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A Chemical Process Design Framework Including Different Stages of Environmental, Health and Safety (EHS) Assessment

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Abstract

In this work, we present a novel framework that comprises four stages of process modeling and multiobjective decision-makings considering monetary and non-monetary aspects. Four stages in early design phases are considered and characterized by the available information for process modeling and assessment. Appropriate modeling methods, and evaluation indicators for economy, life-cycle environmental impacts, EHS hazard and technical aspects are selected for each defined stage. The framework is demonstrated in the case study of methyl methacylrate (MMA) process design. 17 reaction routes are screened step-by-step up to generating optimal flowsheet of a promising route. As a validation, evaluation profiles of 6 routes are compared over stages to identify key factors that should be well estimated in earlier stages.

Keywords: process design, safety, environment, hazard, framework, case study

1. Introduction

Needs are growing to include environmental, health and safety (EHS) aspects in every decision-making throughout process development. In particular, decisions on reaction path, solvents, unit operations and operating conditions affect the EHS performance of the process significantly. Various methods to reflect such aspects of early stages into decision-makings have been proposed [1-3]. Selection of these evaluation methods should be done appropriately to cover EHS aspects comprehensively at every design stage. Some authors distinguished different stages of process design, and applied one environmental evaluation method with different amount of available information in a two-step procedure [4,5]. We present a novel framework comprising four stages of chemical process design. Each stage is characterized by the available information as a basis for process modeling and assessment and the tasks that have to be solved. For each stage appropriate modeling and evaluation methods are selected. This framework is demonstrated and validated in the case study of methyl methacrylate (MMA) process design.

2. Design framework

2.1. Stage definition and process models

Figure 1 shows defined design stages convered in the framework, and selected evaluation indicators at each stage. These stages are typically part of early design stages of grass root design. Product, and production scale should be determined prior to the first stage. In *Process Chemistry I*, reaction routes to synthesize the product are searched, and they are screened on the basis of ideal performance i.e. 100% yield. Here, technical difficulties can be a basis for decisions rather than multiobjective evaluation results. More reaction information such as side reactions, catalysts and solvents are included in *Process Chemistry II*, and promising routes are selected. Proxy indicators are defined to estimate unknown part of the process performance e.g. separation energy. In *Conceptual Design I*, the analysis scope is broadend to the whole process including separation part. Process structure is determined by simulation with simple physical property data e.g. tempreture averaged volatility factors. Such short-cut models are replaced by rigorous ones in *Conceptual Design II* including non-ideality e.g. azeotropes. Precise mass and energy balances, equipment sizes become available here. With this rigorous model, detailed analysis is performed e.g. parameter sensitivity analysis and optimization.

2.2. Evaluation indicators

- Economic aspect

Raw material cost is used in first two states. In *Process Chemistry I*, it is theoretical minimum and is updated with more reaction information in *Process Chemistry II*. In *Conceptual Design I*, production cost is used which is the sum of raw material cost and gate-to-gate utility cost that becomes available here. In the last stage, investment cost is calculated based on the equipment sizes, and together with production cost, net present value (NPV) is used as an indicator.

		Process Chemistry I	Process Chemistry II	Conceptual Design I	Conceptual Design II
Design stages	Considered aspects	Reaction	Reaction	+ Separation + Waste treatment	+Equipment
	Model includes:	Stoichiometry, 100% yield (ideal)	Conversion, selectivity, auxiliary, catalyst, solvent, byproduct, heat of reaction	Shortcut process models, simple property data	Rigorous process models, non-ideality, reaction kinetics, detailed property data,
	Decision characters	**No decision forced** screen routes with serious problems D1	**Filter some routes** D2	**Select process option(s) &/or route(s)** by multiobj. evaluation of all feasible options D3	**Optimize parameters** by sensitivity analysis D4
Multiobjective evaluation indicators	**Economic performance**	**Raw material cost** (theoretical min)	**Raw material cost** (updated)	**Production cost**	**Net present value**
	Proxy for gate-to-gate costs/impacts	**Mass Loss Indices** [6]	**Energy Loss Index**		
	Life-cycle environmental Impacts	**CED**[7] **in RM productions** (theoretical min)	**CED in RM productions** (updated)	**Cradle-to-gate CED**	**Cradle-to-gate CED** (updated)
	EHS hazard	**Substance EHS** [9]	**Process EHS** (around reactor)	**Process EHS** (whole process)	**Process EHS** (updated)
Supplemental indicator	**Technical aspects**	#Reaction steps; Raw material availability; Patents; Blacklist substances	Technical problems (e.g. catalyst activity)	Process complexity	Equipment specification

Figure 1: Proposed design framework: 4 design stages with selected evaluation indicators

- Life-cycle environmental impacts

Life Cycle Assessment (LCA) is the basis in this aspect, where environmental impacts in raw material production and the process itself are quantified. In this work, Cumulative Energy Demand (CED [7]) is selected as an impact category, which is a good proxy for many other energy-related categories [8]. The indicator first considers CED in raw material, and then cradle-to-gate CED.

- Proxy for gate-to-gate cost/impacts

In first two stages, utilities associated to the process e.g. separation energy are not available. To estimate such gate-to-gate utility, we defined proxy indicators there. Energy Loss Indices (ELI) is a new concept in this work which estimates gate-to-gate energy based reaction information at *Process Chemistry II* e.g. product concentration at reactor outlet. At this stage, ELI can be combined with raw material cost or CED, to estimate production cost or cradle-to-gate CED.

- EHS hazard

This is the aspect where hazard to the environment, workers' health and safety are considered. EHS assessment method [9] is selected as an indicator. This method, developed for early design stages, provides index scores of a substance in 11 EHS categories. Such index values of substances can be extended as EHS score of a process by including process information e.g. inventory at different boundary levels e.g. around reactor or the whole process.

- Technical aspects

This additional indicator serves as a supplement to indicators described above. Examples of considered issues are shown in figure 1. This aspect normally serves as a constraint for the decision, and especially in the first stage it could serve as a terminating factor.

3. Case study on MMA process design

The framework is demonstrated in the case study. We considered MMA synthesis routes shown in figure 2, and by mimicking the framework, inferior routes were screened out step-by-step to produce optimal flowsheet of a promising route. In this paper, we present results in *Process Chemistry II* as an example where route A, B, C, D, F and X are considered. In other stages, analysis and decision-makings can be performed in a similar way.

Figure 3 (a) shows the aggregated evaluation score of 6 routes. Indicator results at this stage i.e. economy, life-cycle impacts, gate-to-gate proxy and hazards in E, H and S were aggregated using empirical weighting factors. From the overall height, route C is the best choice. Number of routes to choose depends on company resources e.g. time, or heuristic rule e.g. 30% from the best. Within individual aspects, some differences can be highlighted, for instance, route X is the best one when only economy is concerned. Environmental hazard is highest in route A, which is mainly due to dangerous substances e.g. HCN contained in the system. Route X has 10% conversion in step X1, which requires large throughput of isobutane, the raw material. This leads to higher safety hazard especially in categories of mobility and fire/explosion.

Sensitivity analysis was performed to measure the impact of choosing various weighting factors between cost, CED and EHS hazard. In figure 3 (b), each ternary diagram corresponds to the rank of the route by the aggregated score, and each node within a diagram is a set of weighting factors. The default set of factors i.e. 0.5, 0.2, 0.3 for cost, CED and hazard is indicated by star. It can be seen that route X would be the best choice when economy was strongly favored. This diagrams can be used to check the stability of the decision as well, by looking at nodes around the star.

As a validation of the framework, these 6 routes were modeled and evaluated up to the level of the last stage. Figure 4 shows profile of economic evaluation indicator. Only raw material cost is available in *Process Chemistry II*, and overall production cost (indicated by triangles) which is a sum of all material and utility costs and benefits by selling steam become available in *Conceptual Design I*. In *Conceptual Design II*, NPV is calculated which is a function of investment and production cost. From *Process Chemstry II* to *Conceptual Design I*, it appears here that more precise selectivity and introduction of loss term in the separation update raw material cost, especially in route F. Towards *Conceptual Design II*, inclusion of non-ideality renews production costs, however in this case only slightly. Here, the ranking in production cost is not

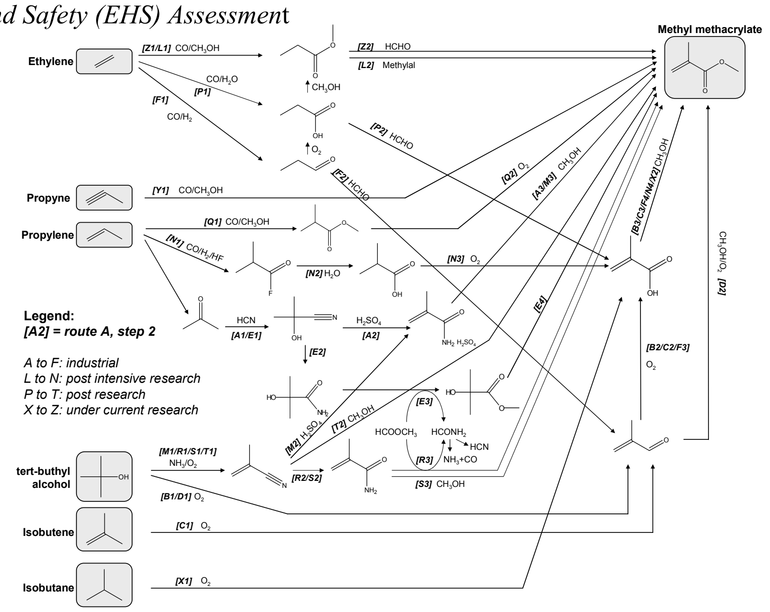
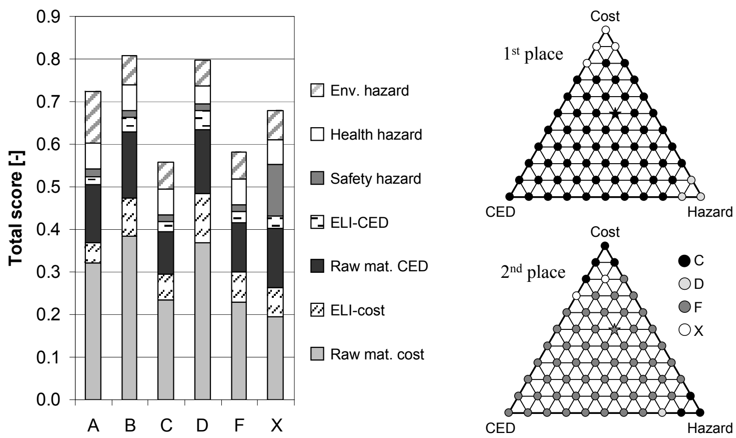


Figure 2: MMA synthesis routes adapted from [10]



(a) (b)

Figure 3: Evaluation and analysis at Process Chemistry II
(a) aggregated evaluation results (b) ranking of routes with different sets of weighting factors

the same as the one in NPV because of investment cost. For instance, route X with lowest production cost has lower NPV than route C because of X's high investment cost. Within economic aspect, investment cost is the factor that changes the ranking significantly which were unknown in earlier stages of this framework. In this way, key factors can be identified for other aspects as well, that should be somehow estimated earlier even with limited information.

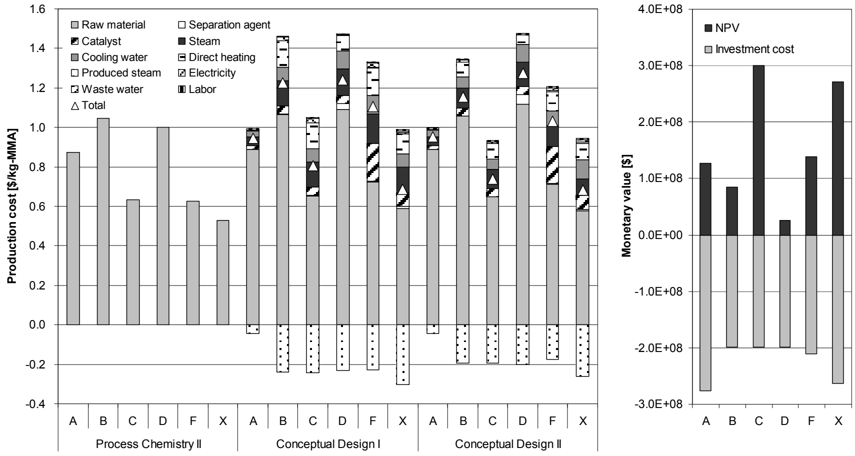


Figure 4: Profile of economic evaluation of 6 MMA synthesis routes over stages

4. Conclusions

We developed a four-stage framework of chemical process design, targeting early design phases that have big impacts on the process development. Evaluation indicators are selected for each defined stage to cover wide range of monetary and non-monetary aspects including life-cycle environmental impacts and EHS hazard. In the case study on MMA process design, it was illustrated that syestematic decision-making and transparent analysis are made possible within the framework. At the same time, key factors that should be well estimated in earlier stages e.g. investment cost were identified.

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