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IDEF0 Activity Modeling for Integrated Process Design Considering Environmental, Health and Safety (EHS) Aspects

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Abstract

We present an activity model of novel chemical process design. This model defines different stages of early process design, i.e. process chemistry and conceptual design, with appropriate process evaluation indicators. Environmental, health and safety (EHS) aspects are considered new assessment criteria together with conventional economic and technical indicators. The type-zero method of Integrated DEFinition language or IDEF0 is selected as a method for activity modeling. The activity model is described from the viewpoint a design-project manager who leads a group of process chemists and engineers. Application of IDEF0 enables systematic and transparent description of complex design activities, where the manager has to consider different types of design constraints and resources at different design stages.

Keywords: IDEF0, activity modeling, integrated process design, multiobjective design

1. Introduction

Companies need a new business process model when implementing a new strategy. Various methods are brought into focus, e.g. traditional block-flow diagram or Gantt chart for analyzing work flow or scheduling, or UML (Unified Modeling Language) for systems development. In chemical engineering, several authors have presented applications and merits of such business-process modeling techniques, e.g. Schneider and Marquardt (2002).

Among other methods, the type-zero method of Integrated DEFinition language or IDEF0 (Ross, 1977; NIST, 1993) is a standardized method of enterprise-resource planning or business-process re-engineering. In process systems engineering, different authors applied this activity modeling technique to the integration of new software tools to existing process- or operation-design (Fuchino et al., 2004; Gabber et al., 2004; Kikuchi and Hirao, 2007). Within ISO's standards development, there is a project called Process Industries Executive for Achieving Business Advantage Using Standards for Data Exchange (PIEBASE, 2007) where IDEF0 is used to standardize work processes and information requirements within process industries.

In regard to new philosophies that will be incorporated in the chemical industry, the concept of sustainable process design is receiving increasing attention. Environment, health and safety (EHS) was the center of the interest of many authors who developed evaluation methods for processes, e.g., Hilaly and Sikdar (1995), Kheawhom and Hirao (2004), Sugiyama et al. (2006, 2007). So far, various indicators or methods have been proposed (see Adu et al., 2007 for review), and they are getting more sophisticated with the incorporation of broader issues. However, many papers left it unclear, how a user can apply it in industrial process development.

We present an IDEF0 activity model based on our multiobjective process design framework (Sugiyama, 2007; Sugiyama et al. 2008). The viewpoint of the activity model is the user of this design framework, i.e., a design-project manager who leads a group of process chemists and engineers. Application of IDEF0 enables us to make systematic and transparent description of complex design activities, where the manager has to consider different types of design constraints and resources at different design stages. We also present important know-how of the design manager in executing the activity model for increasing its industrial applicability.

2. Integrated Process Design Framework

Figure 1 shows an overview of the framework. It covers the early phase of a grass root design and defines four design stages, i.e. *Process Chemistry I/II*, *Conceptual Design I/II*. These stages are separated according to the available information for process modeling and to the character of process assessment. As design objectives the following three aspects are considered: economy, environmental impacts through product's life-cycle, and hazard in terms of EHS. Life Cycle Assessment (LCA) and ETH-EHS (Koller et al., 2000) methods are selected for non-monetary evaluation. As an impact category of LCA, the Cumulative Energy Demand (CED; Verein Deutscher Ingenieure, 1997), which is an energy equivalency of different primary sources used for the production, is selected. At *Process Chemistry I/II*, proxy indicators are defined to estimate consequential process energy consumption, as a complement to raw material cost/LCA. These quantitative indicators are applied with expanding evaluation scopes, e.g., from substance level to process levels for EHS hazard. In contrast to the above objective functions, technical constraints are considered qualitatively throughout all four stages.

A stage-gate approach is taken in our framework: at each stage, reaction and/or process alternatives are modeled and evaluated, and promising one(s) survive(s) to the next design stage. It is assumed that product quality, production scale and location are fixed 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. In *Conceptual Design I*, the analysis scope is broadened to the whole process including separation part. Process structure is determined by simulation with simple physical property data, e.g. temperature 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 such as parameter optimization is performed.

3. Activity Modeling of the Design Framework

3.1. Top-activity A0

Figure 2 shows the top-activity A0: Design a chemical process at early phase levels with syntax of IDEF0. In IDEF0, a box represents a function or an activity, which has a verb as a name. The input arrows entering the activity box from the left side represent the objects that are transformed by the function into the output arrows on the right side. The control arrows associated with the top side indicate the conditions required to produce the correct output. The mechanism arrows on the bottom indicate the means of performing the function. Although inputs and controls generally consist of similar objects, e.g., data, products, information, they are distinguished in terms of whether or not the objects are transformed by the function. Every activity can be decomposed into a sub-level activity model that has the same boundary as the parent activity. Sub-activities can be defined hierarchically with information and tools consistent with the parent activity. The box at the highest level called “top-activity A0” represents the aggregation of all sub-activities.

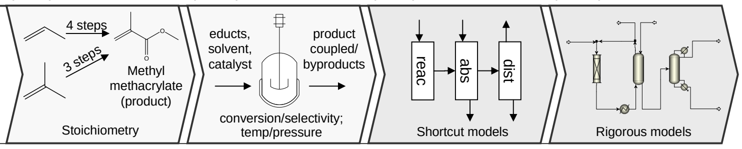
		Process Chemistry I (PC I)	Process Chemistry II (PC II)	Conceptual Design I (CD I)	Conceptual Design II (CD II)
Design stages	Modeled aspects				
	Decision structure	No decision forced	Select some reaction route(s)	Select process option(s) &/or route(s)	Optimize parameters
Design objectives	Economy	Raw material cost + MLI[1] *as proxy*	Raw material cost + ELI[3] *as proxy*	Production cost	Net present value
	Life-cycle environmental impacts	Raw material LCA + MLI *as proxy*	Raw material LCA + ELI *as proxy*	Cradle-to-gate LCA	(updated)
	EHS hazard	ETH-EHS method[2] (substance level)	ETH-EHS method (process level)	(updated)	(updated)
Design Constraints	Technical aspects	e.g. market situation; raw material access; patent situation; blacklist substances	e.g. catalyst activity	e.g. existing know-how; legislation	e.g. equipment specification

Figure 1. Overview of framework: definition of design stages and appropriate modeling approaches as well as evaluation indicators attached to each stage. 1: Mass Loss Indices (MLI) by Heinzle et al. (1998); 2: ETH-EHS method by Koller et al. (2000): 3: Energy Loss Index (ELI) by Sugiyama (2007).

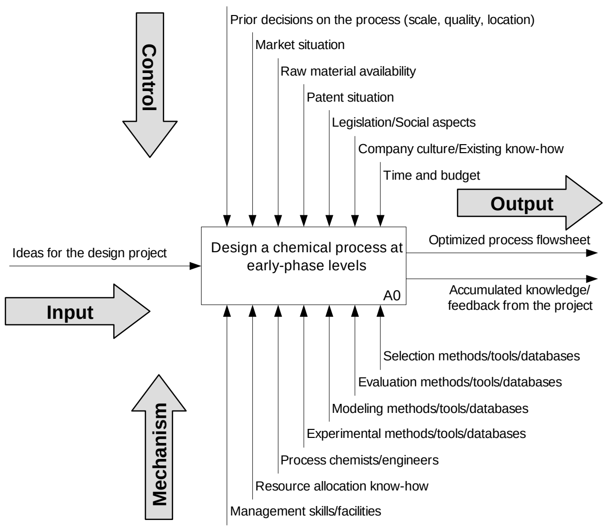


Figure 2. Top-activity A0: Design a chemical process at early-phase levels with syntax of IDEF0.

The viewpoint of this model, i.e. subject of activity boxes, is the manager of a process design project. This manager has the power to make decisions within the framework, i.e., decisions on reaction chemistry and process technology. The overall input is “*Ideas for the design project*” that triggers the whole project. There are seven project-external constraints. “*Prior decisions on the process*” is the necessary constraint of the design regarding production scale, product quality and process location. “*Market situation*”, “*Raw material availability*”, “*Patent situation*”, and “*Legislation/Social aspects*” are enterprise-exogenic constraints, whereas “*Company culture/Existing process*” and “*Time and budget*” are enterprise-endogenic ones. On the side of the mechanism, the “*Management skills/facilities*” and “*Resource allocation know-how*” are defined as general management resources. The remaining mechanism arrows are “*Process chemists/engineers*” and “*Methods/tools/databases*” for experiments, modeling, evaluation and selection. These resources are *available but unallocated* in the beginning of the project, i.e. the manager needs to apply them appropriately during a project. Based on these incoming information and resources, the overall outputs “*Optimized process flowsheet*” and “*Accumulated knowledge/feedback from the project*” are produced. The former output is a direct input for the successive process development phases, e.g., piloting and detailed engineering. The latter can also be used in the following design phase, e.g., as safety warning on a particular part of the process, or can trigger other design projects, e.g., as motivation in improving reaction performance.

3.2. Main-level activities

Figure 3 shows the main-level activities or the decomposition of top-activity A0. Activities A1 and A6 are defined as *managerial activities*, where the design manager receives and allocates design constraints (A1) and resources (A6) appropriately to different design stages. Activities A2 to A5 correspond to four stages in Figure 1. The design-project manager makes individual steps performed by process chemists or engineers that he/she provides in Activity A6. In this activity, these project members are trained to get familiar with methods, data and tools for experiments, modeling and evaluation. Chemists and engineers, when allotted to each design stage, know-how to perform LCA and EHS hazard evaluation. This is new to conventional practice, and this activity A6 determines the quality of EHS-based design. Multiobjective decisions on process alternatives are made step by step in Activities A2 to A5, and “*Optimized process flowsheet*” is finally produced in Activity A5.

Different non-ideal cases of project execution are represented in the iteration loops, e.g., a case when more experimental resources are requested from a design stage. Another particular non-ideal case in process design is the gap between opinions of process chemists and process engineers. For instance, specifications on reaction chemistry considered only by reaction chemists can serve as a severe constraint on designing separation processes. To avoid such a situation, the model shown in Figure 3 defines a direct iteration loop of “*Feedback from process engineers*” between Activities A3 and A4, as a desired exchange of information between chemists and engineers.

3.3. Impact of Design Constraints on Decision-making Characterized by Methyl Methacrylate (MMA) Process Development

Table 1 shows impact of different design constraints on decisions at four design stages. The basis of this analysis is the Japanese MMA process development during the 1970s/80s where several alternative production processes were launched against the dominating acetone cyanohydrin (ACH) process. Project-external constraints listed in the table are more relevant at earlier design stages. At Conceptual Design, decisions on the process at previous stages, i.e. project-internal constraints, becomes also important.

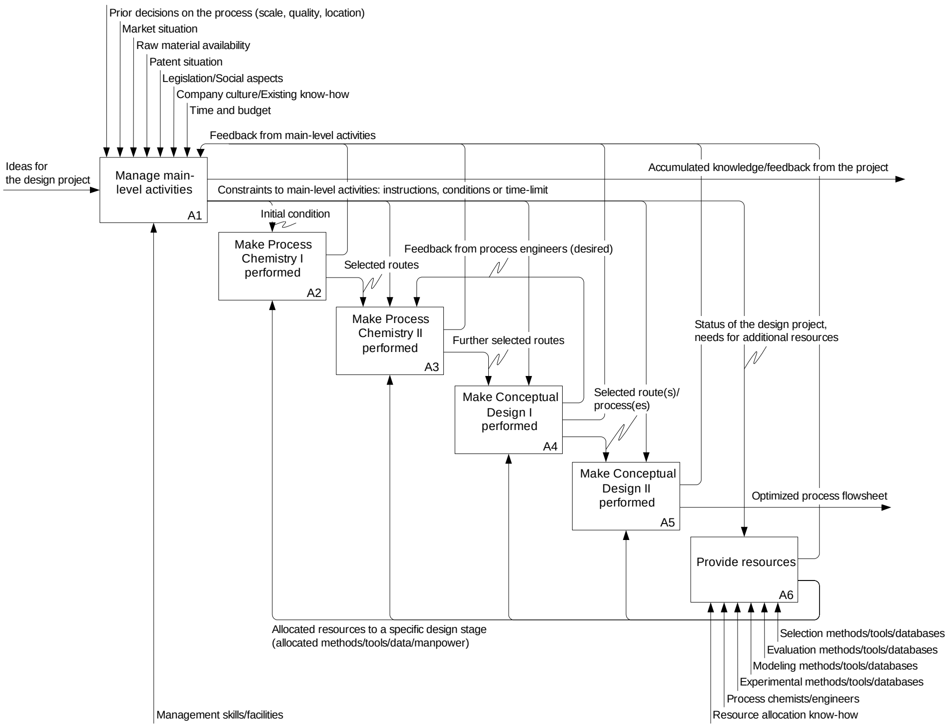


Figure 3: Decomposition of A0 shown in Figure 2.

Table 1. Characterization of project-external design constraints
on the basis of Japanese MMA process development in the 1970s/80s.

Constraints	Effects on decision-making at Process Chemistry (**PC**) or Conceptual Design (**CD**) stages in MMA process development
Market situation	Strong growth in MMA market (**PC**: need to develop a reaction system starting from well-available raw material)
Raw material availability	Limited availability of HCN as a byproduct of acrylonitrile processes (**PC**: hindrance to further develop ACH process starting from HCN)
Patent situation	Competition with domestic MMA producers (**PC**/**CD**: restricted choice for reaction/process technologies)
Legislation/Social aspects	Legislation forbidding MTBE (C4) as a fuel additive (**PC**: motivation to use inexpensive and abundant C4 remaining as a starting material for MMA)
	Pressure against landfilling NH_4HSO_4 (**PC**: motivation to develop H_2SO_4-free reaction system)
Company culture/Existing know-how	Strong motivation in developing catalyst technology (**PC**: potential to purify isobutene as raw material; **CD**: potential to simplify a separation process in sequential oxidation steps)
	Possession of acrylic acid process (**CD**: know-how of operating similar process)

Table 2. Changing characters of decision-making, constraints and mechanisms.

Character	Process Chemistry I/II	Conceptual Design I/II
Decision-making	Highly influential	Fine tuning and optimization
Constraint	Mainly project-external	Both project-external and -internal
Mechanism	General/Wide scoped	Specific/narrow focused

3.4. Summary of Important Know-how for Design-Project Manager

Table 2 summarizes the changing character of decision-making, and mechanisms over design stages. Based on this general summary the following findings are drawn. For making influential decisions at *Process Chemistry* stages, the design-project manager should consider a broad range of project-external constraints and provide wide-scoped resources. For fine-tuning-type decisions at *Conceptual Design* stages, the manager should look for various constraints inside and outside the project, and allocate elaborate mechanisms for specific purposes. This is also the case for EHS assessment of a process. With regard to safety, various categories need to be considered e.g. gas release, fire/explosion, at earlier stages, while at later stages it may be rational to concentrate on a relevant category in a detailed manner, e.g. technical prevention of explosion.

4. Conclusions

We presented an activity model of chemical process design integrating EHS evaluation as a new element with conventional economic and technical considerations. Important know-how is drawn to execute the activity model. IDEF0 modeling can play as a key approach for implementing the concept of integrated process design in practice.

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