

K3 bahan kimia essay



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Diss. ETHNo. 17186 Decision-making Framework for Chemical Process Design Including Different Stages of Environmental, Health and Safety (EHS) Assessment A dissertation submitted to ETH Zurich for the Doctor of Sciences degree (Dr. of ETH sc. Zurich) presented by HIROKAZU SUGIYAMA Master of Engineering, The University of Tokyo born 30. 09. 1978 citizen of Japan accepted on the recommendation of Prof. Dr. Konrad Hungerbuhler, examiner Prof. Dr. Masahiko Prof. Dr. Alexander Hirao, co-examiner Wokaun, co-examiner 2007 Acknowledgement This thesis is the result of almost four years of research at the Safety and Environmental

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Harald and Roland who shared the office G136 but also the ups and downs of research with me. I am particularly powerful thankful to Prisca for her IT friendly help in all administrative issues and to Erol for his and troubleshooting. My great appreciation belongs experiences and discussions as Andrej M, Levente Andrej S who shared many members of the process group, also to Christian, Martin, Stefanie and Matthew who helped I would like to me through their environmental expertise. and dearly thank all members of our group for all the magnificent days nights including SOLA, bike-tours, ski-weekends, and Toggele. ove, support My deepest appreciation and gratitude is reserved for and their my parents, for all their unwavering faith in me. Zurich, May 2007 Hirokazu Sugiyama Abstract In recent years, chemical a core companies have adopted the concept of sustainable development as business value. The basis of various decision-making in their entire business has been extended to cover aspects, especially non-monetary issues, the in addition to economic performance. sustainability This thesis From the viewpoint of chemical engineering, big challenge is to integrate criteria early a in process design for as design objectives. rocess presents framework of chemical design, which incorporates multi objective consideration economic, and environmental, health and safety (EHS) different aspects in decision-making over design stages. With a focus on the early design according phase, to four stages, Process Chemistry as a I/II and Conceptual Design I/II, modeling are defined the available information basis

for process and assessment. For each defined to economy, stage, appropriate modeling methods and evaluation indicators with respect lifethe cycle environmental impacts, EHS hazard and technical aspects are selected. Based at on evaluation esults, multi objective decision-making is performed systematically the each stage. A case study on methyl methacrylate (MMA) production study, which processes is applied throughout routes this thesis. This case uniquely offers 17 potential synthesis and various types of chemicals in the reaction network, is applied for demonstrating the framework. Starting with 17 an possible synthesis routes, optimized inferior routes are eliminated step-by-step and at is the last stage flowsheet of the route with the best multi objective case performance produced. observing Another part of the the evaluation study alidates decisions made within the framework over by profile of six routes when different stages. Most routes are correctly selected at earlier routes. cause design stages are compared are to the detailed assessment results of all six Several factors identified that to available in detail only at later stages, and which significant updates the results. Among these are the magnitude of energy consumption, EHS investment cost, the amount of loss of valuable of materials, and the monetary and a implications newly considered substances. For these parameters there is measures need to have better estimates in the form of proxy lready at earlier stages. Two what-if analyses are presented to examine how the assessment results are change when the different process options or evaluation settings considered. One analysis investigates l impact of specifying process options at the detailed conceptual design stage, i. e. the rigorous flowsheeting stage, economy and and the effect of choosing different setups in evaluation for the criteria of The MMA case life-cycle

environmental impacts. options study quantitatively reveals that, among different types of process and evaluation settings, specifying alternatives in reaction chemistry, e. . synthesis path, has the most significant impact. This result confirms the importance layouts of reliable proxy indicators for for different forecasting unknown aspects, e. g. detailed process synthesis paths, in early design stages. the As the second part of the assessment what-if analysis, Several and impact of method selection can on the EHS results is presented. simple methods that The be applied in the early phases are compared qualitatively on quantitatively. assessment results change significantly depending The overall the hazard evaluation method in the applied in each of the EHS aspects. scope, iscrepancy mathematical result stems from the differences in the manner considered mass parameters, formulation, and especially own that process no information is treated. However, each method has its merit of one background and there is unique or method a over the other in any of the EHS aspects. The appropriate simplicity can degree only of detail of method considering early design phases where it be applied is the characteristic that separates the methods. Finally, the developed framework is serves as represented by using a a standardized activity modeling use technique, IDEFO, enables the which of blueprint f the business model. The same of IDEFO The description complex activities in detail and at the time transparently. activity model is defined for the four I to design stages as of the framework, i. e. from Process Chemistry Conceptual Design II, the activities to which appropriate case instructions and are resources are provided by as a project manager. Findings in the from the studies included in this activity model, know-how to be exploited design. traditional economic criteria with In summary, this dissertation demonstrates

how to integrate non-conventional environment, health and safety criteria in decision-making over different the stages of process design. This systematization will support chemical industry to undergo paradigm shift towards sustainability in developing processes. 11 Zusammenfassung

Während der letzten als Jahre hat die chemische Die Industrie Basis für das die Konzept der nachhaltigen Entwicklung Kerngeschäft eingeführt. um Entscheidungsfindung besonders im gesamten Geschäftsbetrieb wurde finanzielle verschiedene zu Aspekte erweitert, nicht→ Gesichtspunkte des wurden zusätzlich den ökonomischen Kriterien erfasst. Aus der die grosse von Perspektive Chemieingenieurwesens liegt in Herausforderung ahrend in der die Prozessentwicklung Entwicklungsziele. Diese Dissertation welches die der frühen Integration Nachhaltigkeitskriterien präsentiert ein Rahmenkonzept Zielgrossen für die aus Entwicklung chemische Prozesse, aus Berücksichtigung mehrere Wirtschaft, sowie den Bereichen Umwelt, Gesundheit und Sicherheit (UGS) während verschiedener Entwicklungsstufen für eine Entscheidungsfindung beinhaltet. Mit einem Schwerpunkt auf der frühen I/II Planungsphase den werden die vier Stufen Process Chemistry eine Stufe I/II und Conceptual Design entsprechend und verfügbaren definiert. Informationen als Basis für die

Prozessmodellierung Bewertung und UGS Für jede definierte werden entsprechende Modellierungsmethoden ökologischen Auf der Bewertungsindikatoren Gefahren und bezüglich Wirtschaftlichkeit, Belastungen, Grundlage in technischen wird Aspekten die ausgewählt. dieser Stufe Abschätzungsergebnisse multi-kriterielle Entscheidungsfindung jeder systematisch durchgeführt. Die Produktion Dissertation von

Methylmethacrylat (MMA) Diese wird als Fallstudie während der ganzen 17 verwendet. Fallstudie, welche um potentielle Synthesewege zu und verschiedene Chemikalien aufweist, wird benutzt, werden das Rahmenkonzept demonstrieren. o Ausgehend von 17 Synthesewegen minderwertige Wege systematisch eliminiert, für den dass in der letzten Stufe ein multi-kriteriellen optimiertes Flussdiagramm Syntheseweg mit der besten Leistung erhalten wird. Ein anderer Teil der Fallstudie validiert während des Entwicklungsweges Evaluationsprofile Synthesewege detaillierten Detail nur von gemachte Entscheidungen durch Beobachtung der sechs Synthesewegen über verschiedene Stufen. Die meisten der 6 wurden in früheren Stufen korrekt ausgewählt, wie der Vergleich mit den im Abschätzungsergebnissen zeigt. verfügbar Mehrere Faktoren wurden identifiziert, die er in späteren Stufen sind und die grosse Veränderungen Ergebnisse verursachen. Solche Faktoren sind das Ausmass des Energieverbrauchs, Investitionskosten, in der Verlust von Wertstoffen, sowie finanzielle Auswirkungen und UGS-Einfluss von neu berücksichtigen eine bessere Substanzen. Diese Parameter sollten deshalb schon in früheren Stufen für als Einschätzung Proxyindikatoren verfügbar präsentiert um sein. Zwei wenn what-if Analysen unterschiedliche werden abzuschätzen wie sich die Ergebnisse ändern Prozessoptionen oder Bewertungskriterien berücksichtigt werden. Eine d. h. in sowie der beiden der die Analysen erforscht in der detaillierten die konzeptionellen Entwicklungsstufe, von rigorosen Flowsheeting Stufe, Folgen der Wahl von Auswirkungen bestimmten Prozessoptionen verschiedenen Bewertungskriterien bezüglich quantitativ Wirtschaftlichkeit und Umweltbelastung. Typen von Die MMA Fallstudie lässt und den erkennen dass unter verschiedenen Prozessoptionen

Synthesechemie für verlässliche Bewertungskriterien großen Einfluss in die Spezifizierung dieser Alternativen bestärkt die bezüglich Wichtigkeit Aspekte hat. Ergebnisse um Indikatoren z. B. frühen Entwicklungsstufen unbekannte verschiedene abzuschätzen, wie detaillierte Prozess-Auslegung für Synthesewege. Als zweiter Teil der what-if Analyse präsentiert, wird die Einwirkung einfache der Methoden-Wahl auf die UGS

Abschätzungsergebnisse Planungsphase Mehrere Methoden, die in der frühen benutzt werden ändern können, werden qualitativ und quantitativ verglichen. Die sich bedeutsam Abschätzungsergebnisse abhängig Die von der verwendeten UGS Bewertungs-Methode bezüglich stammt von aller UGS Aspekte. allgemeine Abweichung von im Resultat Unterschieden des und besonders berücksichtigten Bereiches, von Parametern, mathematischen Formulierungen der Art, wie Informationen bezüglich es Masse behandelt werden. Jede Methode hat Vorteil einer Methode an jedoch ihren eigenen Hintergrund und gibt keinen eindeutigen gegenüber den anderen. Die entsprechende Einfachheit oder der Grad Genauigkeit einer Methode in Bezug auf die frühe „ Planungsphase“, ist die einzige charakteristische Größe mit welcher die Methoden unterschieden werden können. Zum Schluss wird das entwickelte Rahmenkonzept mittels einer standardisierten Aktivitäts Modellierungs Technik, IDEFO, präsentiert, Die die als ein Entwurf des Business Modells dient. die detaillierte Das Nutzung von IDEFO ermöglicht und