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Comparison of safety indexes for chemical processes under uncertainty

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Abstract

The fatal consequences of industrial incidents have made evident the need for suitable tools to develop inherently safer process designs. Traditionally, in a process design project, the evaluation of safety aspects is left for analysis after the detailed design has been completed. This approach leads to the use of control loops, barriers and protection layers as the only ways to prevent incidents and to reduce the possible outcomes. An alternative to this approach is the application of the concept of inherent safety, which was introduced to set up several principles that aim to enhance process safety by eliminating, avoiding or minimizing sources of risk.

In this work, we present a comparison of different safety metrics in their role to evaluate the risk associated with a given process design. The indices selected for consideration are better applied at the conceptual stage of the process design, and they were the Dow's fire and explosion index (F&EI), the fire and explosion damage index (FEDI), the process route index (PRI) and the process stream index (PSI). All these indices use different input information and their outcomes have different rankings. The metrics were applied to an ethylene production process to identify risk levels, and the location of streams and pieces of equipment that pose the highest risk within the process. An evaluation of the indices in their capability to track design changes in operating conditions aiming to improve the safety level of the process was developed. To perform the assessment of the safety metrics in a more extensive manner, an uncertainty analysis based on a Monte Carlo simulation framework was implemented and compared to the traditional use of single-value design variables. Within this context, an insightful assessment of uncertainty's effect on process safety characteristics was achieved because of the identification of ranges of safety-relevant performance outcomes (zones of risks and opportunities) that can be probabilistically characterized. The approach was applied to a case study related to the production of ethylene from shale gas. The results showed how some indexes are better suited to capture the risk characteristics associated with the process when changes in the operating conditions of the section with highest risk were implemented. The methodology can be extended to other processes of interest, and may serve as a basis for the safety and process design community to propose adjustments in the structure of the safety indices based on a better understanding of their performance and reliability as part of the efforts towards the continued improvement of those safety metrics.

Keywords: Process design, ISD

1. Introduction

Traditionally, safety analysis in a process design project is performed after the detailed design is completed. Within this approach, little can be done to modify the design in order to enhance safety performance (Lee et al., 2019). Instead, control loops, barriers, and protection layers are used to reduce the possible outcomes in case of an incident (Khan et al., 2003). Despite the usefulness of these devices to contain or minimize the consequences of an incident, past events have shown that these devices may fail to cause fatal consequences (Abidin et al., 2016). Inherent safety aims to eliminate, reduce or avoid sources of risk, thus improving the safety properties of the process (Rahman et al., 2005; Kidam et al., 2016).

Inherent safety principles are better applied at early design stages, where the design can be easily modified to include safer features. To assess if the changes introduced to the design result in a safer process, it is necessary the use of proper metrics that evaluate safety levels of the process design. There are different tools to evaluate a process in terms of safety performance. Among the most popular ones are the hazard and operability (HAZOP) method and the quantitative risk assessment (QRA) (Roy et al., 2016). The HAZOP method is a qualitative tool that requires detailed information about the process. Typically, the type of information needed for a HAZOP analysis is not available in early design stages. The QRA is based on the probabilistic estimation of failures and consequences. Although this method may be suitable for the analysis of pieces of equipment (Medina-Herrera et al., 2014a; Medina-Herrera et al., 2014b) its use in a complete process may not be suitable at early design stages.

As an alternative to these tools, safety indices have been developed to consider process characteristics that may result in potential incidents (Roy et al., 2016). The first index reported in the literature was the Dow's fire and explosion index (F&EI). This index is based on material and process factors (AIChE, 1998) and although it considers detailed information of the process, it can be simplified to assess safety characteristics at the conceptual design stage (Suardin et al., 2007; Vázquez et al., 2018; Ruiz-Femenia et al., 2017). The Dow's F&EI relies heavily on the material factor, which only reflects the characteristics of the chemicals but not the operating conditions. The latter aspect motivated the development of other indices that combine both operating conditions and chemical characteristics to obtain a more reliable safety assessment. One such index is the Fire and Explosion Damage Index (FEDI) developed by Khan and Abbasi (1998). This index classifies the units of a process according to its purpose and assesses the potential to cause hazards. Both indices, Dow's F&EI and FEDI, consider the components in the process as individual components, not as mixtures. For the evaluation of both indices, only the characteristics of the most hazardous component are considered, overlooking the contribution of other hazardous components. To overcome this limitation, other indices have been introduced, such as the process route index (PRI) and the process stream index (PSI). These indices consider the hazardous characteristics of mixtures instead of those of single components. Additionally, these indices were developed to obtain information directly from process simulators, which eliminates the tedious procedure of information transfer and thus avoiding errors during the safety evaluation process (Leong & Shariff, 2009; Shariff et al., 2012). The combination of PRI and PSI may be used to identify hazardous areas in process designs, and examine the result of potential changes in the operating conditions of such areas on items such as risk and economic performance (Ortiz-Espinoza et al., 2017). The PSI uses the principle of relative ranking to identify the most hazardous streams in a process in terms of fire and explosions, while PRI considers stream parameters such as combustibility, energy, density and pressure to rank different processes. While Dow's F&EI and FEDI have an established ranking to interpret the results from the evaluation, the PRI index does not classify the results of the evaluation according to the level of hazard.

The evaluation of these indices typically relies on information that, although represented as average values, is commonly uncertain. The use of these types of input values may lead to the misinterpretation of the results, which may affect the decision-making process. The problem then is to formulate the evaluation model so that uncertainty in key design variables is included. One way to accomplish this task is the use of Monte Carlo (MC) simulation methods (Koc et al., 2012) which allows the consideration of multiple uncertain inputs. The uncertainty in the selected inputs is represented using probability distributions and then propagated through the model. Within this framework, distribution profiles are obtained for the evaluated metrics. Such profiles can be statistically characterized, and ranges of performance outcomes can be generated. This type of results provides more valuable insights that can be used by process decision-makers to make more informed decisions when selecting among different design options.

In this work, the Dow's F&EI, the FEDI, the PRI, and PSI indices are compared to identify which one may be more suitable to use at the conceptual stage of a process design. To complete the analysis, the evaluation of the indices is performed under a systematic uncertainty analysis framework. The metrics are applied to an ethylene production process, where the most hazardous areas or pieces of equipment in the process are identified. Modifications to the operating conditions are then implemented to find which index captures better such modifications. Within the proposed uncertainty analysis, framework distribution profiles are obtained and probabilistically characterized for each index. It should be pointed out that these safety indices profiles represent a potential advantage for decision-makers since possible underestimation of process risks in the presence of uncertainty could pose significant adverse effects.

2. Approach

The four indices analyzed in this work, the Dow's fire and explosion index (F&EI), the fire and explosion damage index (FEDI), the process route index (PRI), and the process stream index (PSI), take into account the characteristics of the chemicals and the process conditions that can result in a fire and/or explosion incident. Each index takes into account different types of information from the process design, and their structure is different. A brief description of those indices is given below.

2.1 The Dow's Fire and Explosion Index (F&EI)

The F&EI was developed in 1964 by the Dow Company (Roy et al., 2016). The index is calculated based on the material factor (MF) and the process unit hazards factor (F_{3Dow}). The MF is selected according to the flammability and reactive characteristics of the chemical molecule involved in the process units. When more than one flammable or reactive chemical is present, the material factor is selected based on the most hazardous one. The process unit hazards factor is the result of the product of two other factors named general process hazards factor (F_{1Dow}) and special process factor (F_{2Dow}). Both factors result from the addition of a base factor and the penalties that result from considering some process characteristics. Equations 1 and 2 show how these factors are calculated, while equations 3 and 4 show the way in which F_{3Dow} and the F&EI are computed.

$$F_{1Dow} = 1 + \sum_{i=1}^{6} penalty_{i_{F_1}} \quad (1)$$

$$F_{2Dow} = 1 + \sum_{i=1}^{12} penalty_{i_{F_2}} \quad (2)$$

$$F_{3Dow} = (F_{1Dow})(F_{2Dow}) \quad (3)$$

$$F\&EI = (MF)(F_{3Dow}) \quad (4)$$

The results obtained for the F&EI can be classified according to the degree of hazard proposed by the classification guide by AIChE (1994) (see Table 1).

Table 1. Classification of units according to the F&EI

F&EI range	**Degree of hazard**
1 – 60	Light
61 – 96	Moderate
97 – 127	Intermediate
128 – 158	Heavy
159 – up	Severe

2.2 The Fire and Explosion Damage Index (FEDI)

The FEDI was developed as part of a system named hazard identification and ranking (HIRA) (Khan and Abbasi, 1998). This index classifies the units of an industrial process according to its purpose, as shown in Table 2.

Table 2. Classification of units for FEDI estimation

Group	Type of unit	Examples
I	Storage	Storages tanks, intermediate process inventories
II	Involving physical operation	Pumps, compressors, units involving heat transfer, mass transfer or phase change
III	Involving chemical reactions	Reactors
IV	Transportation	Pipelines
V	Other	Boilers, direct-fired heat exchanger, flares, furnaces

Once the unit to be evaluated has been classified, different energy factors are considered. The first energy factor (F_{1FEDI}) accounts for chemical energy. F_{1FEDI} is given by the amount of chemical processed in the unit (M) and the heat of combustion (H_c). Energy factors F_{2FEDI} and F_{3FEDI} account for energy due to the internal pressure of the unit (physical energy). In the case of a unit of group III, a fourth factor (F_{4FEDI}) is used. Equations 5 to 8 are used to calculate each energy factor,

$$F_{1_{FEDI}} = (0.1)(M)\left(\frac{H_c}{K}\right) \tag{5}$$

$$F_{2_{FEDI}} = (1.304x10^{-3})(PP)(Vol) \tag{6}$$

$$F_{3_{FEDI}} = (1x10^{-3})\left(\frac{1}{T+273}\right)(PP-VP)^2(Vol) \tag{7}$$

$$F_{4_{FEDI}} = (M)\left(\frac{H_{rxn}}{K}\right) \tag{8}$$

where M is in kg/s, PP is the operating pressure in kPa, Vol is the volume of the vessel in m^3, T is the operating temperature in °C, VP is the vapor pressure in kPa and H_{rxn} is the heat released by chemical reactions in kJ/kg.

After the estimation of the energy factors, penalty values are assigned to account for the severity of some process parameters such as temperature, pressure, capacity, and the characteristics of the chemicals. Then, energy factors and penalties are added to estimate the hazard potential (hazpot) according to equations 9 to 13.

$$hazpot_{Group_I} = \left[\left(F_{1_{FEDI}}\right)(pn_1) + (F)(pn_2)\right]\left(\prod_{i=3}^{8} pn_i\right) \tag{9}$$

$$hazpot_{Group_{II}} = \left[\left(F_{1_{FEDI}}\right)(pn_1) + (F)(pn_2)\right]\left(\prod_{i=3}^{8} pn_i\right) \tag{10}$$

$$hazpot_{Group_{III}} = \left[\left(F_{1_{FEDI}}\right)(pn_1) + (F)(pn_2) + (F_{4_{FEDI}})(pn_9)(pn_{10})\right]\left(\prod_{i=3}^{8} pn_i\right) \quad (11)$$

$$hazpot_{Group_{IV}} = \left[\left(F_{1_{FEDI}}\right)(pn_1) + (F)(pn_2)\right]\left(\prod_{i=3}^{9} pn_i\right) \quad (12)$$

$$hazpot_{Group_{V}} = \left(F_{1_{FEDI}}\right)\left(\prod_{i=1}^{8} pn_i\right) \quad (13)$$

Finally, the hazard potential is transformed into the FEDI with the use of Equation 14.

$$FEDI = 4.76\ (hazpot)^{\frac{1}{3}} \quad (14)$$

The results for the FEDI can be ranked according to values in Table 3.

Table 3. Hazard ranking according to FEDI values from the HIRA methodology*

FEDI	**Hazard characterization**
FEDI > 500	Extremely hazardous
500 > FEDI > 400	Highly hazardous
400 > FEDI > 200	Hazardous
200 > FEDI > 100	Moderately hazardous
100 > FEDI > 20	Less hazard
else	No hazard

*Source: Khan and Abbasi (1998)

2.3 Process Route Index (PRI) and Process Stream Index (PSI)

The PRI and the PSI were developed to include the contribution of individual components in mixtures to the process stream parameters associated to those indices (Leong & Shariff, 2009; Shariff et al., 2012). Both indices are based on parameters that impact the outcome of an explosion incident. Such parameters are density, pressure, energy, and combustibility. Although PRI and PSI are based on the same parameters, these indices are structured differently and have different purposes. The PRI is used to rank processes while the PSI is used to identify the most hazardous process streams within a process. An advantage of both indices is that the process stream parameters can be directly obtained from process simulators, easing off the computation process.

2.3.1 Calculation of the Process Route Index (PRI)

To estimate the PRI, values of density, pressure, and mass heating value (energy) for each stream are obtained from process simulations. In addition, to estimate the combustibility of the process streams, information such as stream composition and temperature is also extracted. Then, the information obtained from the process simulation is combined with data related to the lower and upper flammability limits (LFL and UFL) and the heat of combustion (ΔH_c) for each component in the streams.

Equations 15 and 16 show the effect of temperature in the flammability limits. Once the flammability limits of each component are adjusted due to the effect of temperature, flammability limits for the mixtures are computed as shown in equations 17 and 18,

$$LFL_T = LFL_{25}\left[1 - \frac{0.75(T-25)}{\Delta H_c}\right] \tag{15}$$

$$UFL_T = UFL_{25}\left[1 + \frac{0.75(T-25)}{\Delta H_c}\right] \tag{16}$$

$$LFL_{mix} = \frac{1}{\sum_{i=1}^{n}\left(\frac{y_i}{LFL_i}\right)} \tag{17}$$

$$UFL_{mix} = \frac{1}{\sum_{i=1}^{n}\left(\frac{y_i}{UFL_i}\right)} \tag{18}$$

where LFL_T and UFL_T stand for lower and upper flammability limits at a given temperature T, LFL_{25} and UFL_{25} are the lower and upper flammability limits at 25 °C, and ΔH_c is the heat of combustion; LFL_{mix} and UFL_{mix} are the lower and upper flammability limits of the mixture, y_i is the mole fraction of component i, and LFL_i and UFL_i are the lower and upper flammability limits of component i. Combustibility is then estimated with Equation 19.

$$combustibility = UFL_{mix} - LFL_{mix} \tag{19}$$

Once combustibility is obtained, the average values of the parameters can be used to calculate the PRI for the process using Equation 20.

$$PRI = \frac{\left[\begin{pmatrix}average\ mass\\ heating\ value\end{pmatrix}\begin{pmatrix}average\ fluid\\ density\end{pmatrix}\begin{pmatrix}average\\ pressure\end{pmatrix}\begin{pmatrix}average\\ combustibility\end{pmatrix}\right]}{10^8} \tag{20}$$

2.3.2 Calculation of the Process Stream Index (PSI)

PSI uses the principle of relative ranking to determine the more hazardous streams of a process. The index is composed of four sub-indices in which the four parameters (density, pressure, energy, and combustibility) are compared to the average parameter value for the process as in equations 21 to 24.

$$I_e = \frac{heating\ value\ of\ individual\ stream}{average\ heating\ value\ of\ all\ streams} \tag{21}$$

$$I_P = \frac{pressure\ of\ individual\ stream}{average\ pressure\ of\ all\ streams} \tag{22}$$

$$I_\rho = \frac{density\ of\ individual\ stream}{average\ density\ of\ all\ streams} \tag{23}$$

$$I_{FL} = \frac{combusibility\ of\ individual\ stream}{average\ combustibility\ of\ all\ streams} \tag{24}$$

To calculate the value of PSI, the values from equations 21 to 24 are combined as follows,

$$PSI = A_0(I_e I_p I_\rho I_{FL}) \tag{25}$$

where A_0 is a constant used to adjust the order of magnitude of the index (we used a value of 10 in this work).

2.4 Uncertainty evaluation

To account for the uncertainty in the inputs and propagate it through the model, an integrated framework using MC simulations was considered. The approach is based on the one proposed by Ortiz-Espinoza et al. (2019) and described in Figure 1.

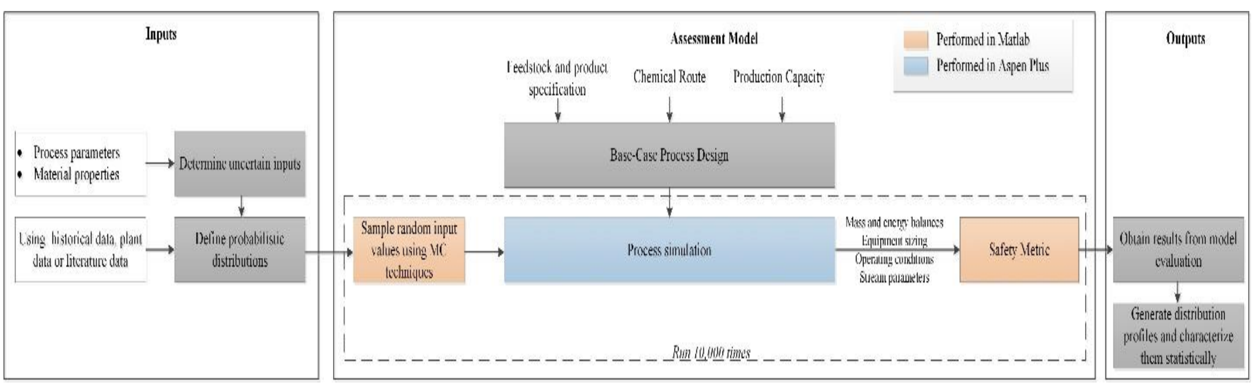

Figure 1. Integrated framework for the inclusion of uncertainty in the evaluation of safety performance of chemical processes

A base case for the process is first developed. Then, it is necessary to select the safety evaluation model and to identify the input information needed, and probabilistic distributions are derived from information obtained from historical, plant, or literature data.

After the probabilistic distributions are established, random values are sampled for each input using MC simulations. These values are then fed to the process simulator and the safety evaluation model. Data from process simulations and external information are used to evaluate the safety metrics. The results are gathered to generate the distribution profiles for the index. This step is repeated a sufficient number of times (10,000 in this case) to generate sufficient results so that a reliable characterization of the profiles can be done. The statistical characterization of the profiles includes minimum and maximum values, mean value, standard deviation, and values of risk and opportunity.

3. Case Study

To compare the selected safety metrics and its performance in the presence of uncertainty, an ethylene production process was evaluated. The process takes the production of ethylene from natural gas via the production of methanol. A great part of this process occurs in gas phase and with the presence of flammable gases (e.g. methane, hydrogen, carbon monoxide). The process consists of three stages, namely reforming, methanol synthesis, and olefins production. A detailed description of the process structure and its conditions may be consulted in Ortiz-Espinoza et al. (2017a).

The safety, economic and sustainable features of this process were previously analyzed by Ortiz-Espinoza et al. (2017b) in which the PSI was used to detect the most hazardous area of the process, and the PRI was used to assess changes in operating conditions. The Dow's F&EI and the FEDI are additionally considered in this work; these indices give a numerical value per piece of equipment, so this helps to identify the most hazardous units in the process. Then, the highest number of all the values obtained is selected as the representative number for the whole process, and changes in the design are evaluated to see if the indices are able to account for the effects of such changes. The first two steps are performed using nominal values, after which the inclusion of uncertainty is carried out using the proposed approach displayed in Figure 1.

3.1 Assumptions for safety evaluation

3.1.1 PSI

For the evaluation of the PSI, the four parameters considered by the index are put together by a multiplication rule. An important characteristic that is observed for this index is that since all factors are weighted equally, the results may be biased by the presence of different stream phases, due to high differences of density. Therefore, liquid and gas streams are considered separately, i.e. the gas phase streams are evaluated with the average value of the gas streams only, and the liquid streams are evaluated only with liquid streams data.

3.1.2 F&EI

For the estimation of the Dow's F&EI, the assumptions and recommendations in the classification guide (AIChE, 1998) are followed. For the estimation of the $penalty_{7_{F_2}}$ term, the amount of flammable material that can be released from the process unit within 10 minutes is considered.

Penalties for unit location ($penalty_{4_{F_1}}$), access ($penalty_{5_{F_1}}$), drainage and spill control ($penalty_{6_{F_1}}$), corrosion and erosion ($penalty_{8_{F_2}}$), and leakage ($penalty_{9_{F_2}}$) are not considered, since the information needed for their calculations is not available at the conceptual design stage of the process.

3.1.3 FEDI

The estimation of the FEDI is made using the methodology reported in Khan et al. (2001). For the assessment of distillation columns, the quantity of material is estimated as proposed in Castillo-Landero et al. (2019) using Equation 26. The conditions at the top of the column are used for safety calculations as suggested in Thiruvenkataswamy et al. (2016).

$$M = Feed + L + V' \qquad (26)$$

Since the index considers the volume of the vessel as an important component to calculate energy factors, small equipment units such as mixers and splitters are not evaluated.

3.1.4 PRI

For the assessment of the PRI only streams in gas phase are considered, since most of the process streams are in the gas phase.

4. Results

4.1 Safety evaluation

4.1.1 PSI

The evaluation of safety indices was performed using the information obtained from Aspen Plus simulations and external data sources (e.g. NFPA, Dow's F&EI guide). The results for the PSI evaluation are summarized in Table 4, and the most hazardous streams are highlighted in Figure 2. As can be observed, the most hazardous gas streams are contained in the methanol synthesis loop. According to the values in Table 4, the main contribution to the PSI values of such streams is the sub-index I_P that accounts for the effect of pressure. The two most hazardous liquid streams are also highlighted in Figure 2.

Although the consideration of the phase stream may be relevant, e.g. a liquid stream leaking will release more material than a gaseous stream at the same conditions, to assess the hazard levels correctly would require the consideration of other factors such as flash point and vapor pressure, and not only the stream density.

Table 4. PSI results for the streams of the ethylene process

Stream	I_e	I_P	I_ρ	I_{FL}	PSI	Stream	I_e	I_P	I_ρ	I_{FL}	PSI
1	0.425	0.712	0.590	0.320	0.573	26	0.608	0.043	0.027	0.628	0.004
2	0.409	0.570	0.527	0.313	0.384	27	1.271	0.370	0.644	0.534	1.619
3	0.409	0.570	0.318	0.464	0.343	28	1.276	0.370	0.641	0.534	1.618
4	0.348	0.570	0.161	2.055	0.654	29	1.331	0.370	0.656	0.534	1.727
5	0.515	0.570	0.525	1.660	2.557	30	1.331	0.698	1.096	0.542	5.517
6	0.515	0.570	0.525	1.660	2.557	31	1.356	0.698	1.580	0.519	7.769
7	0.914	0.570	0.340	1.660	2.943	32	1.367	0.698	1.755	0.963	16.116
8	0.914	0.570	0.340	1.660	2.943	33	1.826	0.251	0.218	0.950	0.949
9	0.394	0.570	0.944	1.073	2.272	^34	1.144	0.380	0.994	1.723	7.437
10	0.914	0.570	0.340	1.660	2.943	^35	1.144	0.872	0.997	1.723	17.124
11	0.760	0.570	0.420	1.571	2.858	^36	1.110	1.057	0.853	0.580	5.812
12	0.758	0.570	0.410	1.577	2.793	37	1.293	0.575	2.212	0.243	3.996
13	0.758	2.364	0.990	1.743	30.956	38	1.293	0.624	2.396	0.243	4.702
14	0.786	2.364	1.081	1.567	31.472	39	1.104	0.817	0.868	0.445	3.716
15	0.751	2.364	1.531	1.186	32.247	C4's	1.276	0.216	0.885	0.231	0.566
16	0.753	2.307	1.928	1.108	37.108	^C5's	1.129	0.328	1.047	0.404	1.567
17	0.759	2.202	1.812	1.105	33.443	^Ethane	1.177	0.880	0.813	0.512	4.308
18	0.860	2.136	1.610	1.045	30.920	Ethylene	1.329	0.581	1.913	0.928	13.709
19	0.860	2.136	1.610	1.128	33.377	Hydrogen	2.814	0.570	0.103	1.967	3.245
20	0.860	2.136	1.610	1.128	33.377	Natural Gas	1.441	0.741	0.885	0.281	2.658
21	0.860	2.136	1.610	1.128	33.377	^Propane	1.117	0.945	0.846	0.458	4.094
22	0.860	2.364	1.706	1.136	39.412	Propylene	1.292	0.624	2.428	0.244	4.776
23	0.860	2.364	1.429	1.177	34.214	Purge	0.866	0.285	0.368	0.552	0.502
^24	0.539	3.236	1.260	1.585	34.799	Syngas Purge	0.860	2.136	1.610	1.128	33.377
^25	1.129	0.328	1.047	0.405	1.567	Tail gas	2.314	0.251	0.196	1.228	1.397

^Liquid streams

4.1.2 Dow's F&EI

The results for the estimation of the Dow's F&EI are reported in Table 5, and the hazzard classification for each piece of equipment is shown in Figure 3. Similarly to the results for PSI, the equipment unit identified as the most hazardous one is the methanol synthesis reactor. Additionally, most of the units in the methanol synthesis loop are classified as intermediate in terms of hazard. The rest of the equipment is classified as moderate or light hazard, except for the reactors in the reforming stage. This result may be due to the penalties considered for exothermic or endothermic reactions, a characteristic that is not addressed in the PSI estimation.

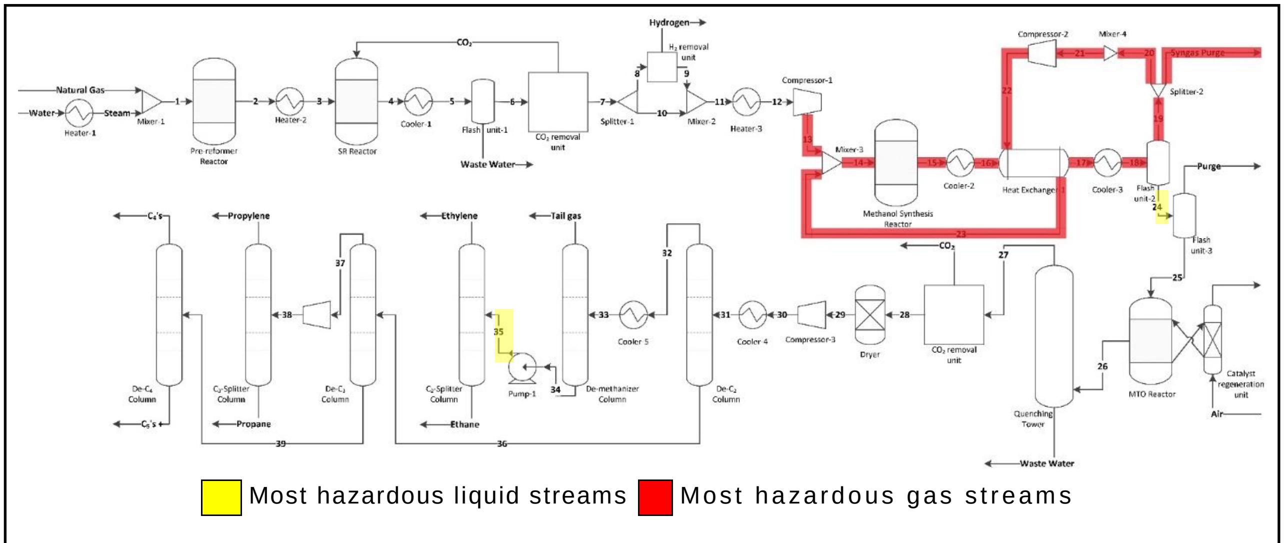

Figure 2. Identification of hazardous streams using process stream index (PSI)

Table 5. Dow's F&EI results for the equipment of the ethylene process

Piece of equipment	F&EI	Classification	Piece of equipment	F&EI	Classification
Heater-1	1.7	Light	Splitter-2	99.6	Intermediate
Mixer-1	85.2	Moderate	Mixer-4	90.9	Moderate
Pre reformer reactor	100.3	Intermediate	Compressor-2	116.0	Intermediate
Heater-2	83.6	Moderate	Flash unit-3	48.7	Light
SR Reactor	125.2	Intermediate	MTO Reactor	90.8	Moderate
Cooler-1	104.3	Intermediate	Catalyst regenerator	94.4	Moderate
Flash unit-1	93.8	Moderate	Quenching tower	82.0	Moderate
CO_2 removal unit	93.8	Moderate	CO_2 removal unit	82.2	Moderate
Splitter-1	93.8	Moderate	Dryer	82.2	Moderate
H_2 removal unit	81.7	Moderate	Compressor-3	99.0	Intermediate
Mixer-2	91.4	Moderate	Cooler-4	94.2	Moderate
Heater-3	91.4	Moderate	De-C_2 column	94.2	Moderate
Compressor-1	112.6	Intermediate	Cooler-5	84.4	Moderate
Mixer-3	105.3	Intermediate	De-methanizer	77.5	Moderate
Methanol synthesis reactor	136.8	Heavy	Pump-1	93.8	Moderate
			C_2-Splitter	81.9	Moderate
Cooler-2	104.7	Intermediate	De-C_3 column	62.9	Moderate
Heat exchanger-1	105.0	Intermediate	Compressor-4	59.0	Light
Cooler-3	103.9	Intermediate	C_3-Splitter	59.0	Light
Flash unit-2	103.9	Intermediate	De-C_4 column	42.8	Light

4.1.3 FEDI

Results for the ethylene process using the FEDI index are presented in Table 6 and Figure 4. Some discrepancies are observed with respect to the PSI and the F&EI results. According to the FEDI evaluation, the most hazardous piece of equipment is the C_3-Splitter column, followed by the de-propanizer unit and the methanol reactor, which are classified as hazardous. One important characteristic of this index is that it considers the volume of the vessel in the estimation of the physical energy factor (F_{2FEDI} and F_{3FEDI}). Therefore, for the biggest units such as distillation columns, the results may be influenced by their size. From the results of the PSI and F&EI, however, this may not necessarily represent an accurate hazard level for the process unit.

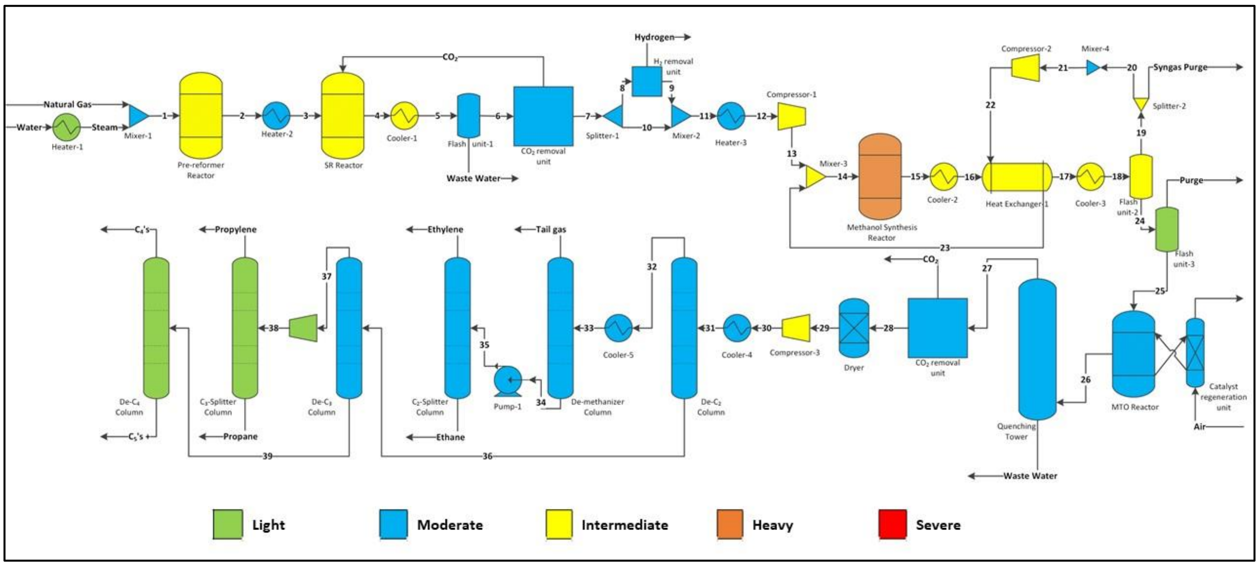

Figure 3. Classification of equipment according to degree of hazard using the Dow's F&EI

4.2 Assessment of design changes

Given that we are dealing with a conceptual design stage of the process and that we have identified the most hazardous pieces of equipment, changes to the design to enhance safety levels can be readily analyzed. To keep track of the effect of the changes in the process safety performance, the safety metrics are evaluated for each individual change implemented for the process conditions. To evaluate the response of the indices on the same basis, the modifications were made to the operating pressure of the methanol synthesis loops, since two out of the three indices identified this area of the process as the most hazardous. The results for the evaluation of the different indices at different operating pressures are reported in Table 7.

Table 6. FEDI results for the equipment of the ethylene process

Piece of equipment	FEDI	Classification	Piece of equipment	FEDI	Classification
Heater-1	18.0	No hazard	Flash unit-3	93.1	Less Hazardous
Pre reformer reactor	140.4	Moderately hazardous	MTO Reactor	123.8	Moderately hazardous
Heater-2	148.1	Moderately hazardous	Quenching tower	119.0	Moderately hazardous
SR Reactor	151.3	Moderately hazardous	CO_2 removal unit	91.3	Less Hazardous
Cooler-1	157.5	Moderately hazardous	Dryer	91.3	Less Hazardous
Flash unit-1	156.9	Moderately hazardous	Compressor-3	89.6	Less Hazardous
CO_2 removal unit	134.9	Moderately hazardous	Cooler-4	89.7	Less Hazardous
Heater-3	107.5	Moderately hazardous	De-C_2 column	199.8	Moderately hazardous
Compressor-1	107.6	Moderately hazardous	Cooler-5	87.4	Less Hazardous
Methanol synthesis reactor	306.6	Hazardous	De-methanizer	113.8	Moderately hazardous
			Pump-1	71.9	Less Hazardous
Cooler-2	119.7	Moderately hazardous	C_2-Splitter	164.8	Moderately hazardous
Heat exchanger-1	119.5	Moderately hazardous	De-C_3 column	300.3	Hazardous
Cooler-3	122.5	Moderately hazardous	Compressor-4	147.9	Moderately hazardous
Flash unit-2	122.4	Moderately hazardous	C_3-Splitter	526.0	Extremely hazardous
Compressor-2	76.9	Less Hazardous	De-C_4 column	187.7	Moderately hazardous

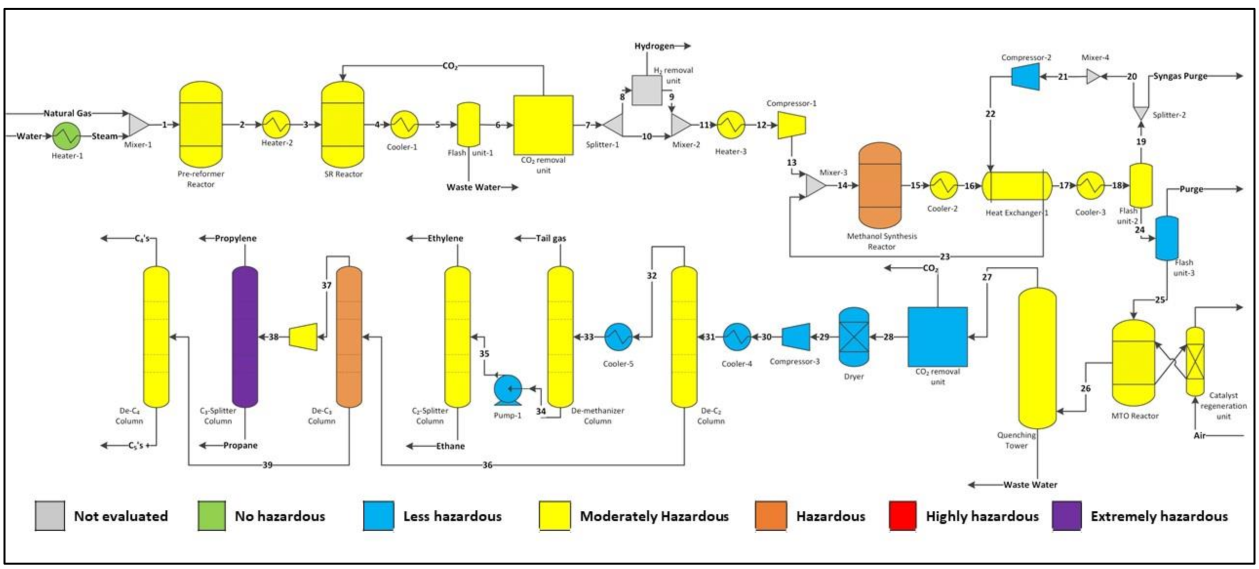

Figure 4. Classification of equipment according to hazard levels using the FEDI

Table 7. Safety indices evaluated for different pressures of the methanol synthesis reactor

Pressure, bar	**PRI**	**F&EI**	**FEDI**
83	9.47	136.8	306.6
70	8.00	135.8	306.5
60	6.84	135.4	306.4
50	5.81	135.3	306.3

The F&EI and the FEDI do not present a significant change. While changes in the PRI values are more notorious, the lack of a ranking for the PRI hinders the possibility to classify these changes in terms of hazard levels. One possible reason for the minor change in the F&EI and FEDI indices is the way in which they are structured, i.e. while there is a decrease of pressure, an increase in the quantity of chemical handled by the unit may compensate the overall effect on the value of the index.

4.3 Uncertainty analysis

The uncertainty analysis was made considering the probability distributions shown in Table 8. These distributions take into account the pressure ratio of the compressors in the methanol synthesis loop, where most of the hazardous equipment or streams are located.

By applying the approach depicted in Figure 1, we obtained the cumulative probability distributions shown in figures 5 to 7. The doted lines in those figures represent the expected (nominal) values.

Table 8. Uncertain inputs and probability distributions[+]

Variable	**Minimum**	**Most likely**	**Maximum**
Compressor-1 pressure ratio (83 bar)	3.94	4.15	4.37
Compressor-2 pressure ratio (83 bar)	1.05	1.11	1.17

[+]Note: Distribution types were triangular.

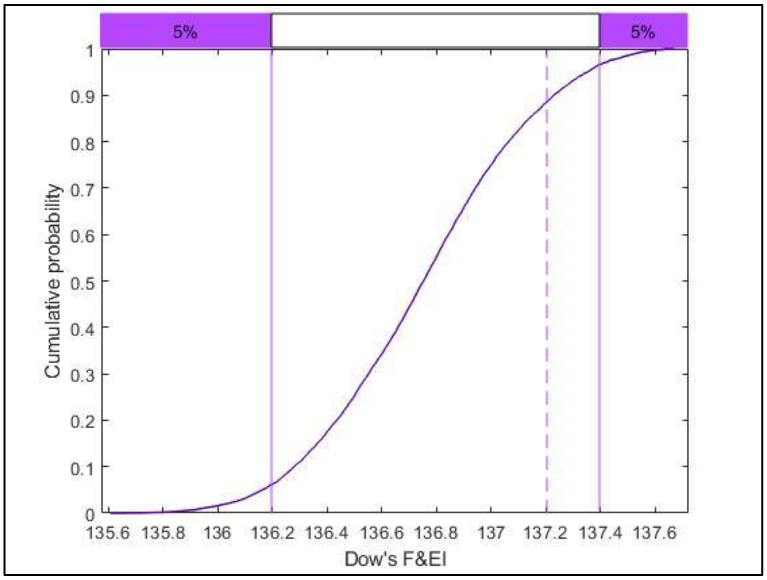

Figure 5. Probability distribution for the Dow's F&EI

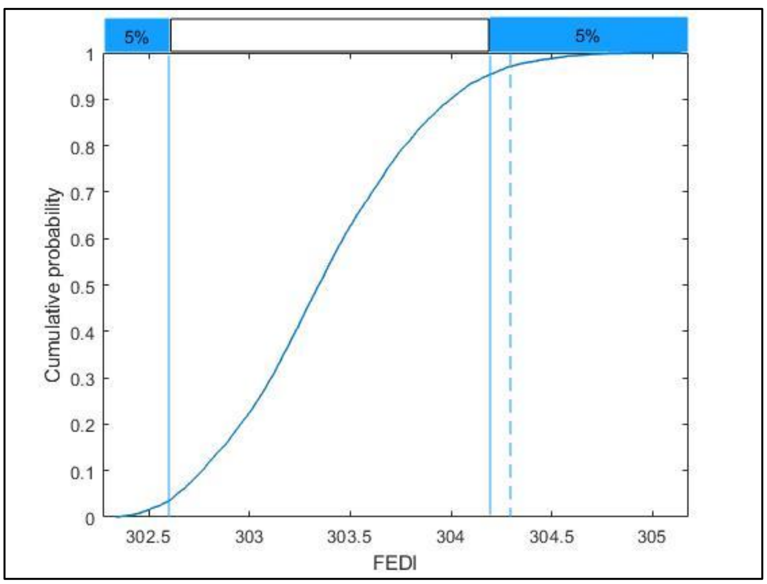

Figure 6. Probability distribution for the FEDI

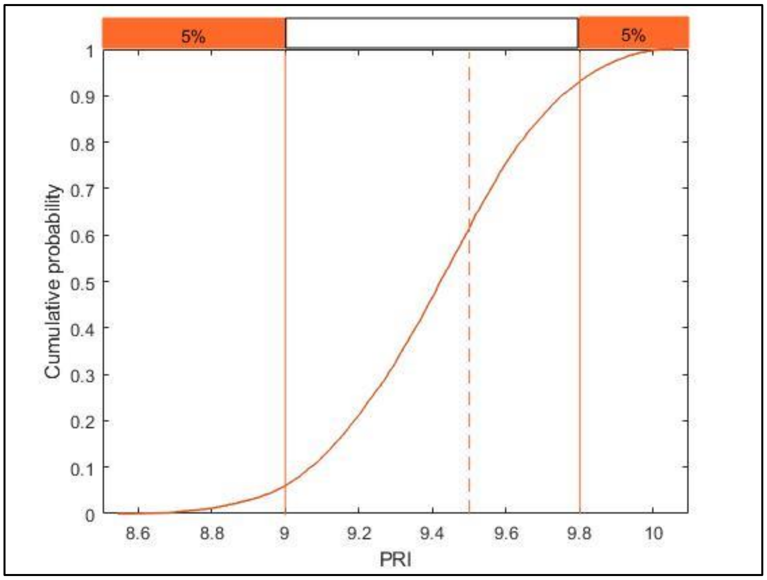

Figure 7. Probability distribution for the PRI

The results show that the expected values for the F&EI and the FEDI have a high probability of occurrence, 87% and 97.3% respectively, while the PRI expected value has only 57%. This observation indicates that the F&EI and the FEDI indices can produce good results with nominal values. It should be pointed out that it is always desirable that the calculated occurrence of an index value is as high as possible, because a low probability could represent an underrating of the indices when using nominal values. The results were complemented by the probabilistic characterization of the three indicators reported in Table 4. Standard deviation values for the three indices as fairly low, in accordance with the minimum and maximum values that were obtained for the calculation of the indices.

Table 4. Probabilistic characterization of results for the MTO process with methanol synthesis

Metric	Mean	Minimum	Maximum	Standard deviation	P5	P95
PRI	9.41	8.54	10.06	0.26	8.98	9.84
F&EI	136.75	135.61	137.67	0.36	136.16	137.35
FEDI	303.37	302.34	305.14	0.47	302.64	304.18

5. Conclusions

Four safety indices were analyzed, out of which three (PRI, F&EI and FEDI) are related to the performance of the overall process and one of them (PSI) to the risk characterization of streams within the process. assessment of safety The indices are conveniently applied during the conceptual design of a process. Regarding the indices related to the overall process performance, their comparison identified some disadvantages of those metrics when evaluating flowsheets that contain processing tasks carried out mostly in the gas phase. The comparison was completed with an uncertainty analysis that provides insightful information about the metrics. It was observed that the PSI and F&EI indices classified the streams and the units within the same process area as the most hazardous. The FEDI also identified the equipment pieces in the same area as hazardous, but with a lower risk level. This result may be influenced by the term of volume that is used in the calculation of the FEDI index. With regard to the usefulness of the indices to track changes in the process design, only the PRI was able to reflect a significant numerical change, but its lack of relationship with respect to a hazard level characterization of the process limits the usefulness of this finding. The results obtained for the indices call for the need to develop a new or modified index through a careful inclusion of the major characteristics of the three indices analyzed in this work, so that items that appear to be relevant for the evaluation of risk are taken into account. On the other hand, elimination of terms that bias the results towards a particular class of streams or equipment units that are not necessarily characterized as risky items within the process should be considered.

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