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Process Synthesis with Simultaneously Considered Inherent Safety

Andreja Nemet[a,*], Jiří J. Klemeš[a], Zdravko Kravanja[b]

[a]Sustainable Process Integration Laboratory – SPIL, NETME Centre, Faculty of Mechanical Engineering, Brno University of Technology - VUT BRNO, Technická 2896/2, 616 69 Brno, Czech Republic
[b]Faculty of Chemistry and Chemical Engineering, University of Maribor, Smetanova ulica 17, 2000 Maribor, Slovenia
nemet@fme.vutbr.cz

Process plants should be designed to be economically viable and environmentally friendly, operable and maintainable when projects are implemented. Process synthesis is a rather challenging task since results obtained should be feasible and acceptable. The safety of processes is among the most important considerations in obtaining more acceptably realistic results. Safety issues have mostly been addressed as retrofit analysis for projects that have already been implemented. There is a reasonably well-developed field of research focusing on deviation events and on predicting their possible consequences. This approach is well suited for making action plans to control deviation events. However, designers are aware that every control system has its weaknesses and gaps. For this reason, safer design can be obtained when inherent safety is considered. Inherent safety can successfully be enhanced at the early stages of the design. There have been some studies dealing with safety metrics at the design stage. The aim of this study is to develop a quantitative risk assessment method and to incorporate it into process synthesis, using a mathematical programming approach. A mixed-integer nonlinear programming (MINLP) model has been used for the synthesis of a methanol production process including risk assessment during the synthesis. The superstructure is extended using a variety of process units in order to enable the selection of safer designs. Risk assessment is performed simultaneously with MINLP process synthesis, where the risk is determined for each unit of the process individually and, after summing up, for the whole process. Since improving the safety of individual units can lead to decreased overall risk, it is obvious that safety at both the individual and overall levels should be considered simultaneously. The results obtained using the method developed are inherently safer, while still obtaining economic viability.

1. Introduction

The inherent safety of process systems should be considered as early as possible, preferably during the design stage of the process, since the potential for affecting the inherent safety of a process decreases once decisions about on investment in design have already been made (Heikkilä, 1999). Increasing inherent safety can lead to much safer design compared to processes where hazard control is applied since every control system follows the Swiss Cheese Model (Reason, 1997). It points out that in the real world, all defensive layers have some weaknesses and gaps (like holes in a cheese) that could lead to an accident. Moreover, when considering the human error that is estimated to cause 70 - 80 % of accidents in high-hazard industries (Reason, 1990), it can be concluded that eliminating hazard is a significantly more efficient approach, compared to hazard control. Safety also enhances the flexibility and maintenance in process design, altogether yielding better operability of processes (Thomaidis and Pistikopoulos, 1995). There have been various methodologies developed for risk assessment in process systems. Ahmad et al. (2016) presented a graphical method for assessing inherent safety. Using graphical approaches can enhance understanding of the source of risk: however, it is very time-consuming when obtaining an appropriate design with acceptable risk level. Various indexes have been proposed for assessing process design. Leong and Shariff (2009) suggested a Process Route Index (PRI) to assess explosiveness. Rathnayaka et al. (2014) proposed a Risk-Based Inherent Safety Index (RISI) to obtain plant design considering inherent safety. Warnasooriya and Gunasekera (2017) presented the Inherent

Chemical Process Route Index (INCPRI). These indexes offer improved quantitative evaluation of inherent safety; however, these methodologies are suited for an iterative approach, assuming some initial process design, after determining the index and proposing a modification of the initial process design. This iterative approach, besides being time-consuming, leaves all the modifications to designer expertise and does not guarantee optimal design, as it is unattainable to exploit all possible process designs. The resulting designs should be economically feasible and, at the same time, acceptably safe.
In this work, a simultaneous process design synthesis and risk assessment with selected acceptable risk limits is proposed. The authors (Nemet et al., 2017a) have already developed a HEN synthesis with embedded safety analysis. Risk assessment was performed by multiplying the frequency of failure by the severity of consequences. Failure frequency can then be related to the quality of the equipment, and severity can be related to the potential hazard of the substances in the equipment. The severity of consequences was based on methodology presented in Uijt de Haag and Ale, (2005). However, taking into account the whole range of equipment in order to evaluate inherent safety. The failure frequency was taken from historical data presented in Handbook Failure Frequencies (Flemish Government, 2009). The scope of the risk assessment was also established and verified for Total Site Synthesis (Nemet et al., 2017b).
The aim of this study was to achieve process synthesis with simultaneously performed risk assessment. For this purpose, a mixed-integer nonlinear programming (MINLP) model was applied, with embedded calculations for risk assessment. The risk limit was set by setting the upper limits on risk assessment either for each unit separately or for overall process risk.

2. Methodology

The MINLP model was applied for methanol process synthesis initially introduced by Kravanja and Grossmann, (1990) and later rehearsed by Kasaš et al. (2012). The superstructure can be found in Figure 1. Different options were included in the superstructure. There were two feeds possible: i) FEED-1, which had lower cost and lower content of H_2 and ii) FEED-2, which was more expensive but had higher H_2 content. The compression could be performed via one-stage or via two-stage compression with cooling in-between. The reaction could be performed via a more expensive reactor with better efficiency, or via a reactor with lower efficiency and lower investment cost. A simultaneous synthesis of HEN was performed, considering different types of HEs (Soršak and Kravanja, 2002).

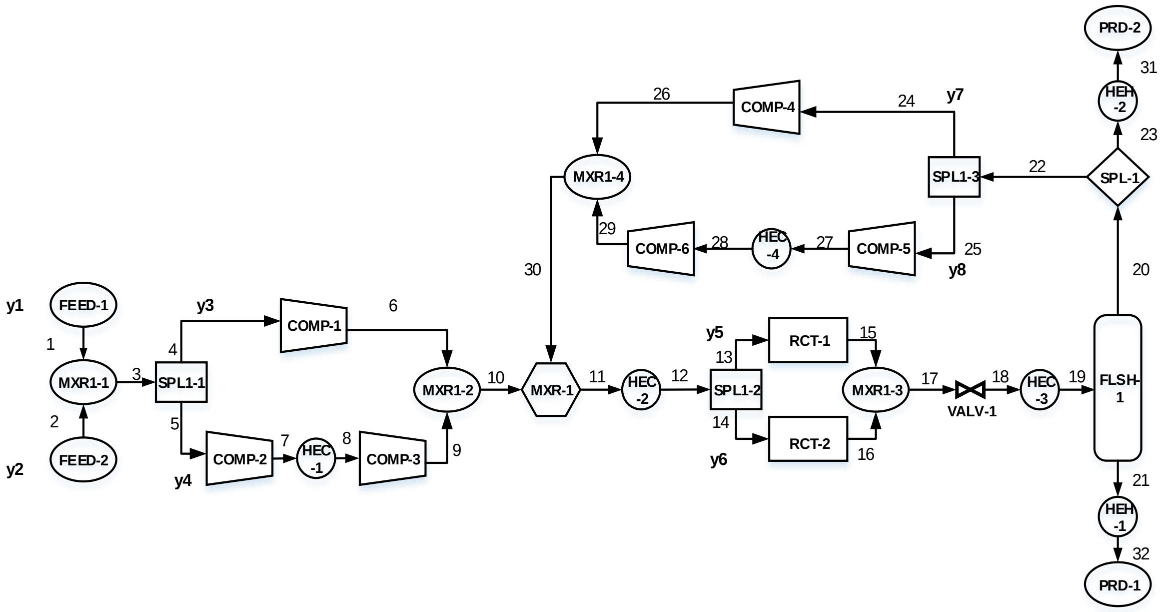

Figure 1: Superstructure for methanol process synthesis (modified from Kasaš et al, 2012)

Risk was assessed by multiplication of frequency of failure f^{fail} and severity of consequences for each component in each unit *j* separately for each type of risk considered (toxicity, flammability, explosiveness) Eq(1).

$$R_{r,i,j}^{\text{ind}} = f_j^{fail}.AI_{r,i,j} \qquad \forall\ r \in RISK,\ i \in COMPON,\ j \in UNITS \qquad (1)$$

The severity of consequences was described with indications number $AI_{r,i,j}$ for each risk type r, for each component i, within each unit j. It was a multiplication of quantity m_i of the substance i present in the installation in kg with the factors for installation type f_j^1, positioning of installation f_j^2, and process conditions f_i^3, divided by limiting value $G_{i,r}$, representing a measure of explosiveness, toxicity and of whether or not the component is flammable.

$$AI_{r,i,j} = \left(m_i \cdot f_j^1 \cdot f_j^2 \cdot f_i^3\right) / G_{i,r} \qquad \forall\ r \in RISK,\ i \in COMPON,\ j \in UNITS \qquad (2)$$

The overall risk of the process was determined as a sum of all risks for each component within each unit. The overall risk was determined separately for each type of risk.

$$R_r^{\text{Process}} = \sum_{j \in UNITS} \sum_{i \in COMPON_j} R_{r,i,j}^{\text{ind}} \qquad \forall\ r \in RISK \qquad (3)$$

Setting safety limits was performed by setting the upper limits either on individual risk $R_{r,i,j}^{\text{ind}}$ or on the overall risk R_r^{Process} .

The objective function was defined as profit after tax P_b, consisting of revenues R, expenditures E and depreciation D. The tax rate was presented by r^{tax}.

$$P_b = R\text{-}E\text{-}D$$

The revenues consisted of product price c^{product} multiplied by the annual amount of production $q_{\text{m}}^{\text{product}}$.

$$R = \sum_{product} c^{\text{product}} \cdot q_{\text{m}}^{\text{product}} \qquad (4)$$

The expenditures were the cost of feed, the electricity cost for the compressor run and the cost of heating and cooling.

$$E = \sum_{feed} c_{feed} \cdot q_{\text{m}\,feed} - \sum_{comp} c^{\text{el}} \cdot elec_{comp} - \sum_{c} c_c^{\text{HU}} \cdot Q_c^{\text{HU}} - \sum_{h} c_h^{\text{CU}} \cdot Q_h^{\text{CU}} \qquad (5)$$

The depreciation consisted of fixed and variable cost for compressors, reactors, flash, mixers, splitters, heat exchangers between hot and cold process streams, coolers and heaters. It should be noted that fixed and variable costs were annualized.

$$\begin{aligned} D = & \sum_{comp} c_{comp}^{\text{fx}} \cdot y_{comp} + \sum_{comp} c_{comp}^{\text{var}} \cdot s_{comp} + \sum_{rct} c_{rct}^{\text{fx}} \cdot y_{rct} + \sum_{rct} c_{rct}^{\text{var}} \cdot s_{rct} + \\ & \sum_{h,c,k,hx} c_{hx}^{fx} \cdot y_{h,c,k,hx} + \sum_{h,c,k,hx} c_{hx}^{\text{var}} \cdot Q_{h,c,k,hx} + \sum_{h,hx} c_{hx}^{\text{fx}} \cdot y_{h,hx} + \sum_{h,hx} c_{hx}^{\text{var}} \cdot Q_{h,hx}^{\text{CU}} + \sum_{c,hx} c_{hx}^{\text{fx}} \cdot y_{c,hx} + \sum_{c,hx} c_{hx}^{var} \cdot Q_{c,hx}^{HU} \end{aligned} \qquad (6)$$

3. Case study

The case study was performed on a process for methanol production. The production of CH_3OH was fixed to 1 kmol/s, and the temperature of the product was set to 127 °C. The feed consisted of 65 % H_2, 30 % CO and 5 % CH_4 (inert component). The feed cost for FEED-1 was 6,375 k\$ /(kmol y), while for FEED-2 it was 7,650 k\$/(kmol.y). The cost of PRD-1 was 80,000 k\$/(kmol.y), while for PRD-2 it was 5,000 k\$/(kmol.y). The electricity cost was 0.255 k\$/(kW.y) Steam at 177 °C was considered as a hot utility, with a cost of 2.22 k\$/(kWh), and temperatures for the cold water inlet at 10 °C and outlet at 22 °C were assumed for cold utility, at a cost of 0.194 k\$/(kWh). The fixed cost of reactor 1 was 500 k\$; for reactor 2, it was 650 \$ and for the compressors, 50 k\$/y. For heat exchangers, the fixed prices were 6.5 k\$/y. The variable cost for reactor 1 was 25 k\$/(y.m^3), and for reactor 2, it was 30 k\$/(y.m^3). The variable cost for the compressors was 87.5 k\$/(y.m^3). The upper and lower limits on temperature and areas for heat exchangers are presented in Table 1, as well as the annualized fixed and variable cost. *Ft* is the correction factor considering the geometric properties of heat exchangers.

Table 1: Input data for heat exchangers.

HE type	T_{hx}^{LO} /°C	T_{hx}^{UP} /°C	A_{hx}^{LO} /m^2	A_{hx}^{UP} /m^2	cf_{hx}/ k€ y^{-1}	cv_{hx}/ k€ m^{-2} y^{-1}	*Ft*
Double pipe	-100	600	0.25	200	3.067	0.1828	1
Plate and frame	-25	250	1	1,200	8.653	0.02313	1
Shell and tube	-200	850	10	1,000	8.093	0.01287	1
Shell and tube with U-tubes	-200	850	10	1,000	6.727	0.0181	0.8

The MINLP process synthesizer MipSyn (Kravanja, 2010) was used to obtain the results. First, a reference design, with no safety limits was obtained. The annual profit after tax was 35,986 k\$/y, and the annualized investment was 5,905 k$/y. The initial design without considering safety is presented in Figure 2. The overall risk of the process, recalculated after optimisation, was 180.70 for toxicity, 12.89 for flammability and 40.27 for explosiveness. The overall conversion of the process was 81%.

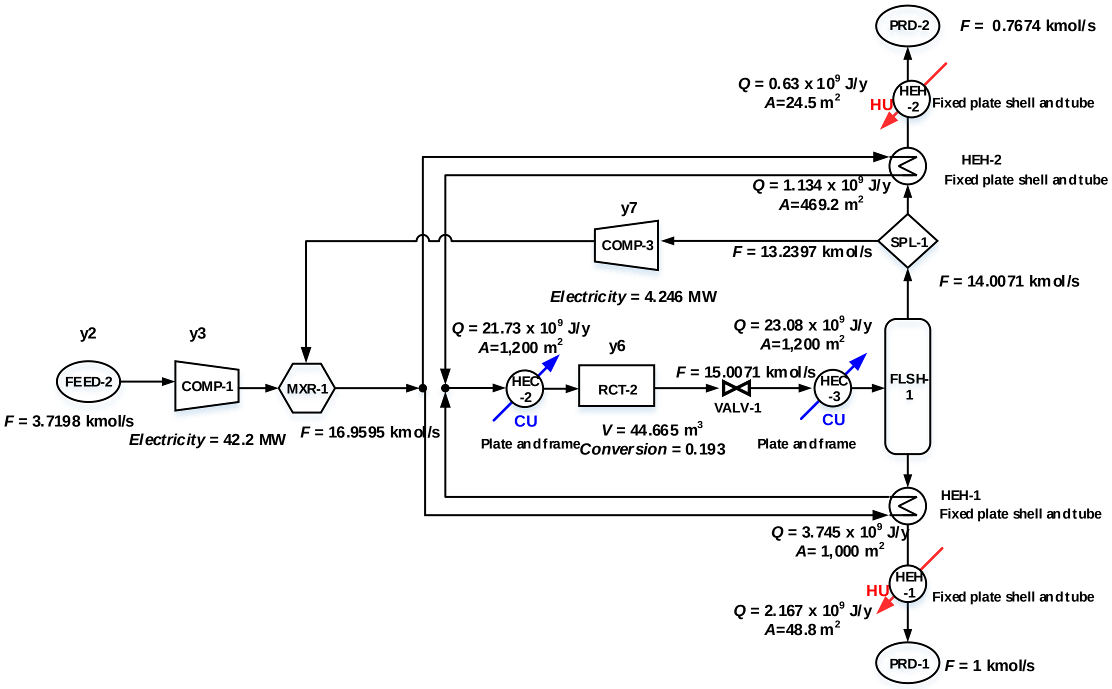

Figure 2: Process design with no safety limits

After obtaining the initial design, the overall safety limit of the process was set to approximately 2/3 (63%) from the initial one, and the design was recalculated (Figure 3).

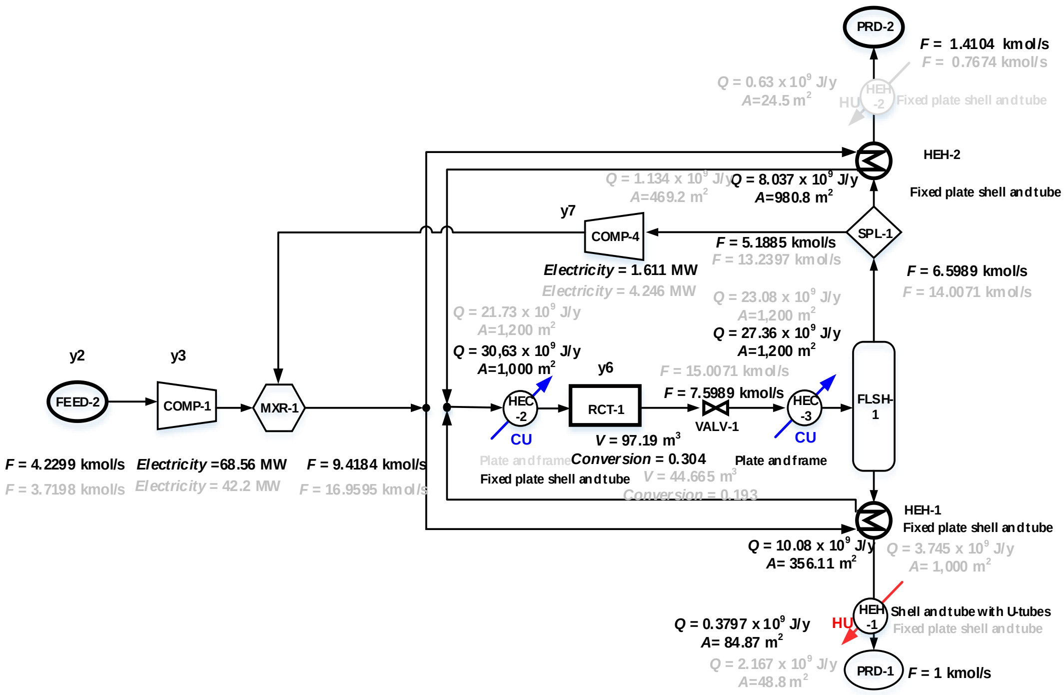

Figure 3: Process design with overall risk limit set at 2/3 of initial overall limit

The annual profit after tax decreased to 26,292 k$/y, which is a 9,694 k$/y (26.9 %) decrease. The investment for this design was 9,170 k$/y, which is 3,265 k$/y (55.3 %) higher compared to the reference case. It should be noted that some structural changes did occur (Figure 3). The heater for product PRD-2 was completely removed, and the reactor type was changed from one with lower efficiency and lower price RCT-2 to a reactor with better efficiency and a higher price. It can be seen that the recycle rate was significantly decreased from 13.2397 kmol/s by 8.0512 kmol/s (61.3 %), to 5.1885 kmol/s. The overall conversion decreased significantly, now reaching only 66 %, compared to 81 % in the reference case. This led to decreased overall risk; instead, reactor efficiency (conversion) was increased. By this change, the mass of a substance was reduced in all heat exchangers, reactors, flash, and compressor COMP-4. Only in compressor COMP-1 was the mass somewhat increased. The overall determined risk was 113.8 for toxicity, 7.12 for flammability and 17.2 for explosiveness.
In further analysis, the individual risk within each unit separately was limited to approximately 2/3 (62 %) of initial overall risk. Figure 4 presents a comparison between the design with no safety and the design obtained when unit risk was set as 62 % of the initial overall risk. The profit after tax was in this case 26,252 k$/y, representing a 9,734 k$/y (27 %) reduction compared to the reference case. The investment was 9,203 k$/y, an increase of 3,298 k$/y (55.8 %) in comparison to the reference case. Some structural changes occurred, compared to the reference case. Both heaters were removed and the reactor volume was higher. A similar trend can be observed when the overall safety was limited, leading to a certain decrease in the recycle rate in order to lower overall conversion. In the case of setting the individual risk limit, the overall conversion rate was 66.5 %. The reactor type did not change; however, the volume did increase from 44.66 m^3 to 74.15 m^3, leading to higher conversion in the reactor. The recalculated overall risk was 114.6 for toxicity, 7.18 for flammability and 17.4 for explosiveness.

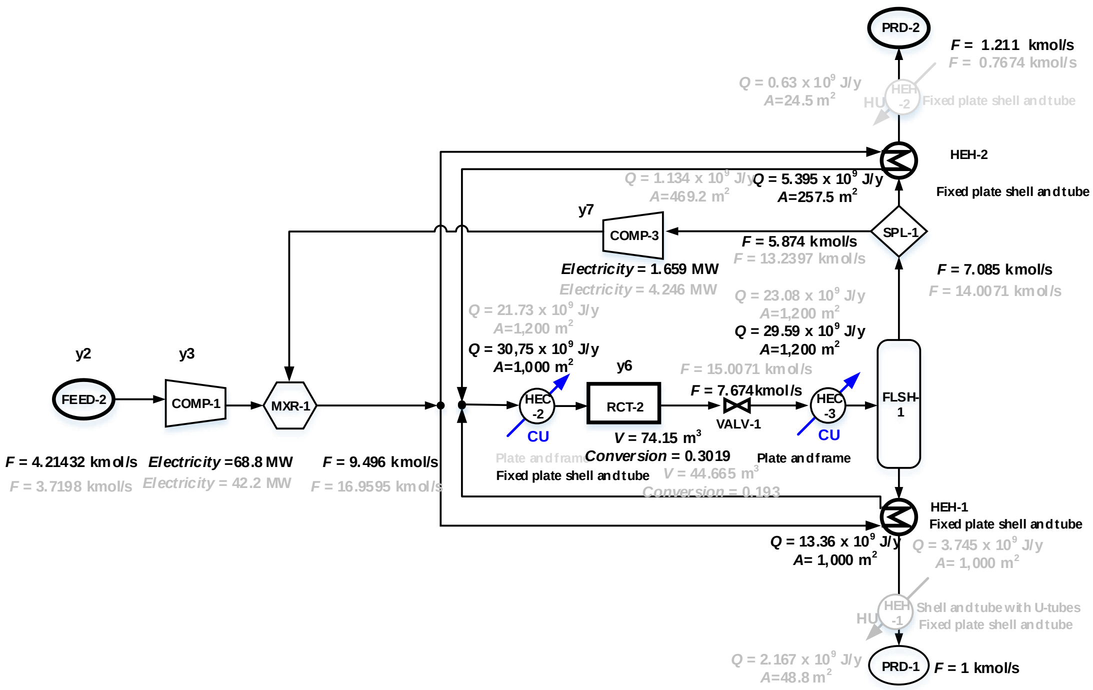

Figure 4: Process design with individual risk limit set at 2/3 of the initial overall limit

Comparison of Figure 3 and Figure 4 reveals that setting limits on overall safety leads to an 11 % lower recycle rate, reaching only 5.1885 kmol/s flow when an overall risk limit is set, compared to 5.874 kmol/s when individual risk limits are set. However, the reactor conversion is higher when an overall risk limit is set. Comparison of overall risk reveals that it is slightly higher when individual unit risk limits are established. In comparing designs, it can be seen that reactor volume is greater when an overall risk limit is set; moreover, the more efficient reactor type is selected. It can be concluded that, when setting an overall risk limit, the risk is concentrated in a few units with high risk, while setting risk limits for each unit separately leads to more evenly distributed risk over each unit. However, setting risk limits by units should be done carefully, since setting too low a limit could lead to increased overall risk.

4. Conclusions

A mixed-integer nonlinear programming (MINLP) model for process synthesis of a methanol production process, simultaneously considering risk assessment, was developed. The results of a case study indicated that considering risk can lead to significantly different results. The upper bound on the risk limit can be set either for overall process risk or for each unit separately. Setting the upper risk limit on overall process risk leads to the accumulation of risk in a smaller number of units while setting the risk on each unit separately leads to distributed risk over the whole process. The methodology presented was tested on a methanol production process; however, it could be applied to other processes, as well.

Acknowledgments

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