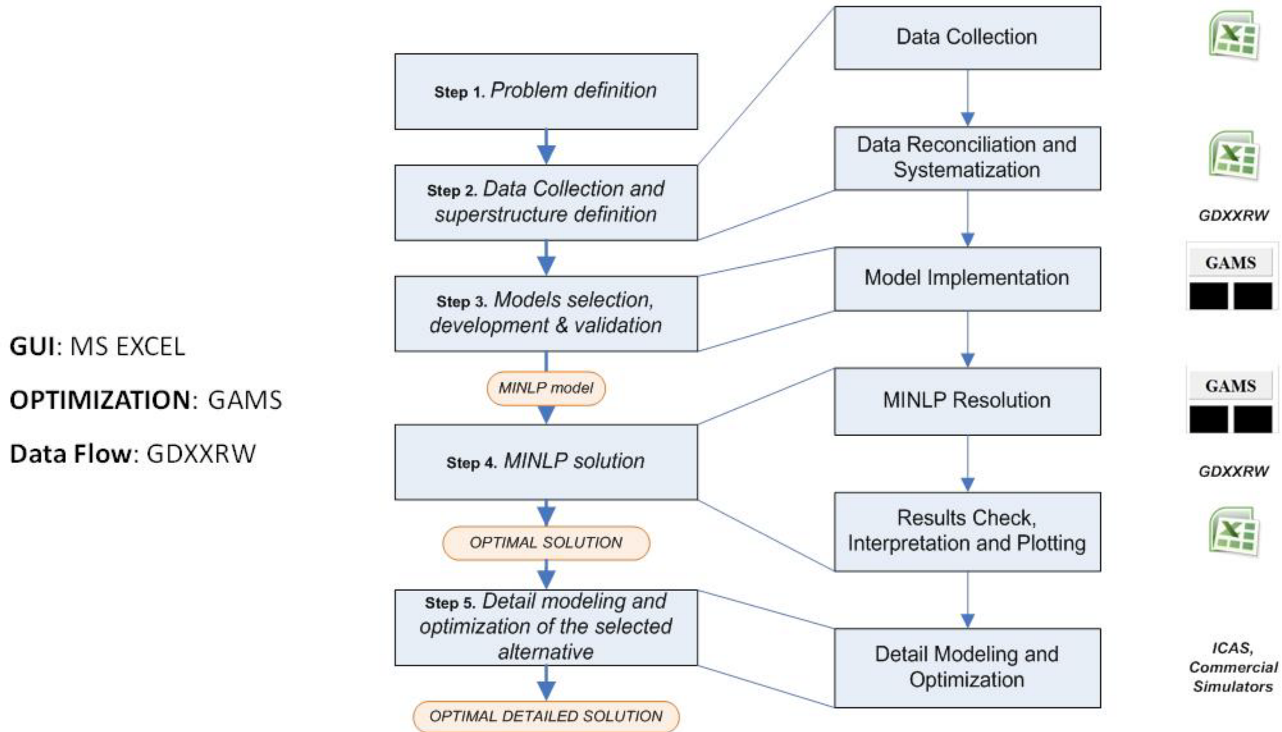

Figure 3 Data Flow and Software infrastructure (Quaglia et al., 2011)

Application highlights of the framework

The application of the framework is highlighted here focusing on the problem of synthesis and design of soybean processing network.

Soybean (*Glycine max*) has become one of the most important agricultural commodities with a steadily increasing global production, which reached 248 MMT in 2009 (Thoenes, 2009).

Soybean can be used as a raw material for a wide range of food, feed and pharma products: soybean oil is widely used as cooking or dressing oil, but can also have feed or technical applications, as well as raw material for biodiesel production. Defatted soy-beans are a low-cost source of protein, used to substitute animal protein in a wide range of feed and food products.

Being a low margin operation, soybean processing profitability can be achieved only by optimizing the allocation of the different seed components to commercially valuable products and by-products (Chicago Board of Trade, 1998). The wide spectrum of potential products and their mutual influence make the determination of the optimal resource allocation a challenging task. Moreover, because of the market volatility of agricultural commodities, this problem needs to be solved frequently in order to have up-to-date solutions.

To solve the problem, we follow step by step the framework outline in Figure 2. In step 1 we define the problem in more generic terms, which follows:

GOAL

Synthesis and Design of Optimal Soybean Processing Network

SCOPE

Entire B2B value chain

Biodiesel production out-of-scope

Generate input for FEED documentation

CONSTRAINTS

Greenfield (no pre-existing plants)

No stream split (one process interval)

OPTIMALITY CONDITION

Maximize Gross Operating Margin

INDICATORS

Wastes Production

Products Yield

Utility consumption

In step 2, the knowledge and data relevant to the problem are collected by integrating the information available in the open literature with the industrial knowledge of Alfa Laval the industrial partner in this project partner.

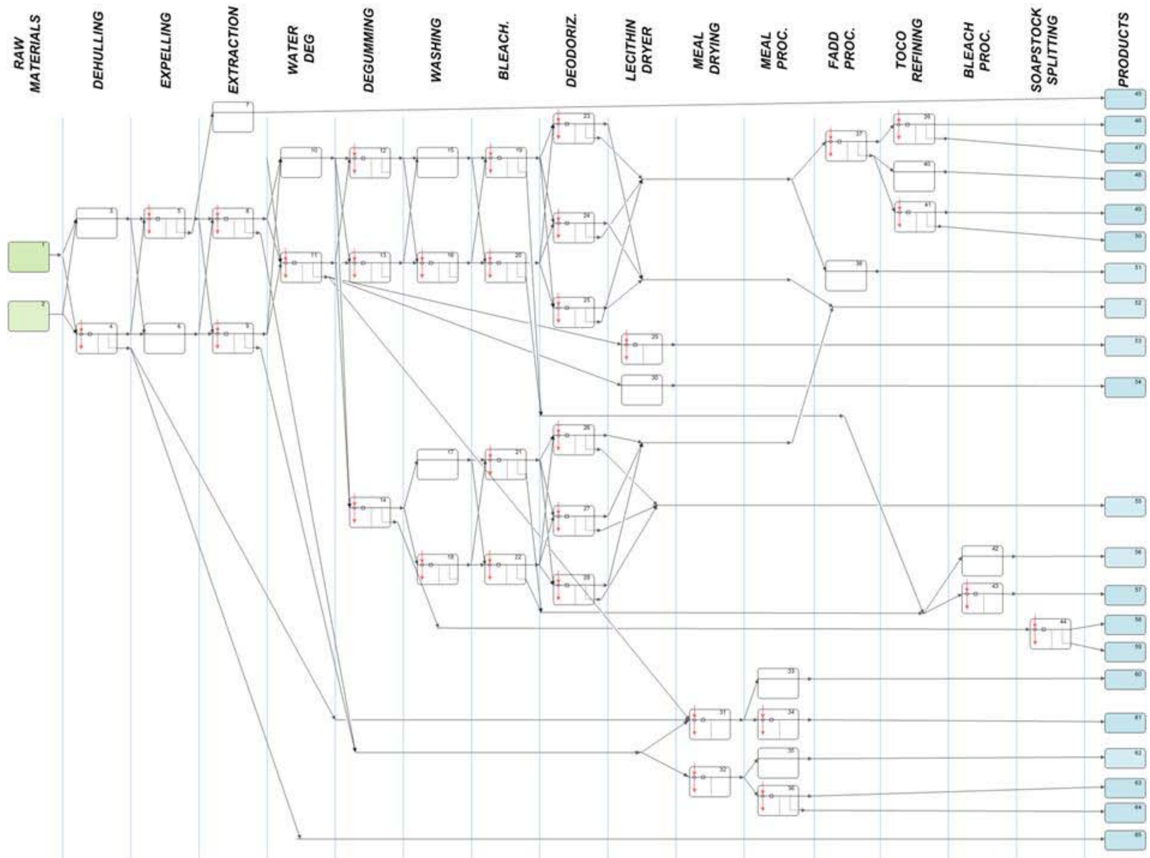

Figure 4. Superstructure of soybean processing networks representing many possible combinations of processing routes

The potential alternatives are represented in a superstructure composed by 65 process intervals: 2 raw material (soybean of different quality), 42 process intervals (organized in 15 process tasks), 20 potential products and 1 special waste (exhausted bleaching clay) are considered. The resulting superstructure is outline in Figure 4, which represents all possible combinations of processing routes from raw materials to products (in order of thousands). Net Present Value (NPV) over a time of 25 years is selected as objective function to maximize. The following two scenarios were evaluated:

- Scenario 1: Base case; the average value of raw material, utilities and products prices is considered.

- Scenario 2: uncertainty analysis: The price of raw materials, some utilities and products, as well as utility consumption is considered to be uncertain, and their correlation is calculated or estimated by expert review.

In step 3, process alternatives are represented by appropriate mathematical models describing degree of conversion or separation performance, utility consumption and waste consumption among others. All model parameters such as raw material compositions, material prices etc. are obtained from data available in the open literature or through Alfa Laval expertise. All secondary model parameter such as specific consumption of hot utility or separation factor are calculated by solving the heat balance or the needed constitutive equation. In step 4,for scenario 1 the resulting mixed integer nonlinear programming (MINLP) is formulated deterministically and solved in GAMS using appropriate solver(see Figure 3). For scenario 2, the problem is formulated as stochastic mixed integer nonlinear programming (SMINLP) problem and solved by translation into deterministic equivalent using sample average approximate method. The results are shown below.

The evaluation results of scenario 1 and scenario 2

For the processing network problem in scenario 1, the following processing route was found optimal with a unit cost 108 (scaled for proprietary reasons): 1 4 6 8 11 13 15 **20** 23 29 32 35 38 42 51 52 53 56 62 65. This processing route is highlighted in the superstructure representation shown in Figure 5. The detailed description of the processing interval indicated by numbers can be found in Quaglia et al., 2011.

In scenario 2, the problem of design of processing network is expanded to include market uncertainties as well as price fluctuation in utilities consumed in the process. The resulting problem is then formulated as a stochastic mixed integer nonlinear programming (SMINLP) and solved using sample average approximation method. The optimal processing network selected included the following processing intervals: 1 4 6 8 11 13 15 **19** 23 29 32 35 38 42 51 52 53 56 62 65. This optimal solution indicates a difference between the deterministic solution, which is basically has to do with the process interval 19, which in the deterministic scenario the interval id 20 was selected as the processing alternative. When tested in the uncertain conditions, the latter showed an NPV of 106.5 unitcost, which allows to calculate the Value of Stochastic

Solution (VSS) as 1.8 unitcost (1.7% of the NPV). The VSS corresponds to the increase in value which can obtained by performing decision making under uncertainty.

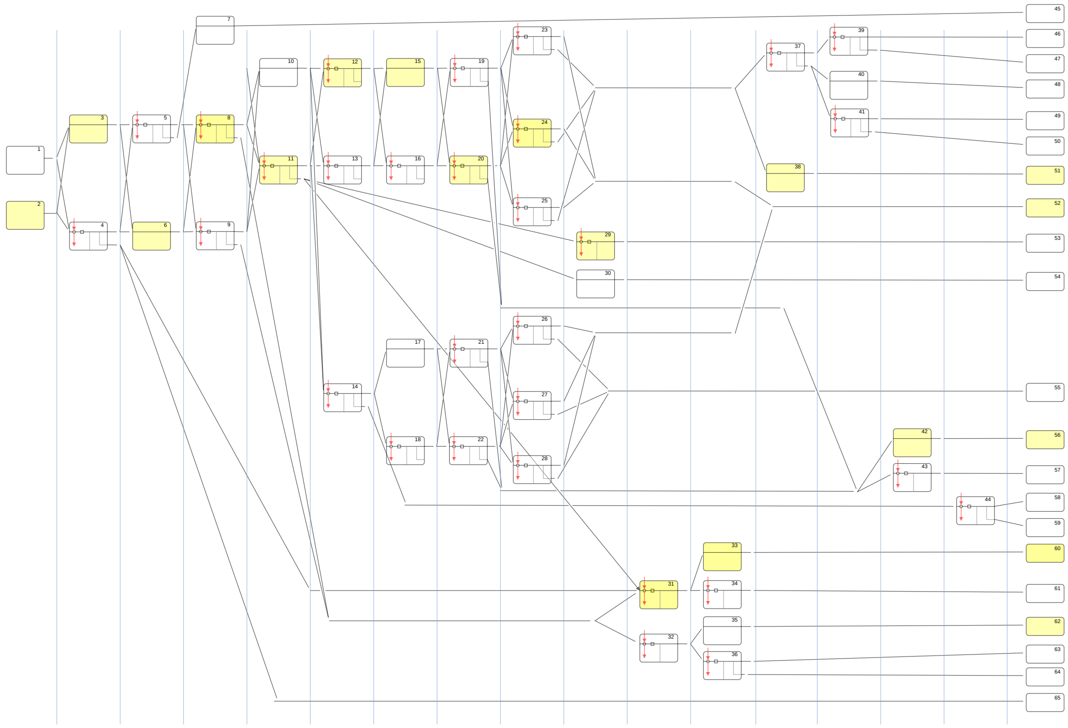

Figure 5. Optimal processing route found in scenario 1

Conclusion

A systematic framework for synthesis and design of processing Networks integrating cross-functional interactions between business and engineering departments in processing industries is successfully developed. The framework is based on integrating the principle of good business practice with focus on “do the right project” , and good engineering practice with focus on “do the project right”.

The framework is implemented as software platform to serve as enabling technology for facilitating the innovation cycle in processing industries. By using a systematic and structured approach, the software implementation of the framework allows processing industries to manage and update and maintain their multi-disciplinary knowledge base composed of business and engineering competences, skills and know-how in one platform.

As a result this enabling technology platform allows business analysts/strategists and engineers/scientists focus on their job idea generation, interpretation, decision making respectively. This is expected to contribute to the companies' efforts to realize the full potential of their activities.

Recommendations

The framework is generic in nature and can be applied across different chemical and processing industries sectors including petrochemical industry, bioprocessing, food and many more. In addition to the case study presented above for soybean processing network, the framework has been successfully applied for designing optimal biorefinery network in which the challenge was to find the optimal processing route/biorefinery network for the production of biofuels (e.g. ethanol, butanol,…) and blends of these chemicals with fossil fuel based gasoline (Zondervan et al., 2010). The framework supports optimal management of industrial water footprint, which involves optimization of water reuse and selection of appropriate treatment technologies.

As regards engineering applications, the framework can serve as a valuable tool in addressing and assessing a number of important problems and challenges such as effects of new technologies? New investment opportunities? Effect of stringent environmental permits? CO_2 footprint? Effect of feedstock grade? to the business portfolio and gross operating margins, among others.

Innovation is and shall remain an important engine for growth of processing industries by churning of new and valuable products for maintaining and improving modern lifestyle of mankind. In future we will increasingly see the integration of information technologies and domain knowledge in multi-disciplinary science and engineering used for facilitating the innovation cycle. Future belongs to knowledge based systems and their software applications for making new generation of product and processes in a fast, effective and intelligent way.

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