Representation of Process Design Rationale for Change Management

Tetsuo Fuchino*[a], Teiji Kitajima[b], and Yukiyasu Shimada[c]
[a] Tokyo Institute of Technology, Tokyo, Japan
[b] Tokyo University of Agriculture and Technology, Tokyo, Japan
[c] National Institute of Occupational Safety and Health, Tokyo, Japan

Abstract: Process design rationale information plays an important role in managing change throughout the lifecycle, especially to judge the change being RIK (replacement in kind) or not. For this purpose, representation of the design rationale should be consistent with the process design process. In this study, the conceptual process design was concerned, and that process design process was clarified by business process model. It was found that the process structure and the operating conditions were designed to prevent the undesired critical phenomena in the conceptual process design stage. Based on such considerations, we proposed to represent the conceptual process design rationale by the causal model of the undesired critical phenomena related to the designed operating conditions of the process modules and/or units associated with the process structure.

Keywords: Design Rationale, Management of Change, Replacement in Kind, Process Conceptual Design

1. INTRODUCTION

The process safety management system intends to realize process safety through the plant life cycle by applying the mechanism of the management of change [1]. However, it isn't exaggerated to express that the defect of the management of change takes the part of the cause for most of the recent major accidents [2].

All the changes except for “replacement in kind” (RIK) to the process, plant, operation and chemicals should be managed through the hazard identification, risk assessment, determination and/or implementation of controls [3]. However, many major accidents, especially occurred in Japan recently, are caused by the changes of which they were judged being RIK. The judgement of whether or not the change is RIK has been made by comparing the change with the results of process and/or plant design. However, this adapts to simple hardware changes, but does not adapt to a little bit more complicated changes such as process operations or process phenomena. This is the cause of accidents caused by changes determined to be RIK. To overcome this problem, it is necessary to judge whether or not the change is RIK based on not the design results but the process design rationales, and the environment for managing the process design rationale information is indispensable.

There exist many researches on the design rationale system [4], and two approaches have been taken for representing the design rationale according to design object; process-oriented and feature-oriented. For industrial design, the former is corrected, and IBIS (Issue Based Information System) has been applied. In IBIS, design activity is expressed by using the relations between three basic elements; i.e. Issue, Position, Argument, which correspond to problem setting, generation of alternatives, and comparison and decision making. The previous studies ([5], [6]) applied IBIS or its equivalent system for the chemical process design. However, the design activity assumed by IBIS and the process design process do not match, so that the represented design rationale by using IBIS cannot be reused in the management of change.

The process is designed step by step through conceptual, basic and detailed stages. We focus on the conceptual process design, which is closely related to the inherently safer process design, here. In the conceptual process design, the process structure and the operating conditions for the respective process modules and/or units composing the process structure are designed to circumvent the constraining

*fuchino@chemeng.titech.ac.jp

critical phenomena such as side reactions, runaway reactions and corrosion, etc. against the required process performance of safety, quality, cost, and productivity. In other words, how to circumvent these constraining critical phenomena against the required process performance by designing the process structure and the operating conditions for respective process module and/or units composing the process structure can be considered as the process design rationale of the conceptual process design stage. Process conceptual design has been carried out implicitly, and the process design rationale has been only the knowledge of the process designer, and until now it has rarely been used as engineering information.

In this study, we explicitly clarify the conceptual process design process, comprehensively derive the critical phenomena that constrain the required process performance, and structure the factors for these phenomena. These structured factors for the critical phenomena are related to the designed operating conditions of the process modules and/or units associated with the process structure. By using these relations, it becomes possible to derive the critical phenomena to be circumvented from the designed operating conditions and/or process structural variables, and also the designed operating conditions and the process structural variables from the constraining critical phenomena against the required process performance. We constructed an environment for managing process design rationale information.

2 CONCEPTUAL PROCESS DESIGN PROCESS

2.1. Process Development and Design

From the view point of lifecycle engineering, three kinds of lifecycles which are process lifecycle, plant lifecycle and product lifecycle, relate to chemical industry. Regarding the production facility design, the first two lifecycles are concerned. In the process lifecycle, process is synthesized, developed, modified and altered finally. On the other hand, the plant lifecycle consists of business steps of design, construction, manufacturing and maintenance, and the design business step is classified into process design and plant design. The process is refined through conceptual design, preliminary design and detailed design stages. The process development in the process lifecycle and the conceptual process design in the plant lifecycle are the point of contact between both lifecycles.

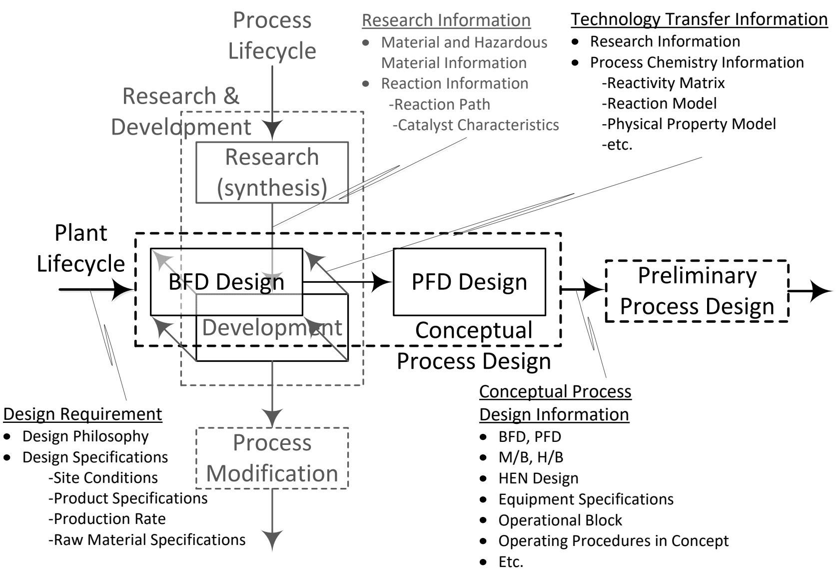

Figure 1: Relation between Process Development and Design

Figure 1 shows relation between the process development stage and the conceptual process design stage in the process and plant lifecycles. The development stage receives the research information including material and reaction information such as the reaction path and catalyst characteristics, and it provides process chemistry information such as reactivity information, reaction models, and physical property models and so on. The research information and process chemistry information are transferred to the conceptual process design stage in the plant lifecycle. On the other hand, the design philosophy and design specifications are given to the conceptual process design stage as the design requirement information, and the conceptual process design information which includes BFD, PFD, heat exchanger network design, operating procedures in concept, and so on, is output. Consequently, the conceptual process design can be considered to be performed on the basis of the design requirement and technology transfer information.

2.2. Business Process Model

In this study, the conceptual process design is investigated on the basis of a generic business process model. To make the generic model, the business process template [7], [8] as shown in Figure 2 is applied across all principal activities. This template configures five types of activities, i.e. "Manage", "Plan", "Do", "Evaluate", and "Provide Resources". The first four types represent the action, plan, do, check of PDCA cycle respectively, and the last one is to prepare information, resources and engineering standards.

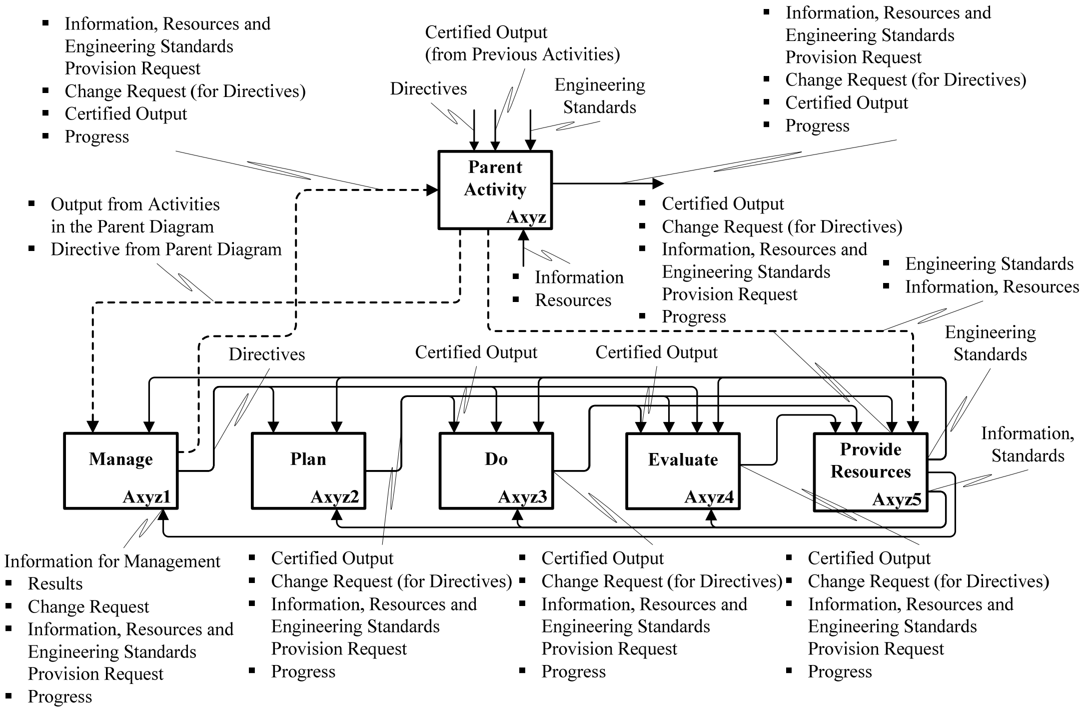

Figure 2: Applied Business Process Template

Figure 3 shows the business process model for conceptual process design which is developed in this study. On the basis of 'Design Requirement' and 'Technology Transfer Information', "A333: Perform Conceptual Process Design" is activated and output 'Conceptual Process Design Information'. The conceptual process design consists of two design levels, i.e. BFD level process design and PFD level process design, and they are performed in this sequence. In Figure 3, "A3333: Perform Block Flow Diagram (BFD) Design" is developed into seven sub-activities of "A33331" to "A33337". First of all, on the basis of the 'Design Requirement' and 'technology Transfer Information', all the critical phenomena that constrain the required process performance and its critical factors for its expression are structured, and operation regions are specified in the "A33332" activity. The structured critical phenomena and its critical factors and specified operation region are informed to the rest of the engineering activities on the "Node-A3333". In the "A33333" activity, operation units are generated, and the process scheme is designed to circumvent the occurrence of the critical phenomena. In the "A33334" activity, the process critical parameters for the designed process scheme to circumvent the critical phenomena are designed for the normal steady state operation. Furthermore, the normal non-steady state operations such as normal startup operation and/or shutdown are considered in the

"A33335" activity. The critical phenomena for the non-steady state operation should be prevented, and the operational block for the block (or circulating) operation is designed.

,

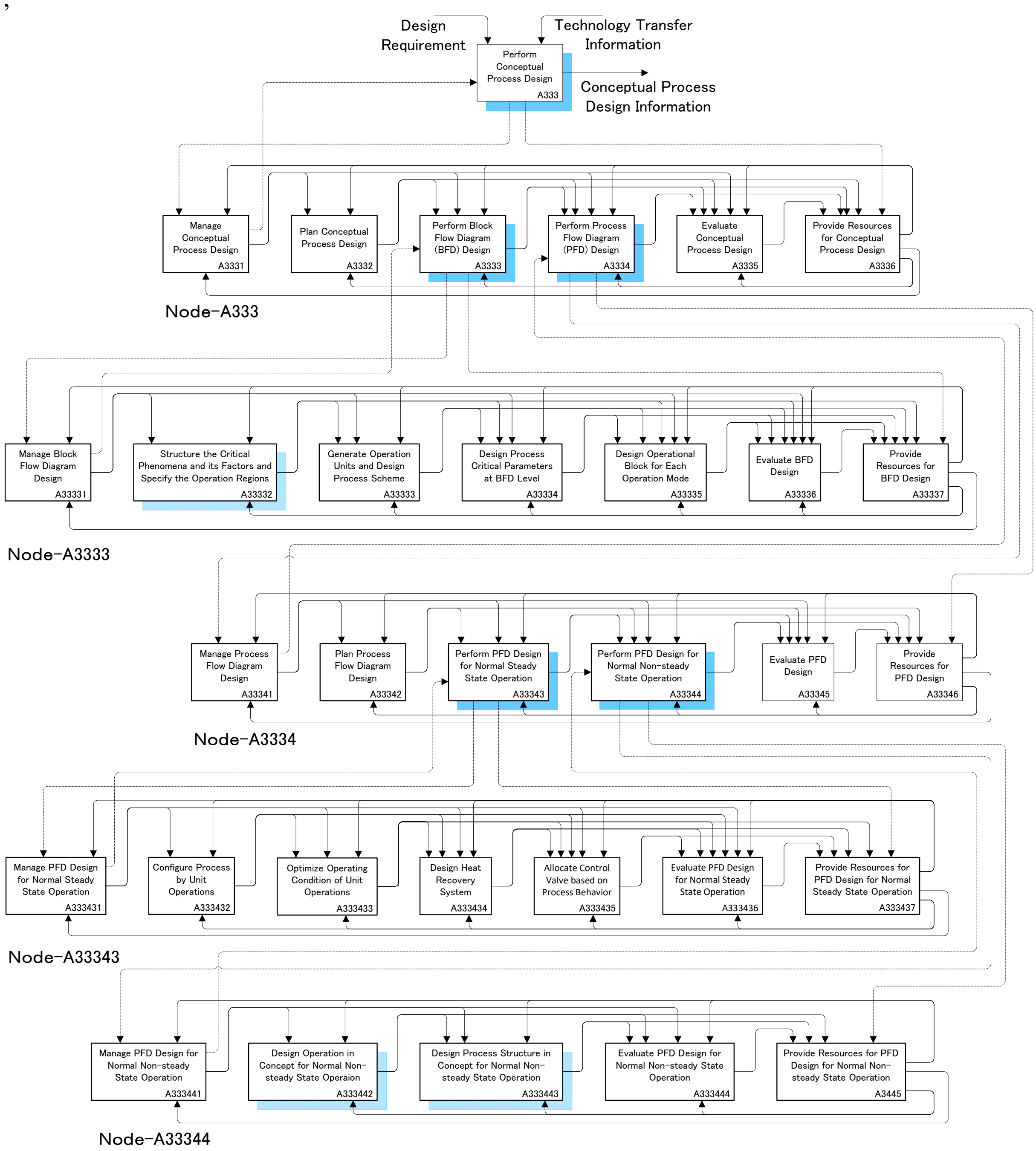

Figure 3: Business Process Model for Conceptual Process Design

All the result of the BFD design output from "A3333" is informed to the "A3334: Perform Process Flow Diagram (PFD) Design". The PFD design can be considered as the PFD level design for the normal steady state operation and for normal non-steady operation. In the "A33343: Perform PFD Design for Normal Steady State Operation" activity, the process units designed at the BFD level design in the "A33333" activity are converted into unit operations, in the "A333432" activity, and the operating conditions of the unit operations are optimized to realize the process critical parameters designed at the BFD level design in the "A33334", in the "A333433" activity. The heat recovery system including heat exchanger network respective for the operational block designed at the BFD level design in the "A33335" activity is designed in the "A333434" activity, and the control valve allocation is designed under the consideration of the operational region specified at the BFD design in the “A33332” activity, in the “A333435” activity. In addition to the PFD design for the normal steady state operation, operational design for normal non-steady state operation is performed in the “A33344: Perform PFD Design for Normal Non-steady State Operation” activity. The operation in concept for normal non-steady state operation for respective for the operational block designed at the BFD level process design in the “A33335” activity, in the “A333442” activity, and the necessary process structure for the normal non-steady state operation is designed in “A333443: Design Process Structure in Concept for Normal Non-steady State Operation” activity.

In Figure 3, the boxes with a blue shadow represent the activities developed in the sub-activities in this study. However, the development of thinly shaded activities into sub-activities is omitted in this paper.

2.3 Conceptual Structure of Design Rationale Information

In summery for the business process for the conceptual process design, the critical phenomena and their factors are structured, and the process scheme, process parameters and the operational block for normal non-steady state operation in the BFD level are designed to circumvent the critical phenomena, in the “A3333: Perform BFD Design”. The process structure, operating conditions and operation are detailed from the BFD level design to the PFD level to prevent the critical phenomena, in the “A3334: Perform PFD Design” activity. Therefore, the design rationale information in the conceptual process design can be interpreted as representing how the design for not expressing the critical phenomena was performed in the BFD level and the PFD level design.

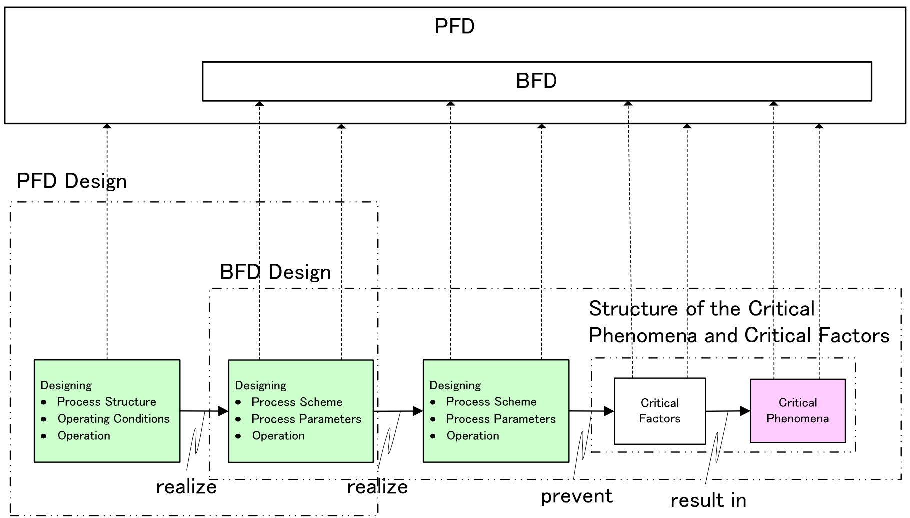

Figure 4: Design Rationale Structure

In this study, the critical phenomena, the critical factors, BFD designing, PFD designing are considered as information objects, and the relations between these objects are defined by connecting these objects using associations such as ‘result in’, ‘prevent’, ‘realize’ and so on to express the conceptual process design rationale circumventing occurrence of the critical phenomena, as shown in Figure 4. Furthermore, this design rationale representation is related to the BFD and/or PFD, and then it will be possible to apply for judging of RIK in change management.

3. APLICATION FOR BFD DESIGN

3.1. Design Requirement and Technology Transfer Information

In this study, dimethyl ether (DME) production process by using crude methanol (Me-OH) as raw material assuming from the crude methanol separator locating at the synthesis loop of methanol process is used to illustrate proposing representation of the conceptual process design rationale. However, in this manuscript, the PFD design and its design rationale representation is omitted from the limitation of the space. A part of the design requirement set up here is as shown in Table 1, and the technology transfer information applied here is as shown in Table 2.

Table 1: A Part of Design Requirement

Item	Specification
Feed Me-OH	75mol % Me-OH+25mol% Water
	30[C], 1.013[bar] Liquid(@BL)
	Impurity: containing a saturated amount of CO_2
Product	99.5 wt% DME (+Me-OH)
	46[C], 11.4[bar] Liquid (@BL)
Production rate	1500 (t/day)
Utilities	Heating Steam: 12[bar] saturated (=190[C])
	Cooling Water: 30[C] supply, 38[C] return
	LP high purity N_2 available
Waste Water	99wt% (less than 1wt% of Me-OH)

Table 2: Technology Transfer Information

Category	Item	Transferred Information
Main Reaction	Thermochemical equation	$2CH_3\text{-}OH(g) \rightarrow CH_3\text{-}O\text{-}CH_3(g)+H_2O(g)+11770$[kJ/kmol]
	Catalyst	Gamma Alumina
	Catalyst Deactivation	Condensed Water
	Normal Operating Region	250[C] to 400[C] without no side reaction
	Kinetic Model	$-r_M=k_0\exp(-Ea/RT)p_{Me\text{-}OH}-k'_0\exp(-E'_a/RT)p_W$ r_M [kmol/m^{3}cat-h], $P_{Me\text{-}OH}$[kPa], P_W[kPa], $k_0=1.21\times10^6$[kmol/m^{3}cat-h-kPa], $E_a=80.48\times10^3$[kJ/kmol] $k'_0=5.07\times108$[kmol/m^{3}cat-h-kPa], $E'_a=11.83\times10^4$[kJ/kmol] T[K], R=8.314[kJ/K-kmol]
	Equilibrium Model	Refer to Ghavipour, M. and R,M.Behbahani, J of Ind. Eng. Chem., 20,1941-1951(2014)
Side Reactions	Me-Oh reaction	Me-OH ⇔ $2H_2$ + CO, Me-OH ⇔$3H_2$+CO_2 (less than 250[C])
	Olefin reaction	nDME ⇔$2C_nH_{2n}$ + n H_2O (more than 400[C])
Corrosion	SUS	Deposits under carbonate pitting
	CS	Deposits under carbonate uniform corrosion
Physical properties estimating equation		PRSV

3.2. Structuring Critical Phenomena and their Critical Factors

For the first step the critical phenomena and their critical factors are structured. On the basis of Table 2, it is found that the critical phenomena to be circumvented are catalyst deactivation, methanol reaction, olefin reaction, and corrosion. These critical phenomena and their critical factors are structured as shown in Figure 5(a) to 5(d). Where, the critical factors painted with dark blue color indicate that they cannot be circumvented by process design. For example, existence of DME for the olefin reaction in the DME reactor as shown in Figure 5(c) cannot be circumvented by process design. For corrosion and/or pitting under deposit as shown in Figure 5(d), existence of deposit is critical, and where deposit sediments depends on the plant structural property. However it is designed in the preliminary plant design and it cannot be controlled in the conceptual process design. Furthermore, very small amount of water cannot be controlled originally, and the material for construction (CS or SUS) will be decided in the conceptual plant design, which material is to be selected cannot be decided in the BFD level design.

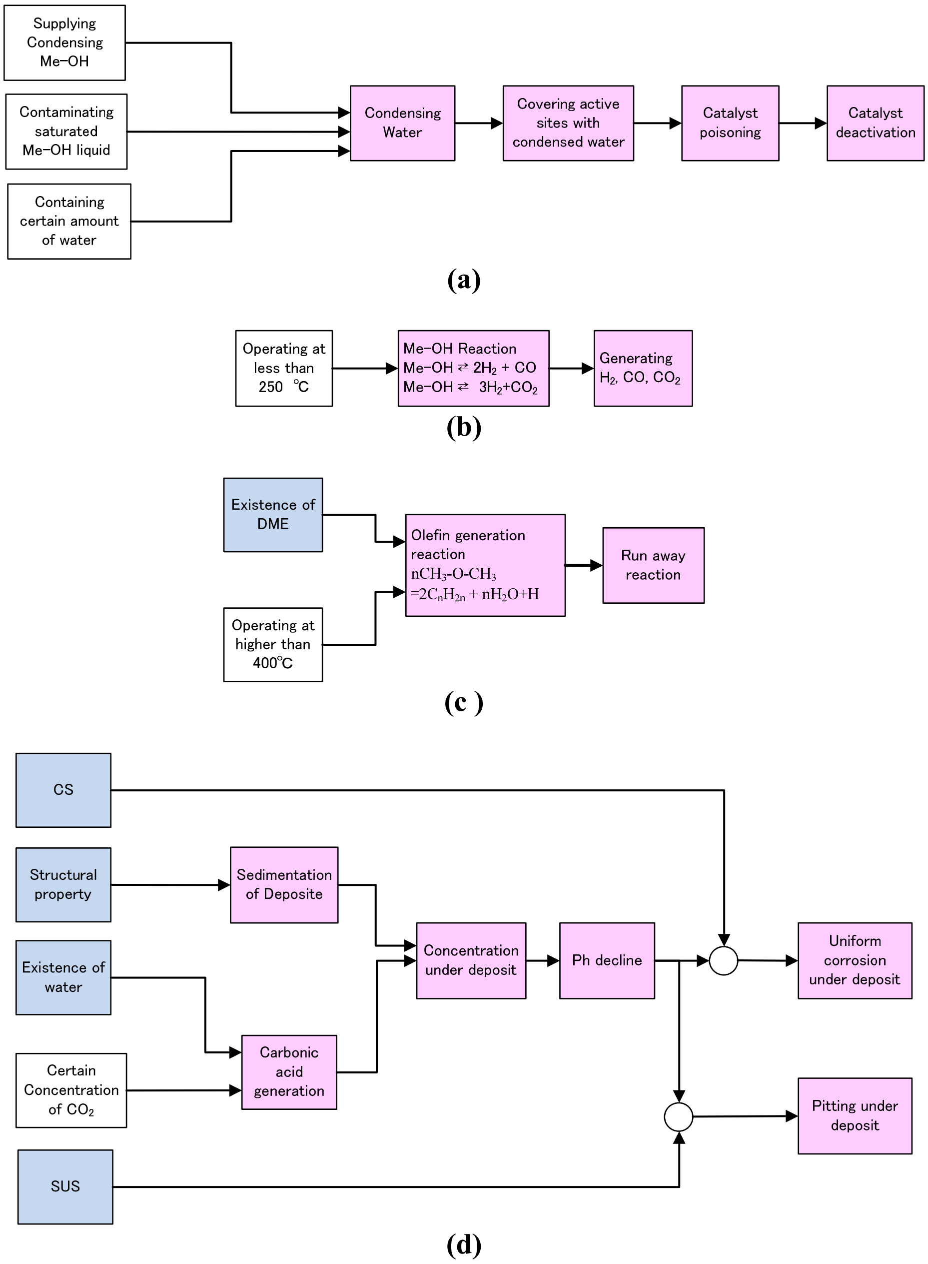

Figure 5: Structure of Critical Phenomena and their Factors

3.3. Process Schematic Design

In the next step, process scheme to circumvent the occurrence of the critical phenomena mentioned above is designed. In designing process schemes, quantitative consideration is not necessarily required rather qualitative analysis such as existence of critical components and operation with sufficient margin from the critical conditions is important, in many cases, and process scheme is to be constructed from the 'Feed Me-OH', here.

In the 'Feed Me-OH', about 25mol% water and 0.5mol% CO_2 are included and there is a possibility of the uniform corrosion or pitting under deposit as shown in Figure 5(d). To reduce this possibility, removing CO_2 at the upstream of the process is preferable so that "CO_2 Stripper" is configured firstly. After CO_2 is removed, the remaining fluid contains about 75mol% methanol and about 25mol% water. In order to avoid the catalyst deactivation shown in Figure 5(a), water is separated from the reactor feed fluid. For this purpose, "Me-OH/H_2O Distillate" is configured next, as shown in Figure 6.

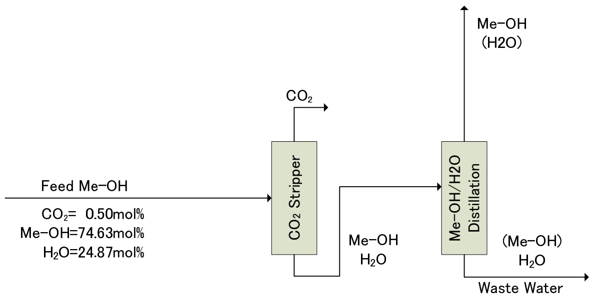

Figure 6: Process Scheme up to "Me-OH/H_2O Distillation"

The distillate of the "Me-OH/H_2O Distillate" containing high concentration of Me-OH with small amount of water is liquid, but the superheated methanol at more than 250 Cels. is necessary to be supplied to the reactor. For that purpose, after the distillate is pressurized to the reactor operating pressure, it is heated up to the boiling point with "Me-OH Heater", to the dew point with "Me-OH Boiler", and to 250 Cels. or more with "Me-OH SH(Supper Heater)". Since Table 2 shows that the DME synthesis reaction is an equilibrium one, the "Me-OH SH" should be designed as a heat exchanger with the reactor outlet stream, and to control the inlet temperature of the reactor, the bypass of "Me-OH SH" is to be used. As shown in Figure 5(a), in order to avoid the risk of condensation of water on the catalyst, it is desirable not to use saturated methanol vapor but superheated methanol vapor as the bypass fluid for temperature control, and "Me-OH SH" is divided into "Me-OH SH Low" and "Me-OH SH High", and a bypass is provided to "Me-OH SH High" as shown in Figure 7.

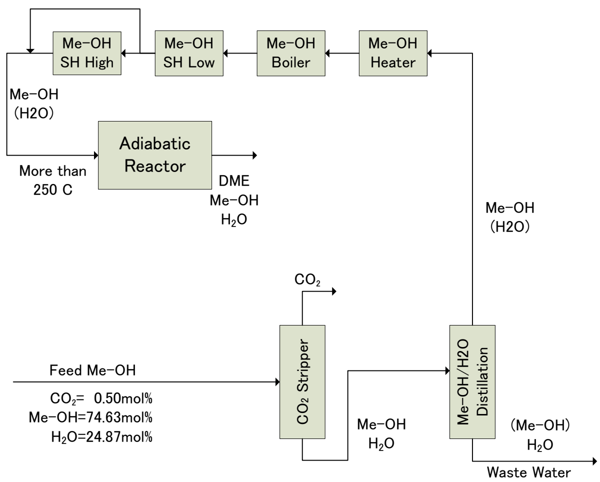

Figure 7: Process Scheme up to DME Reactor

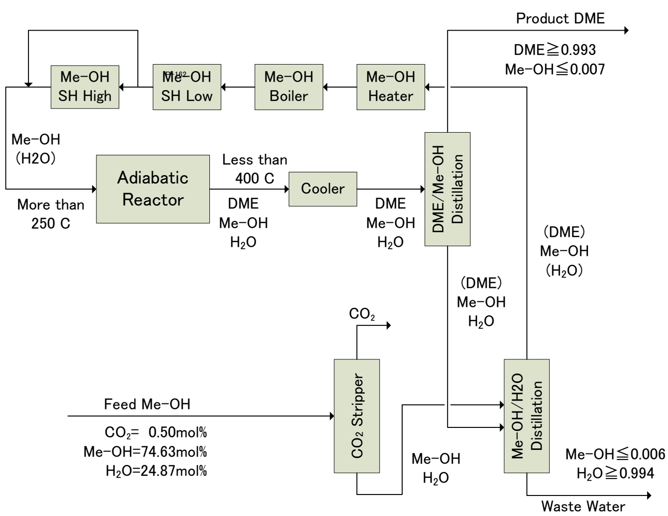

Figure 8: DME Process Scheme

Methanol vapor superheated to 250 Cels. or higher is sent to the DME adiabatic reactor system and DME is synthesized under the operating condition of 400 Cels. or less so as not to cause runaway reaction shown in Figure 5(c). The reactor outlet includes DME, Me-OH and water in the order of vapor pressure. In order to separate the product DME by a distillation column, the reactor outlet fluid is cooled to a saturated liquid and then fed to the "DME/Me-OH Distillate". In the "DME/Me-OH Distillate", the product DEM is refined so as to satisfy the product specification shown in Table 1, and the bottoms contain a very small amount of DME, unreacted Me-OH, and byproduct water. In order to recycle unreacted methanol, the by-product water is separated by distillation. In order to integrate the distillation of the same cut point, the bottom fluid of "DME/Me-OH Distillate" is introduced to "ME-OH/H_2O Distillate". However, because the water concentration in the raw material is different from the water concentration in the bottom of the "DME/Me-OH Distillate", it is decided to design twin feed column for stable operation in startup. As described above, the process scheme shown in Figure 8 can be designed by step-by-step configuring process units so as to avoid occurrence of critical phenomena from 'Feed Me-OH'.

3.4. Parameter Design for BFD Level Design

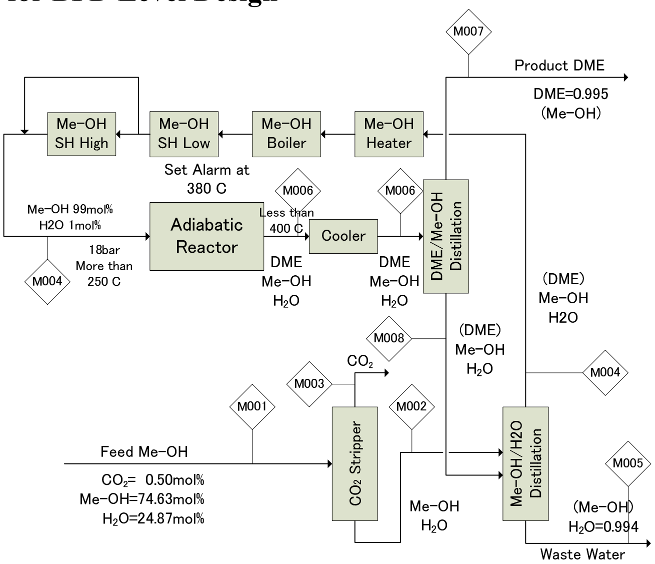

Figure 9: BFD for the Steady State Operation

In the next step, for critical process schemes, the critical process parameters to avoid the occurrence of critical phenomena are to be designed, as shown in Figure 9. To prevent olefin generation resulting run away reaction shown in Figure 5(c), the maximum operation temperature is set to 380 Cels. lower than 400 Cels.. Furthermore, in order to reduce the possibility of catalyst deactivation shown in Figure 5 (a), it is necessary that the reactor inlet fluid is necessarily superheated methanol vapor. The maximum allowable water concentration in the reactor inlet stream is fixed to 1 mol%, and the operating pressure of the reactor is set at 18 bar so that a sufficient temperature difference can be obtained between the reactor inlet temperature and the saturated temperature of the reactor inlet fluid. Although, the fluid numbers are attached in Figure 9, the material balance table is omitted in this paper.

3.5. Operational Block Design

At the final of the BFD level design, the operational block for normal non-steady (especially start-up) operation is designed. The startup of the unit differs somewhat depending on whether the target unit is a unit handling liquid or a unit handling gas, but in general it is done by displacing the substances, boosting, raising temperature, and connecting with another unit. In addition, some units may be operated independently as in a distillation unit, others may require a circulating operation together with other units, such as a heat exchange unit. The operational block to be designed here is a group of units that perform stable operation as an intermediate state of the startup for the whole process.

The conceptual startup operations for deriving operational blocks must be designed not to include the operational factors that derive undesirable critical phenomena, as same as the normal steady state operation in process scheme design. In the DME process design case considering here, it is obvious that the start-up of the reaction unit is critical, and it is required to design the operation so as to avoid the generation of condensed water on the catalyst in the replacement, boosting, temperature rising process from Figure 5. For that purpose, the reactor unit is made to be independent as an operational block assuming the hot nitrogen circulation system for raising the pressure and temperature, and the other operational blocks are as shown in Figure 10 by different colors.

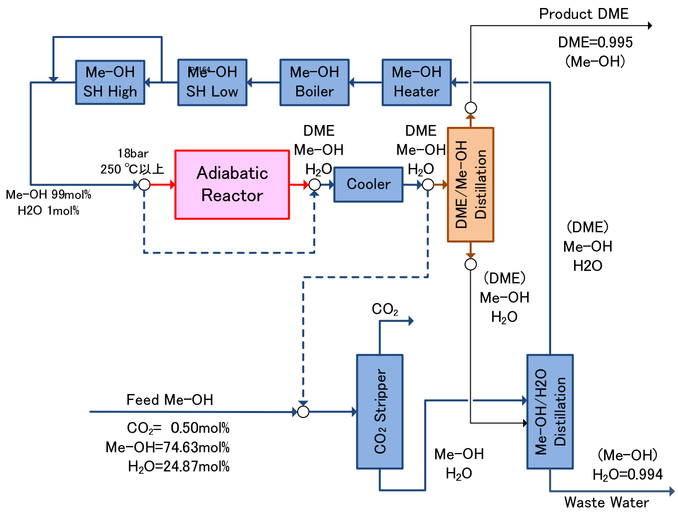

Figure 10: Operational Blocks

3.6. Representing Design Rationale

In designing BFD, the functions of process units to prevent the occurrence of the critical phenomena are considered along with the material flow and/or process flow. On the other hand, in capturing the design rationale, from the critical factor of respective critical phenomenon as shown in Figure 5, how the critical process condition was prevented by BFD design is to be tracked back according to the design rationale structure as shown in Figure 4.

The catalyst deactivation in normal steady state operation is concerned. The direct cause of the phenomenon is existence of condensed water and its critical factors or critical conditions are "Contaminating saturated Me-OH liquid", "Supplying Condensing Me-OH" and "Containing certain amount of water" as shown in Figure 5(a). To avoid the situation of "Contaminating saturated Me-OH liquid", "Super-heated Me-OH vapor for controlling reactor inlet temperature" was considered, "Low temperature super-heated Me-OH" was required and "Low temperature Me-OH super heater" was configured in the BFD design. Each action done in the BFD design is related to the BFD; i.e., "Low temperature Me-OH super heater" connecting with "Me-OH SH low", "Super-heated Me-OH vapor for controlling reactor inlet temperature" connecting with "Me-OH SH low" outlet line and "Super-heated Me-OH vapor for controlling reactor inlet temperature" connecting with "Me-OH SH High" bypass line, here as shown in Figure 11. Contrary to capturing the design rationale information, if the tracing forward to the critical phenomenon is performed from these connected points in the BFD; i.e. from "Me-OH SH low", from "Me-OH SH low" outlet line and from "Me-OH SH High" bypass line, then the necessity of "Me-OH SH low", necessary condition of "Me-OH SH low" outlet line and the role of the "Me-OH SH High" bypass line" would be able to be retrieved.

Similarly for other critical factors of the catalyst deactivation in normal steady state operation, to avoid the situation of "Supplying Condensing Me-OH", "Sufficient delta temperature between supply temperature and dew point" was considered, "Setting dew point of Me-OH vapor around 160℃ (250℃-90℃)" was decided, and "Designing operating pressure of reaction" was done in BFD design.

To avoid the situation of "Containing certain amount of water", "Separating water from Raw material" was considered, and "Configure Me-OH/H2O Distillation before Reactor" was done in BFD design. Each action done in the BFD design is related to the BFD as shown in Figure 11, Contrary to capturing the design rationale information, if the tracing forward to the critical phenomenon is performed from these connected points in the BFD, the reason for the BFD design would be able to be retrieved.

The run-away reaction in normal steady state operation is concerned. As same as above mentioned manner, to avoid the run-away reaction, what was done in the BFD design is considered. The BFD design for preventing the critical phenomenon is related to the BFD, and the representation of BFD design rationale to avoid run-away reaction in normal steady state operation as shown in Figure 12 can be made.

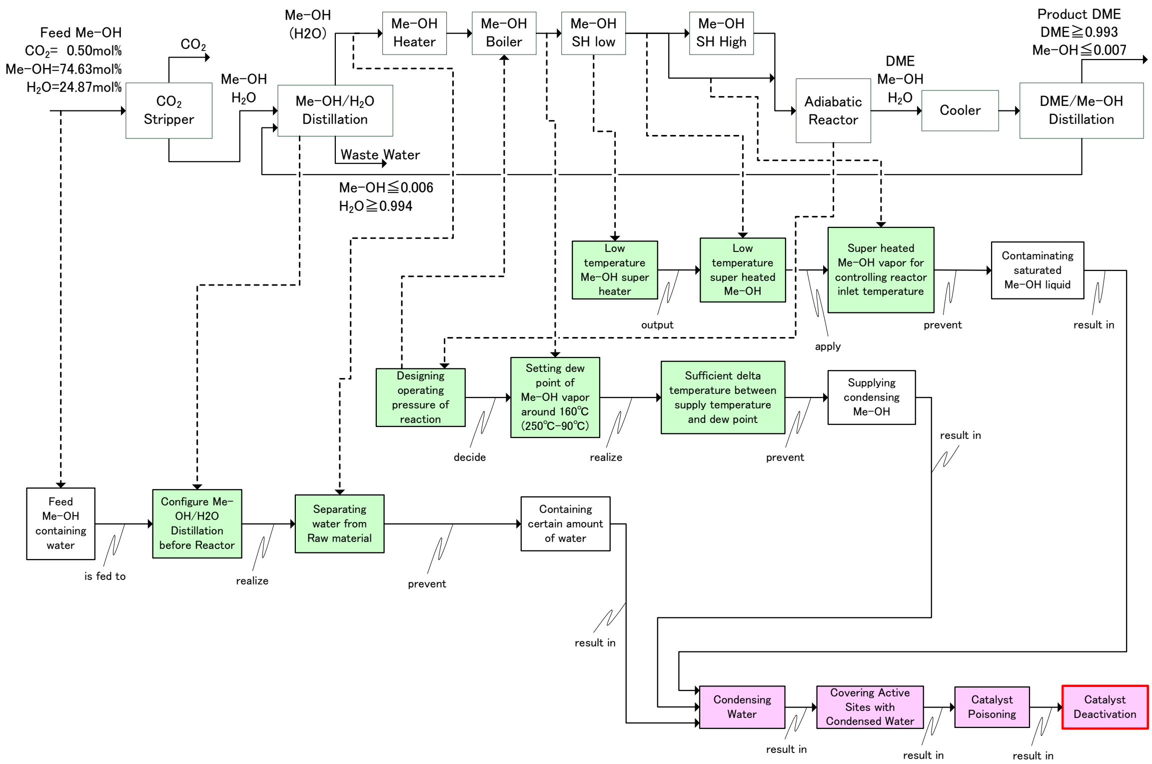

Figure 11: Representation of BFD Design Rationale to Avoid Catalyst Deactivation in Normal Steady State Operation.

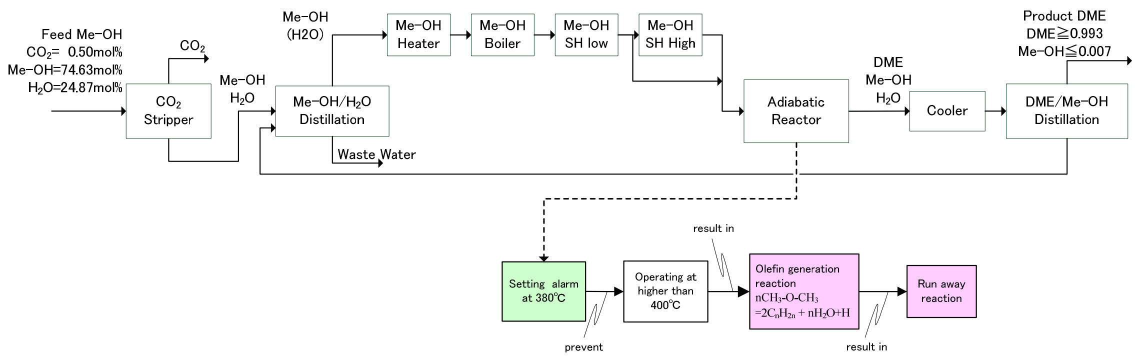

Figure 12: Representation of BFD Design Rationale to Avoid Run-away Reaction in Normal Steady State Operation.

In this manuscript, concerning to the other critical phenomena for the normal steady stage operation, and the all the critical phenomenon for the normal non-steady state operation, representations of the BFD design are omitted for the limitation of the space.

4. CONCLUSION

Many of the accidents in the chemical industry are due to inadequacies in change management, especially accidents due to erroneous judgment on RIK are becoming noticeable in Japan recently. To avoid this problem, it is necessary to judge whether or not the changes are RIKs based on the design rationales, not based on the design results, and an engineering environment for utilizing the design rational information throughout the life cycle is required. In this study, the conceptual process design stage which is most closely related to the inherently safer process design is focused attention to, and a method to represent the captured process design rationale information is developed.

In order to define what is the process design rationale at the conceptual design stage, we developed the IDEF0 business process model explicitly expressing the concept process design process. On the basis of the business process model, the critical phenomena and their factors are structured, and the process scheme, process parameters and the operational block for normal non-steady state operation in the BFD level are designed to circumvent the critical phenomena. The process structure, operating conditions and operation are detailed from the BFD level design to the PFD level to prevent the critical phenomena. Therefore, the design rationale information in the conceptual process design can be interpreted as representing how the design for not expressing the critical phenomena was performed in the BFD level and the PFD level design.

In this study, BFD and PFD designing processes to circumvent the critical phenomena and factors were considered as information objects, and were related to the BFD and/or PFD using associations, to represent the conceptual process design rationale. The effectiveness of the developed design rationale representation, DME process design case from crude methanol was applied.

Acknowledgements

This work was supported by JSPS KAKENHI Grant Numbers JP17K01316, JP16K06843. The authors are grateful to following experts on process engineering: Dr. Koichi Iwakabe (Mitsui Chemicals), Mr. Kensuke Iuchi (SCEJ Safety), Mr. Kuniharu Ueda (Chiyoda Corporation), Mr. Shoichiro Yori (former Mitsubishi Chemical) for helpful discussions.

References

[1] Center for Chemical Process Safety (CCPS), "Guidelines for Risk Based Process Safety," John Wiley & Sons, 2007, Hoboken.
[2] U.S. Chemical Safety Board (CSB); www.csb.gov/.
[3] Center for Chemical Process Safety (CCPS), "Guidelines for Guidelines for the Management of Change," John Wiley & Sons, 2008, Hoboken.
[4] W. C. Regli, X. Hu, M. Atwood and W. Sun, "A Survey of Design Rationale Systems, Approach, Representation, Capture and Retrieval," Engineering with Computers, 16, PP. 209-235, (2000).
[5] R. Banares-Alcantara, and J. M. P King, "Design Support Systems for Process Engineering iii – Design Rationale as a Requirement for Effective Support," Comput. and Chem. Eng., 21, PP 263-276 (1997).
[6] P. W. H. Chung and R. Goodwin, "An Integrated Approach to Representing and Accessing Design Rationale," Eng. Applic of Artif. Intell., 11, PP 149-159 (1999).
[7] Tetsuo Fuchino, Kazuhiro Takeda, Yukiyasu Shimada and Atsushi Aoyama, "Business Process Model Based Incident Investigation for Process Saety Leading Metrics," J. of Chem. Eng. of Japan, 48, PP. 626-633 (2015).
[8] Tetsuo Fuchino, Yukiyasu Shimada, Teiji Kitajima,Kazuhiro Takeda and Masazumi Miyazawa, "Framework to Manage Engineering Technology for Plant Maintenance," J. of Chem. Eng. of Japan, 48, PP. 662-669 (2015).