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Multivariate risk analysis of an intensified modular hydroformylation process

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ABSTRACT

Reduction of investment risk is a major challenge in chemical process design. To minimize financial risks a paradigm shift is necessary. Therefore, risk analysis will have to gain importance already during process development. Only in this way can plant designs be identified that cover the expected demand uncertainty at optimal costs. Stepwise expansion is one option to reduce risks as investments can be spread over a certain time period. This allows waiting for more precise market information and adapting production output to changing market development. The drawback of this approach is the loss in economy of scale. Potentially higher investment costs have to be balanced against an achievable risk reduction which makes the integration of risk assessment in process design indispensable. Furthermore, equipment allowing for an efficient numbering up in plant expansion is needed. Here one of the most promising options is the application of intensified equipment.

This work shows how process intensified equipment can be used to reduce the investment risk of a large scale hydroformylation plant. Two methods for risk quantification are applied. Both show that investment risk is reduced by numbering up unit operations and adapting their size. Influencing parameters are the cost structure and process boundaries.

1. Introduction

The investment decision for a new chemical plant is associated with multiple risks. These risks concern e.g. technical risks, calculated risks or scheduled risks for equipment delivery and construction [15]. Besides these project and process related risks changes in market demand are another important risk factor which is gaining importance in times of economic crisis and globalization. In this context the integration of risk assessment taking uncertain market demand and changes in raw material prices into account, will gain further importance in chemical plant design [13].

As projects in chemical engineering take years until they are finished, market forecast will change multiple times during project duration. Process parameters and equipment dimensions are adapted to changing market reports and new design capacity estimates. This leads to an increase in project time and effort. If project engineers were able to react quickly to these changes and with limited effort, plant design would become more efficient. Therefore, market uncertainties have to be taken into consideration in early project phases and plants have to be designed such that it becomes possible to cope with a wide range of uncertainties. This makes flexibility in capacity one of the most important characteristics of the designed plant.

The usage of equipment modules is a promising approach to limit the impact of changing market forecasts on the project. In this context modules are predefined apparatuses available in fixed sizes. This will in most cases lead to the situation that the apparatus is not available with optimum dimensions so that either

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Nomenclature

K	Covariance matrix
k_{ij}	Correlation coefficients
D	Lower triangular matrix
D^T	Transposed of matrix D
d_{ij}	Coefficients in matrix D
X	Uncorrelated parameters
Y	Correlated parameters
p	Probability
α	Confidence level
X_α	α-quantile
$E(X)$	Mean of a distribution
$q_{1-\alpha}$	Quantile of the normal distribution
$\sigma(X)$	Standard deviation
γ	Skewnes
δ	Kurtosis
CFaR(X)	Cash flow at risk (M €/a)
EMV	Expected monetary value (M €)
p_i	Probability of scenario i
X_i	Profit less the expected risk in scenario i (M €)

numbering up or oversizing of unit operations is inevitable. In the light of market uncertainty these non-ideal equipment dimensions do not necessarily represent a disadvantage as it is no longer the aim to solely optimize a plant for one design capacity but to cover a wide capacity range. Thus modules have to be combined in a way, which limits additional costs for numbering up and oversizing and at the same time achieves the required flexibility. Two prerequisites have to be fulfilled to realize this approach. First, equipment is needed, which can easily be numbered up from a technical point of view. Second, the increase in investment costs as a result of numbering up should not be too high. Both points can be realized with intensified equipment.

The development of modular and intensified production concepts has been pushed in the recent years by European research projects like F^3-Factory and Copiride [10,11]. One of the main focuses of these projects is to develop modular equipment and to demonstrate the operability of modular plants. In this context Bramsiepe et al. [4] estimated that a lead time reduction of about 20% for design and construction of new plants seems reasonable. However, to take benefit from these newly developed technologies, design and evaluation methods are required which take the characteristics of modular plants into consideration. Technical literature already provides some publications dealing with the economic evaluation and the design of modular plants. Wiesner et al. [6] and Oldenburg et al. [5] developed an approach for stepwise plant expansion. Aim of the optimization method is to find an expansion strategy that fits optimal to an estimated market development. Even though both authors did not use the term module in their approach, the idea to copying identical production lines fits quite well to a modular design. The idea of stepwise expansion was picked up by Lier et al. They investigated the economic benefits of a modular plant by applying discounted cash flow calculation [1]. In their approach a complete production line was defined as a module. They have also used real options analysis to show the flexibility of their approach in increasing markets [2]. Harwardt et al. [3] developed an approach for optimized selection of modular equipment with the aim of investment and operating cost minimization. As process example they used distillation columns and optimized the sizes of the heat exchangers and the colmun. Sizes of the equipment available for optimization were fixed in a module data base. Seifert et al. [7] have presented an approach to turn a multiproduct batch plant into a continuously operated modular plant. Here the main focus was on the design of the plant and the economic benefits that can be achieved by a shorter lead time. Calculation results were evaluated using net present value (NPV) calculation.

As it can be seen from the literature examples presented, calculating investment and operating costs as well as NPV calculation are the common methods used in the evaluation of modular plants. However using these cost calculation approaches is not sufficient to show how a modular design can help minimizing investment risk. As the opportunity to split an investment and to wait for more detailed information about market development is one of the main advantages of a module based plant design is, this benefit has to be integrated in an economic evaluation.

It is the aim of this work to show how modularly designed processes can be adapted to economic uncertainties by generating flexibility in capacity. Multivariate risk analysis will be used to investigate a process design in order to identify most suitable plant setups and investment strategies for given uncertainties. The focus will be on risks arising from volatilities in demand and product prices. Risk analysis will be applied exemplarily for an intensified hydroformylation process developed by Evonik Industries within the F^3-Factory Project. The impact of the new intensified technology and its application in a modular design on investment risk will be evaluated. It will be shown that modular design can also prepare a benefit in large scale applications. Finally two suitable risk analysis tools will be described and used to optimize the plant structure for the given process example. The key question in this context will be to identify the minimum degree of uncertainty, beyond which modular design exhibits a benefit over dedicated design.

2. Process example

In the process example *n*-butyraldehyde is produced by hydroformylation of propene. Byproducts are propane, butanol and different dimers. The reaction system is simplified by taking formation of 2-ethyl-2-hexenal as the representative for all possible aldol reactions into account. The reaction equations are shown in Table 1.

One of the common processes for hydroformylation is the Ruhrchemie process [9]. In this design bubble column reactors are used. After the reaction step catalyst and solvent are separated in a flash drum by lowering pressure from 21 bar to 1 bar. The liquid stream is recycled to the reactor. After condensing the gas stream a gas liquid separator is used to remove most of the light components like propane, propene and syngas. The gas stream is recycled to the reactor too. In a desorber column dissolved propane and propene are removed by stripping with syngas. Next propane and propene are separated from the product stream in a distillation column. High boilers are removed in a second distillation column. Finally, *n*- and *iso*-butyraldehyde are separated in a third distillation column. The conventional process is characterized by a large gas recycle stream which has to be compressed from 1 bar to the reaction pressure of 21 bar and operating costs which are dominated by propene and syngas consumption [14]. The goal for process improvement must

Table 1
Reaction system for propene hydroformylation.

Main reaction:	Propene + $CO/H_2 \rightarrow$ *n-/iso-* butyraldehyde
Side reaction:	Propene + $H_2 \rightarrow$ propane
Consecutive reaction 1	Butyraldehyde + $H_2 \rightarrow$ Butanol
Consecutive reaction 2	2butyraldehyde $\rightarrow$ 2-ethyl-2-hexenal + H_2O