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# Industrial best practices of conceptual process design

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## Abstract

The chemical process industry aims particularly at energy, capital expenditure and variable feedstock cost savings due to fierce global competition, the Kyoto Protocol and requirements for sustainable development.

Increasingly conceptual process design methods are used in the industry to achieve these aims. They are used in:

- existing processes to renew parts;
- process re-designs based on existing feedstocks and catalysts;
- innovative processes (new feed stocks, new catalysts, new process routes, new multifunctional equipment).

This article is focused on the best industrial conceptual design practices applied for these application areas. To this end we have reviewed methods, which are used in the chemical process industry in the last 15 years. Capital, energy and variable cost savings are indicated for each method.

Specific attention is paid to:

- functional integration to multi-functional equipment;
- heuristic based selection of unit operations and recycle structure;
- superstructure based design optimisation with mixed-integer-non-linear programming (MINLP).

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## 1. Introduction

This article describes the industrial best practices of conceptual process design as publicised in the open literature over the last 15 years. In view of the Kyoto Protocol and the requirements for sustainable development energy savings become more and more important for the process designer [1]. To stay competitive in the global market capital and operating cost savings are needed. This is why this article focuses particularly at industrially applied design methods resulting in new designs with savings of energy, capital expenditure and feedstock cost compared to old processes.

Any design contains the steps:

- problem definition,
- synthesis of solutions,

- analysis of solutions,
- evaluation,
- reporting.

This article focuses on methods for the synthesis of promising solutions, as this step has a large impact on the development and design of novel process designs and several methods for this step have been developed recently, while in the past little to nothing was available.

Where available, commercial scale novel processes resulting from the new design methods are reported, with resulting savings on energy, capital expenditure and feedstock cost.

Because of the industrial scope of this article many methods reported by academic researchers are not mentioned. This is no implicit negative judgement on those methods. Several of those methods are probably applied in the process industry but are not publicised so far and could therefore not be included in this article.

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## 2. Basic principle for energy savings in combination with capital expenditure reduction

Before we start to describe conceptual process design it is useful to explain the basis principle of energy requirements for any chemical process.

The basic principle to save on requirements of high quality energy carriers (fossil fuels, solar energy) follows from thermodynamics. All process steps are carried out in a finite time and are therefore irreversible, by which high quality energy is converted to lower quality energy. This is defined as exergy loss. By reducing the irreversibility of the process this exergy loss can be reduced [2].

This reduction in irreversibility can be achieved by combining process functions in one process step, by selecting the best unit operations with their recycle structure, by heat integration, and by variable optimisation; spreading the irreversibility evenly over the process [2]. Often the exergy loss reduction also results in lower capital expenditure cost due to number of steps reduction [3].

## 3. Conceptual process design position in the life cycle

From Siirola, Eastman Chemicals Company [4], Kaibel, BASF [5] and the authors experience in Shell a general picture of all life cycle steps of industrial projects could be compiled as shown in Table 1.

The steps chemical route synthesis, conceptual design and process development are sometimes carried out con-currently. As more information becomes available from the development experiments the conceptual design becomes

Table 1  
Overview of all steps to commercial operation and end of life

Life cycle step	Involves
Chemical route synthesis	Development of chemical synthesis steps Selection of best chemical synthesis steps
Conceptual process design	Function integration Heuristic selecting unit operations and recycle structure Superstructure optimisation
Process development	Experiments for kinetic, physical data Reaction and separation tests Pilot plant Cold flow scale-up tests
Process engineering	Definition of all equipment and control for accurate economic evaluation
Site integration	Connect energy and mass flows with other processes and utilities
Detailed engineering	Definition of all process details to allow purchasing and construction
Plant operation	
End of life	Find second use Deconstruct and reuse parts

Table 2  
Functions in conceptual process design

Function	Example
Molecular identity change	Chemical reaction
Amount change	Add component
Composition change	Separate, mix
Phase change	Evaporate
Temperature change	Cool
Pressure change	Pumping
Form change	Extrusion

better defined. A sketch of an industrial method for this combination of these steps is given by Siirola [4]. A detailed publicised method is however lacking for this combination of chemical route synthesis, process design and process development in industry. In the remaining part of this article, we will therefore concentrate on conceptual process design methods, etc. Some generic steps in process development will also be briefly discussed at the end of this article.

Before we describe the elements of conceptual design shown in Table 2, it may be useful for clarity to explain two other terms used in the literature for conceptual process design.

The first term to explain is process synthesis. In 1972, AIChE organised for the first time a meeting devoted to process synthesis [6]. Since then more and more companies are using it and now some consensus in industry is reached about the definition of the term. According to Siirola of Eastman Chemical Company, process synthesis is the invention of chemical process designs [4]. To cite him: "It involves the generation of alternatives in all process engineering steps within the innovation process. There is some overlap with the preceding chemistry stage and the subsequent basic engineering stage. The goal is to develop a flow scheme". According to O'Young, Mitsubishi Chemical Corporation it is distinguished from the subsequent steps modelling and optimisation [7]. It is to be noted however, that superstructure optimisation is part of process synthesis [6]. Hence, process synthesis can be seen as the second step in modern conceptual process design.

Process Intensification is a term that is becoming prominent in publications. A definition is given by Stankiewicz, DSM [8]: "Process intensification consists of the development of novel apparatuses and techniques that compared to commonly used today are expected to bring dramatic improvements in manufacturing and processing, substantially decreasing equipment-size/production-capacity ratio, energy consumption or waste production and ultimately resulting in cheaper, sustainable technologies". He distinguishes between process intensification equipment and process intensification methods. The methods contain multifunctional reactors, hybrid separations alternative energy sources and other methods. He provides however no generic design method.

From Stankiewicz description, it can be concluded that process intensification is not a conceptual design method,

but the result of successful conceptual designing with tight sustainability goals and constraints.

#### 4. Conceptual process design by function-integration

The conceptual process design can start with defining functions (tasks) and integrating these into a process design containing novel process units. Siirola, Eastman Chemicals Corporation describes his method in general terms with the following functions most common to the chemical process industry [4].

After the functions have been synthesised. The functions are combined as much as possible by shifting to common pressure and temperature ranges. After this a set of multi-functional equipment can be defined.

He explains the method with the design of the methyl acetate process as an example [9,10]. A conventional process would consist of 11 different process steps. By designing first in functions the problem could be reduced to six steps, which could be combined in one column. This design is factor 5 lower in energy requirements and capital expenditure [4].

In the authors experience only very experienced process designers can understand and work with Siirola's method and no other publication has been found of industrial use of his method.

The advantage of designing by functions and combinations of functions is that the freedom of action is large. This enhances creativity and increases the number of attractive process alternatives. Functions operating at the same temperature and pressure range can be combined in one piece of equipment. In this way capital expenditure and energy losses are often reduced.

Many cases of function-integrated novel commercial processes or process steps are available in the open literature. Green gives an overview of commercially applied types of process intensifications [11]. Stankiewicz reports also several types of industrial applications [8]. The energy and capital expenditure savings range between 20 and 80% [4,12,13].

A major sub-class of multi-functional design in the industry is reactive distillation [14–16]. CDTECH alone reports 79 commercial processes on reactive distillation, of which 60 ether units, 15 selective hydrogenation units and 4 aromatic alkylation units [14].

For reactive distillation many conceptual design methods are available. For the industry, the method of Schoenmakers, BASF, is most useful as it does also include non-equilibrium and non-azeotropic systems like hydrogenations [17].

Multi-functional reactors is an other sub-class. Dautzenberg, ABB Lumus provides us with many industrial examples [18]. For multi-functional reactors however no generic industrially applied conceptual design method is yet available [3].

Dividing wall column distillations is also an important sub-class. It combines both separation and thermal coupling.

BASF alone reports 30 columns in commercial operation [5]. Typical energy savings over conventional column systems are around 30% [5].

The field of conceptual design methods for reactive separation is under rapid development and methods are emerging, see Schembecker, Process Design Center [19], so widening the scope of applicability of multi-functional design in the industry.

The resulting novel multifunctional process steps require in general a large development effort as all knowledge for design and scale-up of the novel unit operations has to be developed. So this type of design is only selected if large improvements in a design are needed. At the end of this article a development path for novel processes is outlined.

If the time is lacking for radically new designs other conceptual design methods can be applied as described in the next sections.

#### 5. Conceptual process design by heuristic selection of unit operations and recycle structure

Conceptual process design by heuristics is about the selection of the best unit operations, their sequence and recycle structure [20]. An easy to use method is described by Douglas [20] and is used in Shell training classes as a first introduction to conceptual process design. Especially the exercises are well chosen for an industrial environment. The main disadvantage is that it is targeted at economics, while other criteria like safety, health and environment are hardly addressed.

A comprehensive expert software system supporting conceptual process design is the software package "PROSYN". An overview description is given by Schembecker et al. [21]. Special attention is given by PROSYN on selection of reactors and separators. For reactor selection a specific software module READPERT is available. It also can be used on its own [22,23].

PROSYN is used by BASF [5], Shell [24] and others, often with the support of Process Design Centre [25]. The conceptual design with PROSYN is in general carried out by a multi-discipline team, consisting of at least a chemist and a chemical engineer [21,24].

The energy saving by process synthesis depends strongly on the exothermicity of the reaction. For a strongly exothermic reaction the energy savings can be 100% [24]. The total cost savings by industrial applications of process synthesis range from 20 to 60% [24].

#### 6. Superstructure optimisation by mixed integer non-linear programming (MINLP)

Conceptual process design by superstructure optimisation contains five steps:

- All conceivable unit operations are generated using the creativity of the process engineer [5].
- All individual units are connected in all possible ways into a so-called superstructure.
- A large mathematical model is made for this superstructure, containing all components mass flow, enthalpy flows, cost expressions for feed stocks, capital expenditure and fixed cost related to the sizing of equipment.
- A cost optimisation function is defined together with all constraints of the variables.
- The optimum selection of equipment and conditions is determined by numerical optimisation using MINLP methods.

The method described by Seider et al. [26], Biegler et al. [27] and Floudas [28], is industrially applied for optimising existing processes [5,29] and for optimising a design resulting from a heuristic method [24]. For these cases a small design section is optimised with a few alternative options.

So far the industrial does not apply the method for generating completely new process designs [5]. This is due to the complexity of the models, the time needed to set up the models with their equations and the large size of the numerical optimisation problems.

## 7. Development plan for novel processes or process steps

The development effort for a novel process or a novel process step is in general considerable. The following industrial development programme could be compiled from descriptions by Sirola, Eastman Chemicals Corporation [4], Kaibel, BASF [5], and the experience of the author in Shell.

### 1. First make a first scouting conceptual design.

This design is to evaluate the feasibility, safety, health, environment, sustainability, product quality, and economy aspects. It also is used to estimate the development effort required in knowledge, time and money and the risk of failure.

### 2. Determine the physical and chemical properties, crude kinetics and critical construction material choice parameters required for the design, and some proof of principle experiments.

### 3. Make a second conceptual design for the commercial scale plant and a downscaled pilot plant.

Based on these designs and costing a decision is taken to continue with constructing and operating the pilot plant.

If scale-up effects on certain phenomena, like mass transfer, or mixing are not sufficiently known a computational fluid dynamics model will be developed and a so-called cold flow large scale experimental model will be designed and operated to validate the CFD model.

### 4. Operate the pilot plant.

### 5. Design the commercial plant based on the pilot plant findings.

## 8. Conclusions and recommendation

Conceptual process design methods are applied successfully in the industry to obtain processes at lower cost and energy requirements.

The largest savings in capital expenditure and energy requirements are obtained by function integration methods resulting in processes with novel unit operations.

Further research in design methods and simulation tools are required to increase the number of application areas for function integration.

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