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Integration Of Inherent Safety Assessment Into Process Simulation

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This paper describes the integration of Inherent Safety Index (ISI) assessment into process simulation. A framework for integrating the ISI with process simulation performed on iCON® process simulator was developed. The Microsoft Excel® was utilized as an interface. For illustration purposes, the above described technique was implemented in the process simulation of an acetaldehyde production plant. The ISI was utilized to assess the reaction unit by applying the intensification and moderation approach. The results from this investigation show that the integration of ISI with the process simulation provides a tool to assess safety improvement via the implementation of inherent safety principles. Any changes that is made on the process simulation is immediately captured and new set of calculation is triggered automatically, thus enabling a process design and safety assessment to be carried out simultaneously

1. Introduction

The main objective of a process design is to create a process that is economic, safe, and environmentally benign throughout the whole lifetime of the plant. This can be achieved by optimizing the process alternatives according to economic and functional criteria. In addition, due general society expectation, company image and economic reasons, the safety of a processing plant must reach a certain minimum level (Hurme & Rahman, 2005). The application of inherent safety principles since its introduction by Trevor Kletz 1970s has gain popularity as an approach for safety improvement. The primary principles of inherent safety are intensification, substitution, moderation and limitation of effects (Kletz, 1998). Inherent safety principles use properties and characteristics that are intrinsic to the materials or process to effect hazard elimination or reduction (Etowa et al., 2002). Inherent safety strives to enhance process safety by introducing fundamentally safer characteristics into process design. Implementation of inherent safety means selecting and designing the process to eliminate hazards, rather than accepting the hazards and implementing add-on systems to control it (Rahman et al., 2005). The opportunity for installing the inherent safety features decreases exponentially from conceptual design stage to operational stage (Kletz, 1998). Thus, it's best to implement the inherent safety principles at early stages of process design and to assess their effectiveness in improving the process safety.

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Takriff et al. (2008) summarizes the works of several authors on the inherent safety assessment at early process design stage and part of the information is reproduced in Table 1. Despite the various development efforts on inherent safety assessment in the early design stage that have been put forward by various investigators, minimal work has been carried out to integrate the assessment with process simulation. Based on the features and the requirements of the inherent safety assessment techniques presented in Table1, the ISI appears to be the most suitable for integration with at early stage of process simulation. According to Hekkilä (1999) the ISI considers both the chemical (reaction heats, flammability, explosiveness, toxicity, corrosiveness, chemical interaction) and the process (inventory, process temperature, pressure and the safety of equipment and process structure). At the process simulation stage, it is possible to consider various possibilities of process improvement via the implementation of inherent safety principles. Thus, the integration of inherent safety assessment with process simulation is much desired.

Table 1: Methods for inherent safety assessment in the early design stage

Evaluation Method	Description
Inherent Safety Index – ISI (Heikkilä in year 1999)	ISI is based on PIIS that classifies safety factors into two categories: chemical and process inherent safety. However both the PIIS index and ISI index have sudden jump in the score value at the sub-range boundary, e.g., based on Gupta & Edwards (2003), the scoring of parameter changes to one score added only for small escalation.
Integrated Inherent Safety Index (I2SI) (Khan and Amyotte in 2004)	I2SI considers the life cycle of the process with economic evaluation and hazard potential identification for each option. I2SI is comprised of sub-indices which account for hazard potential, inherent safety potential, and add-on control requirements.
Dow's F&EI and Dow's CEI (Etowa et al. 2002, Suardin et al., 2007).)	Automatic F&EI calculation and perform sensitivity analysis using Microsoft® Visual Basic. Not intended to determine business interruption and loss control credit factors, to conduct process unit risk analyses, to automate the sensitivity analysis in order to integrate F&EI calculation into process design and optimization framework

2. Framework for Integration of ISI into Process Simulation

The framework for integrating inherent safety assessment at the process simulation design stage is shown in Figure 1. The first step is to simulate a base design case using iCON® process simulator and was later used as a basis for comparison. The excel® worksheet is than call upon using the worksheet option that is provided in iCON®. The PFD for the base case simulation with the excel® worksheet interface is shown in Figure 2. The required input variables were identified and the necessary equations for ISI calculations were then set-up in the worksheet. Details of the ISI calculations may be obtained from Hekkilä (1999). A unit operation was then selected and the inherent safety principles was applied for process improvement e.g. moderation or attenuation by varying the temperature, pressure or flow rate. The input data as listed in Table 2 were then transferred from the process simulator to the excel® worksheet using the import/export features of iCON® as shown by the a window on the top upper right-hand side of Figure 2. The ISI score was then calculated from the input data. Once the link between the worksheet and the process simulator has been established, any changes that are made in the simulation condition (e.g. Operating pressure or flow rate) is also captured by the worksheet and thus triggering a new set of calculation. The above described features enable process design and inherent safety assessment to be carried out simultaneously. The consequence of changes that have been made on the process simulation on the safety of the process can then be analysed by comparing the ISI scores. The iCON® - excel® interface allows for two ways data transfer. Any input data may be exported from excel® to iCON®. With this features, once the base simulation case has been established the users are not required to go back and forth between the two softwares to change any of the input values. Once the assessment is completed for a given unit operation, the same procedure are repeated for the other unit operations.

Table 2: Data required based on safety hazard categories

Safety Hazard Categories	Input data required
Process conditions	Pressure, temperature
Fire and explosion	Flash point, boiling point and flammable limits
Reaction and decomposition	Heat of main reaction and heat of side reaction
Toxicity	TLV
Inventory	Mass flow rate
Others	Corrosiveness and chemical interaction

3. Case study

An acetaldehyde production plant as described in (*http://www.che.cemr.wvu.edu/publications/projects*) was used as a case study to illustrate the implementation of the framework for integrating index based inherent safety assessment at early process design stage. The plant capacity that is selected for this illustration was 60,000 ton/yr. In this process, acetaldehyde was produced from the dehydrogenation of ethanol in an isothermal reaction. The feed to the reactor was made-up of fresh ethanol and unreacted ethanol that is recycled to the front end of the process. The product recovery was carried out in a few separation units involving a phase separator, an absorber and three distillation columns. Acetaldehyde with a purity of 99.9 wt% was recovered in the final product stream and the unreacted ethanol was recycled to the reactor. The PFD for the process simulation of the acetaldehyde plant along with the Excel® worksheet is shown in Figure 2. Most of the chemical substances in the process are flammable and/or toxic of varying degrees. The ISI scores for the main unit operation for the base design case are presented in the Table 4. Based on this table, the reactor is rated the most severe hazard source. For this reason, the reactor is selected to illustrate how the safety level can be improved via the implementation of the intensification and moderation principles of inherent safety.

The objective of intensification in inherent safety is to reduce the inventories of hazardous materials. The higher inventories of hazardous chemicals mean the more severe is the potential consequence from the hazard. The use of smaller and simpler equipment is also part of the approach. No unit operation, except for the storage facility, offers more scope for reduction of inventory than reaction. A process becomes inherently less safe as the quantity of material increase for potentially hazardous materials. An exact calculation of inventory is difficult in the conceptual design phase, since the size of equipment is not usually known. As suggested by Hekkilä (1999), the inventory of hazardous material may be estimated based on the flow rate and residence time. Similarly in this case study the inventory was based 1 hour residence time, thus capacity of the reactor was varied by varying the flow rate. The ISI scores for the reactor at various feed flow rate are presented in Table 4. This table shows that the total ISI score changes only slightly as the flow rate was varied from 5 tones/hr to 25 tones/hr.

Pressure if one of the most important operation and design variable. Operating at high pressure indicates high potential energy that affects the leak rates in the case of loss of containment. On the other hand, any leaks in vacuum equipment may cause inlet of air and consequent explosion. Equipment design and maintenance become more critical when the spillage potentially increase as the operating pressure increase. The changes in equipment pressure will affect the score of ISI which means either increased or decreased the degree of hazard. Table 4 shows that the ISI score of the reactor only slightly changed as the pressure was varied between 6.6 bars to 3 bar.

Table 3 and 4 show that the hazard rating for the reactor which was selected as illustration of safety improvement via process intensification and moderation. These results indicate that for the range of process variables investigated in the case study, the hazard rating is only slightly improved based on process intensification and moderation approach. Practically however, it is not possible to keep lowering the flow rate or pressure to improve the hazard rating. Thus, safety improvement via inherently safer design should be implemented by looking at the whole the spectrum of process and operating parameters.

Table 3: Safety analysis for the unit operation based on ISI

Unit Operation	ISI
Reactor	**32**
Phase Separator	18
Absorber	12
Column 1	21
Column 2	18
Column 3	14
Column 4	14

Table 4: ISI score for the variation in reactor capacity and reaction pressure.

Total Mass Flow rate (tonne/hr)	ISI score	Pressure (Bar)	ISI score
25.44	31	6.63	31
20.36	31	6.00	31
15.27	31	5.00	30
10.18	30	4.00	30
5.09	30	3.00	30

4. Discussion

Index based inherent safety assessment was successfully integrated into iCON® process simulator software for safety assessment in the early design stage. Inherent Safety Index (ISI) was used in this study. The inherent safety out assessment was carried using Excel® worksheet that is directly linked and allows for two way data transfer with iCON® process simulator software. In addition, the user may manipulate any process parameter from MS Excel® to meet the safety criteria. Any changes that is made on the process simulation is immediately captured and new set of calculation is triggered automatically, thus enabling a process design and safety assessment to be carried out simultaneously. The results presented in Tables 3 and 4 show that the ISI scores, both total or based on subindex, may be calculated based on the framework that has been developed. It allows for simultaneous assessment of inherent safety as various design alternatives are considered. With simultaneous technical and safety assessments are done at early stage of the process design, the process designers are provided with better information to make an informed decision on the process design.

5. Conclusion

A framework for integrating ISI with process simulation was sucessfully developed and implemented in this work. The process simulation was performed using iCON® and the ISI quantification was carried out in microsoft excel® that is liked with iCON®. Once the link between the worksheet and the process simulator has been established, any change that is made in the process simulation is captured by the worksheet and thus triggering a new set of calculation. Thus, allowing for simultaneous assessments of process design and inherent safety as various design alternatives are considered. The framework that has been developed in this work allow for quantification of the total index as well as the subindex. With simultaneous technical and inherent safety assessment, the process designers are provided with better information to make an informed decision on the process design.

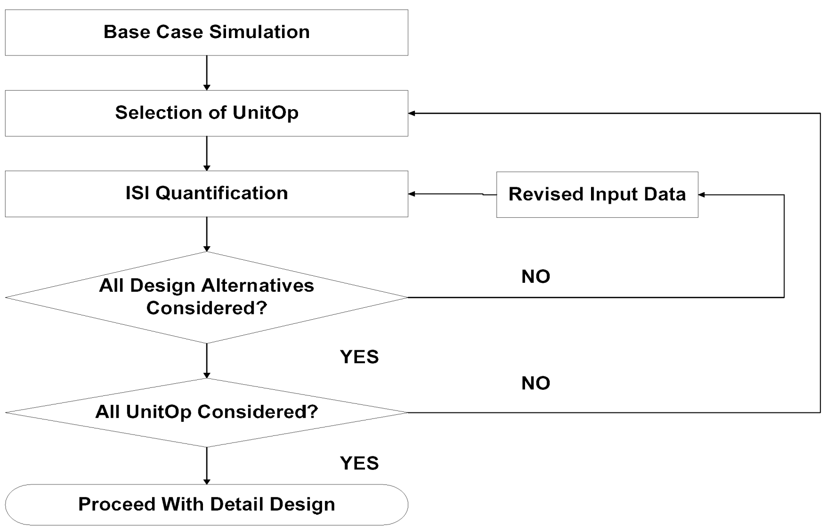

Figure 1: Connection between iCON simulator software and Excel Spreadsheet to determine inherent safety level.

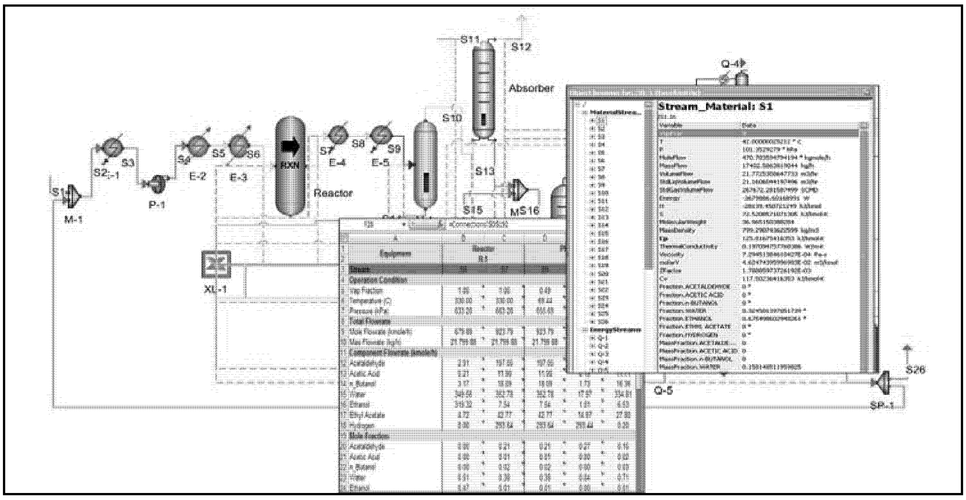

Figure 2: Process flow diagram for acetaldehyde plant and excel® worksheet interface

References

Etowa, C.B., Amyotte, P.R., Pegg, M.J. and Khan, F.I. 2002. Quantification of inherent safety aspects of Dow indices. Journal of Loss Prevention in the Process Industries. 15: 477-487

Hekkilä, A-M., Hurme, M. and Järveläinen, M. 1996. Safety considerations in process synthesis. *Computers and Chemical Engineering.* **20**: 115-120.

Hekkilä, A.-M. (1999). Inherent Safety in Process Plant Design. D.Tech. Thesis, VTT Publication 384. Espoo: Technical Research Centre of Finland, www.inf.vtt.fi/pdf/publications/1999/P384.pdf

Hurme, M., and Rahman, M. 2005. Implementing inherent safety throughout process lifecycle. *Journal of Loss Prevention in the Process Industries*. **18**: 238-244.

Khan, F. I. and Amyotte, P. R. 2005. I2SI: A comprehensive quantitative tool for inherent safety and cost evaluation. Journal of Loss Prevention in the Process Industries. 18: 310-326

Kletz, T. 1998. *Process Plants: A Handbook for Inherently Safer Design.* United States of America: Taylor & Francis.

Rahman, M., Hekkilä, A-M., and Hurme, M. 2005. Comparison of inherent safety indices in process concept evaluation. *Journal of Loss Prevention in the Process Industries*. **18**: 327-334.

Suardin, J., Mannan, M. S. and El-Halwagi, M. 2007. The integration of Dow's fire and explosion index (F&EI) into process design and optimization to achieve inherently safer design. *Journal of Loss Prevention in the Process Industries.* **20**: 79-90.

Takriff, M.S, Bahnudin, N.N, Mohammad, A.W, Sheikh Ahdullah, S.R and Wan Daud, W.R, 2008, Integrating Inherent Safety At Early Stage Of Process Design: Index Based Approach, Regional Symposium of Chemical Engineers, Kuala Lumpur.