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A Consequence Based Approach to the Quantitative Assessment of Inherent Safety

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The availability of inherent safety drivers for early process design is a critical issue for the further development of the chemical and process industry. In this study, a consequence-based method for the inherent safety assessment of process alternatives was developed. Key performance indicators (KPIs) for inherent safety were defined and a procedure for their quantitative assessment was developed. A specific equipment classification and the related failure modes were identified, in order to define the potential accidental scenarios associated to each process unit. Rules for the calculation, by physical model runs, of the damage distances for conventional effects were also defined. Credit factors to account for the safety score of the different equipment classes were introduced. KPIs were defined by the combination of the expected damage distances and of credit factors. The methodology was demonstrated through a case study, and provided useful results both for the identification of safety critical units, and for the assessment of the inherent safety of alternative processes. The comparison of the results with those obtained from other literature methods for inherent safety assessment showed that the KPIs introduced allowed considering the hazards coming from auxiliary equipment, that are often overlooked in conventional inherent safety assessment methods. © 2007 American Institute of Chemical Engineers *AIChE J,* 53: 3171–3182, 2007
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Introduction

Inherent safety promotes the elimination or the extensive reduction of process hazards by proper design choices. The idea of limiting process hazards rather than controlling the risk was introduced by Kletz,[1–2] who proposed the five fundamental principles of inherent safety: minimization, substitution, attenuation, simplification and limitation of effects. Several studies further developed these concepts, outlining the technical and economic advantages of the inherent approach to process safety.[3–5]

Although inherent safety analysis may be applied to any of the different stages of process design and even during process operation, the major opportunities for cost-effective hazard reduction by inherent safety criteria were identified during early process design. Thus, the inherent assessment tools developed should cope with the limited amount of information suitable in initial process and/or plant design

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stages. Indexing approaches were usually proposed to represent the process hazards, allowing the identification of inherently safer design alternatives. Several quantitative tools were developed for inherent safety assessment in process design. Table 1 reports a summary of the inherent safety indexes proposed in the literature, and the detail of process data required for their calculation. The index proposed by Edwards and Lawrence[6] represents the first effort toward quantification of inherent safety. The method, also revisited by Gupta,[18] is based on scoring a limited number of hazardous proprieties (e.g., flammability, toxicity, pressure, etc.) for each reaction step of a process. The same approach was used by Heikkilä,[7] and by Gentile,[19] that proposed the adoption of a fuzzy approach in order to smooth some biases generated by the former crisp approach in assigning scores. These specific scoring methods for inherent safety calculation may be easily applied even having limited details on the process. However, these methodologies are heavily based on simplifications and built-in assumptions that strongly rely on the specific experience of the developers, and may hardly retain their value when further information on the process become available. Methods requiring a higher level of detail on the process were also proposed. The safety tools of the INSET toolkit[9] provide an evaluation of the hazard based on inventories and factors scored from the proprieties of a substance. A similar approach is followed by the safety subindexes of EHS.[10] Nevertheless the assessment procedure is still based on the evaluation of inherent safety scores. The Dow Fire & Explosion Index (F&EI),[14] the Dow Chemical Exposure Index (CEI),[15] and the Mond Fire, Explosion and Toxicity Index (F,E&T),[16,17] were as well proposed as possible tools for quantitative inherent safety assessment.[5,7,20–22] However, since these methods were originally developed for the assessment of existing plants, the complete calculation of the indexes requires several details that usually are not available during early process development. Recently, a new approach, named IS2I, was developed by Khan and Amyotte[11,12] in order to integrate the assessment of inherent safety guidewords application, hazard potential and safety costs. However, the approach resorts to scoring based on expert judgment of the analyst, thus introducing some subjective elements in the comparison of alternatives.

Therefore, despite the valuable research effort that resulted in the presented approaches, there is still a recognized concern on the availability of reliable inherent safety assessment tools, suitable for decision-making and for the comparison of alternatives during process design and optimization. In particular, no broadly accepted methodologies are available and some of them are based on subjective judgment in the scoring process. These problems were identified as one of the main reasons for the limited diffusion of inherent safety in the current engineering practice.[5]

In this article, a specific effort is made to develop an alternative method for inherent safety assessment in early process design. Key performance indicators (KPIs) for inherent safety are defined and a procedure for their quantitative assessment is developed. In order to overcome the dependence of the scores on the experience and on expert judgment, the procedure is strongly based on consequence assessment of potential accidents. A specific equipment classification and the related failure modes are identified, in order to define the

Table 1. Data Required for the Calculation of Some Quantitative Indexes Proposed for Inherent Safety Assessment

Data Required	PIIS[6]	ISI[7]	i-safe Index[8]	INSET (I, J)[9]	ESH[10]	I2SI[11,12]	SWeHI[13]	Dow F&EI[14]	Dow CEI[15]	Mond F,E&T[16,17]	This study
Chemicals and their proprieties	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Reactions and interactions	✓	✓	✓	✓	✓	✓	✓	✓		✓	✓
Operative conditions	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Process Flow Diagram		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Equipment inventory				✓	✓	✓	✓	✓	✓	✓	✓
Material balances						✓	✓	✓	✓	✓	✓
P&ID						✓	✓	✓		✓	
Layout definition						✓	✓	✓		✓	
Equipment design data								✓	✓	✓	

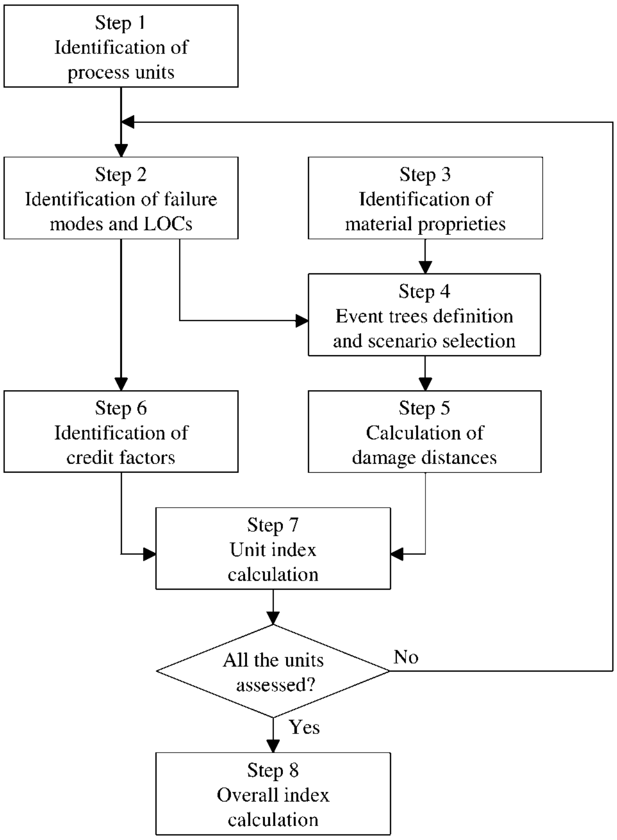

Figure 1. Flow diagram of the method.

potential accidental scenarios associated to each process unit. Rules for the calculation, by physical model runs, of reference damage distances are also defined. Credit factors to account for the safety score of the different equipment classes are introduced. The methodology is applied to a case study in order to demonstrate its suitability for the identification of safety critical units, and for the assessment of the inherent safety of alternative processes.

Methdology Developed for Inherent Safety Assessment

General features

The aim of the method is to compare the inherent safety of alternative process schemes by the calculation of quantitative hazard and risk indexes for single units and for the overall process. The conceptual flow diagram of the method is reported in Figure 1. As most of the methods requiring the assessment of safety indexes, the procedure starts from the identification of the equipment units of each process, based on a specific equipment classification. KPIs are then calculated for each unit, based on the consequence analysis of credible scenarios. The single unit indexes may be further added in order to provide an overall hazard index.

The estimation of the KPIs of the single units is directly based on the assessment of the expected consequences of credible scenarios, whose straightforward calculation is presently possible with the aid of commercial software codes for consequence analysis. The use of a procedure based on consequence assessment contributes to limit the problems of built-in judgment on the relative importance of some parameters, that resulted a critical point in the application of score-based indexes (e.g., PIIS and ISI)[18,19]. Moreover, the rigid and sometimes unclear assessment structure of some index structure of some methods may lead to difficulties in their application. In particular, some indexes were designed only for specific process applications,[10,22] and their evaluation in other types of processes is not straightforward. In the methodology proposed, the approach introduced and the use of consequence analysis allow a more general application of the procedure.

Required data on process alternatives

The input data required for the application of the method to the process alternatives of concern are preliminary data on process equipment, and the data contained in a simplified process flow diagram (PFD): (1) substances and operating conditions (pressure, temperature, phase) in each unit of the process; (2) material flows in process lines; (3) general technical specifications of the equipment units; and (4) a preliminary estimation of substance inventories in each process unit.

Identification of process units

As shown in Figure 1, the starting point for the application of the procedure is the identification of relevant equipment units to which the method should be applied. The units identified at this stage represent the basic elements of the assessment. Equipment units to be considered were sorted by a specifically defined classification, that was based on the geometrical structure of the units. Table 2 reports the main general unit categories defined for process equipment. For each unit category, subcategories featuring the specific characteristics of the units related to their function/operative condition were also defined.

Definition of the failure modes and of the events leading to the loss of containment

The following step of the method consists in the identification of reference failure modes which lead to a loss of containment (LOC). Reference LOCs were associated to the more common classes of pieces of equipment, following the classification reported in Table 2, on the basis of approaches suggested in the technical literature.[23–25] Table 3 reports an example of the LOC events associated to different equipment categories on the basis of the approach suggested by the TNO "purple book".[23] When nonstandard equipment needs to be considered in the analysis, Failure Mode and Effect Analysis (FMEA), may be applied to identify the credible events leading to loss of containment.

Several LOC events are possible for each piece of equipment. "Credit factors" may be determined in order to assess the credibility of the LOCs identified. In this approach, the likelihood of the reference LOCs was estimated from statistical data. Reference failure frequency data may be easily used to evaluate the hazard linked to each class of equipment,[7] and to represent the susceptibility to particular failure modes of the equipment class. Equipment frequency failure data are reported in several publications.[23,25–28] The reference frequencies reported for a given equipment failure mode by the

Table 2. Main General Categories Proposed for the Classification of Process Units

General Categories	Subcategories	Code
Vessel-like equipment	Atmospheric vessel (storage, process, etc.)	EQ1.1
	Pressurized vessel (storage, column, reactor, etc.)	EQ1.2
	Mobile vessel (tank wagon, road tanker)	EQ1.3
Tube bundle equipment	S&T heat exchanger, reactor, etc.	EQ2.1
Plate and frame equipment	Filter, plate heat exchanger, etc.	EQ3.1
Pipe	Pipeline, manifold, etc.	EQ4.1
Pumping equipment	Pump (centrifuge, alternative, etc.)	EQ5.1
	Compressor (centrifuge, alternative, etc.)	EQ5.2
Warehouse	Packed materials (bags, barrels, etc.)	EQ6.1
	Spare materials (piles, etc.)	EQ6.2
Special equipment	Solid handling (conveyors, crushers, etc.)	EQ7.1
	Other	EQ7.2

''purple book''[23] or, if not available, by API publications[26] were used in this approach as "credit factors" for standard technologies. Specific failure frequency data, e.g., derived from available statistical data or from conventional fault-tree analysis,[25] can be introduced to account for the credit factors derived from the adoption of technologies with higher safety standards. This approach allows the estimation of "standard" credit vectors for each reference class of equipment. The elements of the credit vector are the aforementioned defined credit factors for each LOC considered for the unit. Table 3 gives an example of credit vectors defined for some common pieces of equipment. Clearly enough, the standard credit vectors reported in Table 3 may be modified to account for improved safety standards of specific pieces of equipment.

Event tree definition and scenario selection

As previously discussed, this methodology is based on the calculation of equipment hazard indexes derived from the consequences of the accidental scenarios that may be associated to each unit. Thus, a necessary step in the application of the procedure is the identification of the accidental scenarios that may be associated with each unit. A set of reference event trees, derived from conventional approaches proposed in the technical literature,[23–25] were defined to identify the expected incidental scenarios associated with each LOC. The selection of the proper event tree follows the criteria used in conventional risk analysis, that are based on the characteristics of the LOC event and on the type of hazard, of the physical properties, the temperature, the pressure and the phase of the released stream. Further details on the criteria for event tree definition and selection are reported in the literature.[24,29] Table 4 summarizes the scenarios associated with the different release categories considered for flammable/toxic substances.

Calculation of damage distances

The calculation of the equipment hazard indexes requires the estimation of a parameter representing the severity of each scenario that may be triggered by the identified LOC events. Different types of physical effects (thermal radiation, overpressure or toxic concentration) are taken into account and compared in the analysis. Thus, in order to obtain a homogeneous severity parameter of each scenario, the damage distances corresponding to a given effect threshold were calculated. The effects on humans were taken into consideration to define threshold values for each physical effect. Table 5 shows the threshold values selected, that are suggested in technical documents as representing the 1% mortality level of exposed population.[24,30–32] Damage distances, are, thus, defined as the maximum distance where, at a fixed height (1m in this study), the physical effect of the scenario (thermal radiation, overpressure or concentration) reaches the threshold value. Damage distances may, thus, be calculated for each scenario using consequence analysis models, on the basis of the LOC characterization performed in the previous steps. Several models and commercial software tools are available in the literature for consequence analysis, and may be used for the purpose. The only limitation is that the same model should be used in the comparative assessment of different LOC events to obtain coherent results and to avoid at least the possible "bias" in the comparison derived from

Table 3. LOCs and Related "Credit Factors" for Different Categories of Process Equipment

LOC	Horizontal gas storage (EQ1.2)	Floating roof tank (EQ1.1)	Centrifugal pump (EQ5.1)	Centrifugal compressor (EQ5.2)	Shell and tube heat exchanger (EQ2.1)
R1: small leak, continuous release from a 10 mm equivalent diameter hole	1×10^{-5}	1×10^{-4}	*n.a.*	*n.a.*	1×10^{-3}
R2: catastrophic rupture, release of the entire inventory in 600 s	5×10^{-7}	5×10^{-6}	*n.a.*	*n.a.*	5×10^{-5}
R3: catastrophic rupture, instantaneous release of the entire inventory and release from the full-bore feed pipe	5×10^{-7}	5×10^{-6}	*n.a.*	*n.a.*	5×10^{-5}
R4: pipe leak, continuous release from a hole having 10% of pipe diameter	*n.c.*	*n.c.*	5×10^{-4}	1×10^{-3}	*n.c.*
R5: pipe rupture, continuous release from the full-bore pipe	*n.c.*	*n.c.*	1×10^{-4}	1×10^{-4}	*n.c.*

Data for credit factors derived from the literature[23,26]. *n.a.*: not applicable; *n.c.*: not considered.

Table 4. Summary of Conventional Scenarios considered by the Reference Set of Event Trees for the More Common LOC Events Involving Flammable or Toxic Fluids, Listed as a Function of Release Conditions

	FB	JF	VE	FF	TD	PF	BV
Continuous releases							
Gas or vapor		✓	✓	✓	✓		
Pressurized liquefied gas		✓	✓	✓	✓		
Cryogenic/Boiling liquid			✓	✓	✓	✓	
Non-boiling liquid					✓	✓	
Instantaneous releases							
Gas or vapor			✓	✓	✓		
Pressurized liquefied gas	✓		✓	✓	✓		✓
Boiling liquid			✓	✓	✓	✓	
Cryogenic liquid	✓		✓	✓	✓		
Non-boiling liquid					✓	✓	

Fireball (FB), Jet Fire (JF), Vapor Cloud Explosion (VE), Flash Fire (FF), Toxic Dispersion (TD), Pool Fire (PF), BLEVE (BV).

model differences. In the case study discussed in the following, the set of consequence analysis models reported by the TNO "yellow book"[33] were used.

Thus, for each unit it is possible to calculate an impact matrix, having a number of rows equal to all the credible LOC events and a number of columns equal to the maximum number of accidental scenarios related to each LOC event. Each element of the impact matrix for the k-th unit, $m_{i,j,k}$, is related to the expected damage distance calculated for the j-th scenario of the i-th LOC event by the following expression

$$m_{i,j,k} = \max(d_{i,j,k}, c) \tag{1}$$

where $d_{i,j,k}$ is the calculated damage distance and c is a constant, considered equal to 5 m in this study. The use of the constant c in Eq. 1 allows the definition of a "near field" zone, in which the consequences of the event are neglected. This takes into account the unreliability of conventional consequence assessment models in describing correctly the consequences of the events in the "near field", thus, avoiding biases in the analysis due to these uncertainties.

Starting from the impact matrix, a unit hazard vector h may be defined, whose elements are the maximum damage distances calculated for each LOC event considered in the analysis

$$h_{i,k} = \max_j(m_{i,j,k}) \tag{2}$$

where $h_{i,k}$ is the maximum damage distance of the i-th LOC event considered for k-th unit.

Calculation of hazard indexes

The key performance indicators (KPIs) are obtained starting from the hazard and credit vectors calculated for each unit. A unit potential hazard index may be defined as follows

$$UPI_k = \max_i(h_{i,k})^2 \tag{3}$$

where UPI_k is the unit potential hazard index of the k-th unit, and $h_{i,k}$ is the corresponding hazard vector. The unit hazard index, is, thus, representative of the maximum impact area that may derive from the worst-case scenario considered for the unit.

Credit factors may be introduced in the analysis in order to consider the safety scores of the equipment, and to consider differences in inherent safety performance deriving from equipment technology

$$UHI_k = \sum_{i=1}^{n_k} cf_{i,k} \cdot h_{i,k}^2 \tag{4}$$

where UHI_k is the unit inherent hazard index of the k-th unit, n_k is the number of LOC events considered for the k-th unit, $cf_{i,k}$ and $h_{i,k}$ are, respectively, the credit factor, and the maximum damage distance calculated for the i-th LOC event. The value of the index is higher for units having higher potential hazards or a higher record of LOC events.

The overall indexes of a group of N units (e.g., the entire plant) are calculated as follows starting from the unit indexes

$$PI = \sum_{k=1}^{N} UPI_k \tag{5}$$

and

$$HI = \sum_{k=1}^{N} UHI_k \tag{6}$$

Thus, the methodology developed allows the calculation of indexes representing the inherent safety performance of the plant, based either on a direct assessment of potential worst-case scenarios (PI) or of likely safety performance and release scenarios of process units (HI). Both indexes represent a quantification of the inherent safety of a process, hav-

Table 5. Threshold Values Assumed for Damage Distance Evaluation*

Physical effect	Threshold Value
Flash Fire	1/2 LFL
Fireball	7 kW/m^2
Jet Fire	7 kW/m^2
Pool Fire	7 kW/m^2
Vapor Cloud Explosion	14 kPa
Physical/mechanical explosion	14 kPa
BLEVE	14 kPa
Toxic exposure	IDLH

*LFL: Lower Flammability Limit; IDLH: Toxic Concentration Immediately Dangerous to Life and Health.

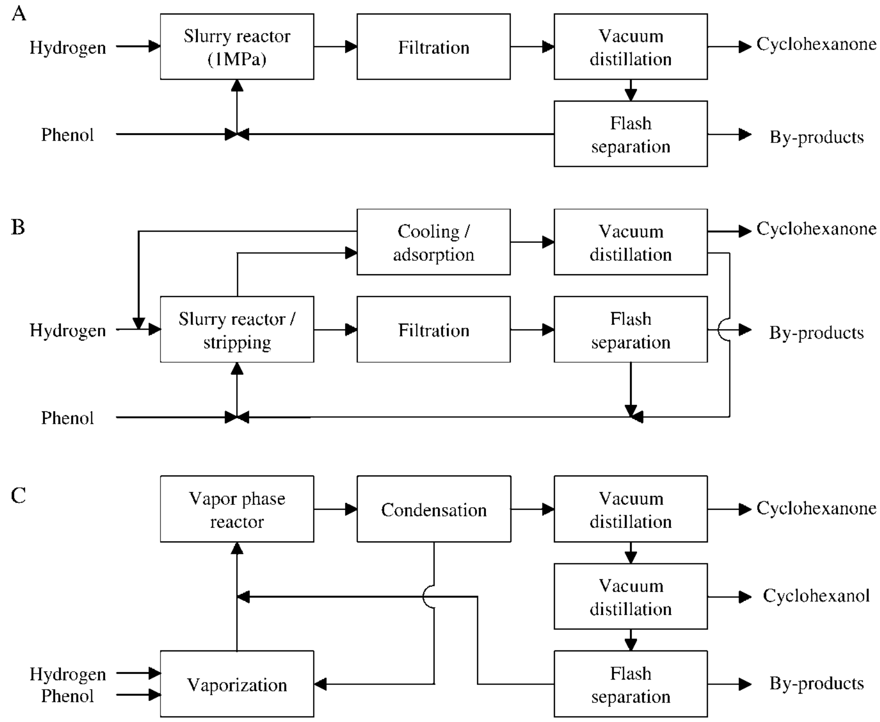

Figure 2. Three process options for the catalytic cyclohexanone synthesis by phenol hydrogenation discussed in the case study.

(A) liquid-phase pressurized hydrogenation; (B) liquid-phase hydrogenation and striping, (C) gas-phase hydrogenation.

ing lower values as the inherent safety of the process is increased.

This methodology was applied to several case studies, in order to test its suitability for the assessment of the inherent safety of alternative process schemes. The results obtained were also compared to those from several methods previously proposed in the literature for the assessment of inherent safety (see Table 1), in order to understand the potential advantages and the limitations of the proposed technique. The results of one of these case studies are discussed in the following.

Description of the Case Study

The inherent safety of three options for cyclohexanone production was assessed. The process options taken into account represent three alternative industrial production processes used in the last 50 years for the production of this organic intermediate.[34] All the options are based on the catalytic hydrogenation of phenol according to the reaction

$$C_6H_5OH + 2H_2 \xrightarrow{Pd} C_6H_{10}O \tag{7}$$

Cyclohexanone yield is 96% or higher, according to the technology used. Cyclohexanol and high-boiling byproducts are formed in side reactions and have to be separated to reach the required product quality. Figure 2 reports the simplified block diagram of the three process alternatives considered. The conditions under which the phenol hydrogenation reaction is carried out are the key difference among the assessed options. In alternative A, the reaction takes places in a slurry pressurized reactor (1 MPa and 408 K). The reacted stream is filtered to remove the catalyst, and the product is vacuum-distilled. The bottoms are recycled back to the reactor after a flash distillation to remove the high-boiling byproducts. In alternative B the slurry (418 K) in not pressurized and products are continuously stripped by a gas flow. The condensable fraction of this stream is recovered in a train of two quenching/absorption columns by recycling of the cooled condensate. The product is vacuum-distilled from this stream. A minor liquid side stream from the reactor allows the continuous separation of high-boiling byproducts, preventing their accumulation in the reactor. In alternative C a gas-phase reaction occurs in a fixed-bed reactor. Phenol feed is vaporized and mixed with hydrogen. Reaction products are condensed and distilled. In this process, a valuable co-product stream of cyclohexanol is separated in a dedicated vacuum column. Further details on the processes considered are reported elsewhere.[34]

In order to carry out the analysis, a basis of 98Gg/year cyclohexanone production was assumed. A simplified PFD was defined for each process (an example for alternative A is reported in Figure 3 to show the level of detail required for the analysis), and the heat and mass balances were carried out. A preliminary estimation of the operating conditions, of the substance inventory and of the hold-up was also carried out for each process unit considered in the PFDs.

Results and Discussion

Assessment of the case study

Table 6 reports, for alterative A, the damage distances and credit factors resulting from the application of the method

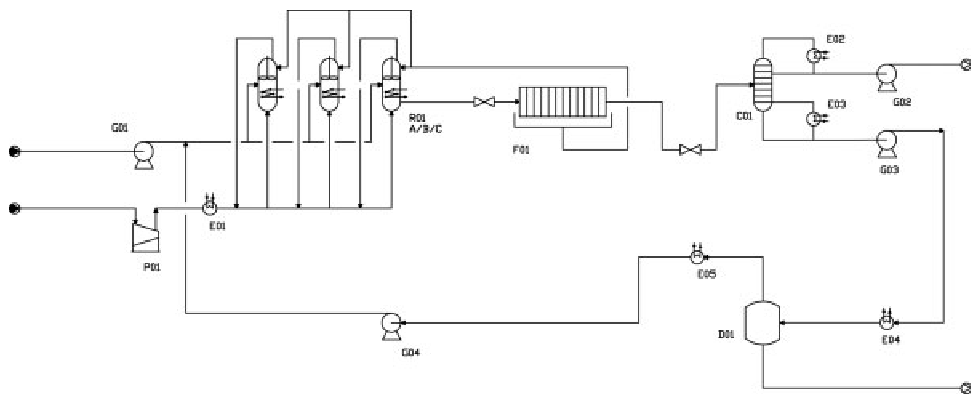

Figure 3. Case study, alternative A: liquid-phase pressurized hydrogenation for cyclohexanone synthesis.

Example of the level of detail required for the simplified PFD used in the assessment of case studies. Phenol feed pump (G01); hydrogen compressor (P01); hydrogen cooler (E01); slurry reactors (R01 A/B/C); filter (F01); vacuum distillation column (C01); condenser (E02); reboiler (E03); cyclohexanone pump (G02); bottom pump (G03); evaporator (E04); flash drum (D01); condenser (E05); recycle pump (G04).

described previously. The table shows that important differences (up to some orders of magnitude) may be present both in the damage distances, and in the credit factors for different LOCs concerning the same piece of equipment. As expected, scenarios involving toxic dispersions are those resulting in higher damage distances. On the other hand, higher credit factors are obtained for units that are more likely to cause loss of containment (e.g., heat exchangers, compressors and pumps etc.). Table 7 shows the results obtained in the calculation of the equipment potential, and of the inherent hazard indexes. The potential hazard index only gives information on the equipment that may potentially trigger the most severe scenario, while the inherent hazard index also includes information concerning the credibility of the possible scenarios. Thus, the inherent hazard index yields a more realistic description of the credible accidental events that may be associated to plant operation. In particular, this index points out the importance of the safety performance of small pieces of equipment, as compressors and heat exchangers, on the inherent safety of the plant, since these components may have per se relatively small damage distances, but are more vulnerable to undergo loss of containment events. As shown in the table, these units have inherent hazard indexes that are often comparable to those of major process units (e.g., columns or reactors) that have potentially more severe scenarios, but higher safety scores, and, thus, lower credit factors.

The analysis of the results in Table 7 allows the addressing of some important features of the different alternatives for cyclohexanone production. The unit potential hazard indexes show that, as expected, LOCs in reactors and distillation columns may cause high-damage areas due to the quantities of toxic material that may be released. Nevertheless, the units employed in the recovery of the product from the gas-phase in options B and C yield as well very high values of the UPI. These components handle both the gas-phase stream collected from all the reaction units, and the hot volatile liquids resulting from condensation. Long-distance toxic dispersions and vapor cloud explosions, are, thus, possible following LOC events in these units.

If the overall indexes are considered, the ranking among alternatives given by potential indexes becomes straightforward, due to the presence of different numbers of units that may trigger long-distance scenarios in the alternative processes, process A being the more penalized. However, the potential hazard gap between options A and B is decreased if credit factors are considered, since the three reactors of option A results more hazardous, due to the higher operating pressure, and the effect of the UPI index of the quenching columns in option B is limited by the low credit factor of catastrophic failure scenarios.

Alternative C is identified as the preferable option by both inherent safety performance indicators, PI and HI. This is a direct consequence of the low UPI and UHI values of the single units. In particular, the choice of a nonpressurized gas-phase reaction minimizes both hazard distances and the hazard related to small, but highly credible, leaks, that played a major role in the reactor hazard of former options. The hazard related to the cyclohexanol distillation is suggested to be limited if compared to cyclohexanone separation, since minor inventories are involved. Moreover, also the hazard related to vaporization of reagents and condensation of products is much lower than in option B.

Comparison of results with those from existing inherent safety assessment methods

The case study was also analyzed using literature methodologies for inherent safety index assessment. In particular, the following methods were considered:

- Prototype Index of Inherent Safety (PIIS) proposed by Edwards and Lawrence[6];
- Inherent Safety Index (ISI) proposed by Heikkilä[7];
- Potential of Danger for safety in Environmental Safety and Health (ESH) by Koller et al.[10];
- Tools I and J of INSET Toolkit (INSET);[9]
- Safety Weighted Hazard Index (SWeHI) by Khan at al.[13]
- Integrated Inherent Safety Index (I2SI) by Khan and Amyotte;[11,12]
- Dow Fire and Explosion Index (F&EI);[14]
- Dow Chemical Exposure Index (CEI).[15]

The comparison of the results obtained by the methods listed ealier required some further assumptions. In particular, some methods (e.g., ESH, INSET) yield a cluster of indexes

Table 6. Alternative A of the Case Study: Calculated Damage Distances ($d_{i,j,k}$) and Credibility Factors ($cf_{i,k}$) for each Scenario of Each Process Unit (see Figure 3)

	Unit	Eq. Class	LOC	Scenario	$cf_{i,k}$ (1/a)	$d_{i,j,k}$ (m)
R01	Single slurry reactor	EQ1.2	R1	JF	1×10^{-4}	7.6
				VE	1×10^{-4}	12
				FF	1×10^{-4}	7.4
				TD	1×10^{-4}	58
				PF	1×10^{-4}	14
			R2	TD	5×10^{-6}	66
				PF	5×10^{-6}	14
			R3	JF	5×10^{-6}	23
				VE	5×10^{-6}	19
				PF	5×10^{-6}	13
C01	Vacuum distillation column	EQ1.2	R3	VE	1×10^{-5}	30
				TD	1×10^{-5}	61
				PF	1×10^{-5}	17
				EX	1×10^{-4}	36
D01	Flash drum	EQ1.2	R3	JF	1×10^{-7}	20
				VE	1×10^{-7}	9.6
				FF	1×10^{-7}	6.4
				TD	1×10^{-7}	16
F01	Filter	EQ3.1	R4	TD	6×10^{-4}	8
				PF	6×10^{-4}	15
			R5	TD	1×10^{-5}	61
				PF	1×10^{-5}	17
E01	Hydrogen cooler	EQ2.1	R1	JF	1×10^{-3}	8.2
				VE	1×10^{-3}	13
				FF	1×10^{-3}	7.5
			R3	JF	1×10^{-5}	22
				VE	1×10^{-5}	14
E02	Condenser	EQ2.1	R3	TD	2×10^{-5}	16
				PF	2×10^{-5}	17
				EX	1×10^{-3}	6.3
E03	Reboiler	EQ2.1	R3	VE	2×10^{-5}	14
				TD	2×10^{-5}	8.2
				PF	2×10^{-5}	16
				EX	1×10^{-3}	7.7
E04	Evaporator	EQ2.1	R1	PF	1×10^{-3}	8.5
			R3	TD	5×10^{-5}	17
				PF	5×10^{-5}	8.5
E05	Condenser	EQ2.1	R1	PF	1×10^{-3}	7.7
			R2	TD	1×10^{-5}	6.2
				PF	1×10^{-5}	7.7
			R3	JF	1×10^{-5}	20
				VE	1×10^{-5}	9.6
				FF	1×10^{-5}	19
				TD	1×10^{-5}	16
				PF	1×10^{-5}	7.7
G01	Phenol feed pump	EQ5.1	R4	PF	5×10^{-4}	8.1
			R5	PF	1×10^{-4}	13
G02	Cyclohexanone pump	EQ5.1	R5	TD	1×10^{-4}	16
				PF	1×10^{-4}	17
P01	Hydrogen compressor	EQ5.2	R4	JF	1×10^{-3}	13
				VE	1×10^{-3}	18
				FF	1×10^{-3}	10
			R5	JF	1×10^{-4}	22
				VE	1×10^{-4}	14

For equipment class identification see Table 2, for LOC description see Table 3, for type of scenario see Table 4.

for specific types of unit hazards. Thus, additional assumptions were necessary to obtain overall combined indexes: in accordance with the literature, the maximum expected values and an equal weight of the indexes were considered in normalization and aggregation.[9,21] Whenever single indexes are expressed in terms of damage distance (Dow F&EI, Dow CEI) the use of the higher distance was preferred, in accordance with the approach suggested by the SWeHI method,[13] and by the methodology developed in this article. Furthermore, several methods do not define clear and homogeneous procedures to calculate the material quantities to be considered in the unit assessment, requiring specific assumptions to limit potential biases in results.

Figure 4 shows an example of comparison of the results obtained in the inherent safety assessment of a single unit. The hydrogenation reactor was selected, since the assessment of a reaction unit is considered in most of the literature methods. Since the indexes calculated by the different methods

Table 7. Case Study: Values of Unit and Overall Inherent Safety Key Performance Indicators for the Alternative Processes Considered in the Analysis

Alternative A: liquid-phase pressurized hydrogenation			Alternative B: liquid-phase hydrogenation and stripping			Alternative C: gas-phase hydrogenation		
	UHI_k	UPI_k		UHI_k	UPI_k		UHI_k	UPI_k
R01A Slurry reactor	3.7×10^{-1}	4.3×10^{3}	R01A Slurry reactor	2.2×10^{-1}	7.9×10^{3}	R01A Fixed bed reactor	2.6×10^{-2}	2.5×10^{3}
R01B Slurry reactor	3.7×10^{-1}	4.3×10^{3}	R01B Slurry reactor	2.2×10^{-1}	7.9×10^{3}	R01B Fixed bed reactor	2.6×10^{-2}	2.5×10^{3}
R01C Slurry reactor	3.7×10^{-1}	4.3×10^{3}	R01C Slurry reactor	2.2×10^{-1}	7.9×10^{3}	C01 Vacuum distillation of cyclohexanone	2.2×10^{-1}	2.1×10^{3}
C01 Vacuum distillation column	1.7×10^{-1}	3.7×10^{3}	C01 Quenching column	3.0×10^{-1}	5.2×10^{4}	C02 Vacuum distillation of cyclohexanol	2.8×10^{-2}	2.7×10^{2}
D01 Flash drum	4.2×10^{-5}	4.2×10^{2}	C02 Quenching column	7.2×10^{-2}	8.6×10^{3}	D01 Flash drum	5.2×10^{-5}	5.2×10^{2}
F01 Filter	1.8×10^{-1}	3.7×10^{3}	C03 Vacuum distillation column	1.5×10^{-1}	1.4×10^{3}	E01 Feed evaporator	9.2×10^{-2}	1.8×10^{3}
E01 Hydrogen cooler	1.7×10^{-1}	4.8×10^{2}	D01 Flash drum	8.6×10^{-4}	8.5×10^{1}	E02 Product condenser	1.2×10^{-1}	4.6×10^{3}
E02 Condenser of C01	4.5×10^{-2}	2.9×10^{2}	F01 Filter	7.6×10^{-4}	7.6×10^{1}	E03 Condenser of C01	4.6×10^{-2}	3.6×10^{2}
E03 Reboiler of C01	6.4×10^{-2}	2.6×10^{2}	E01 Quencher C01 cooler	2.5×10^{-1}	4.2×10^{3}	E04 Reboiler of C01	8.2×10^{-2}	2.8×10^{2}
E04 Evaporator of D01	1.4×10^{-2}	2.8×10^{2}	E02 Quencher C02 cooler	2.3×10^{-1}	2.4×10^{3}	E05 Condenser of C02	1.4×10^{-3}	1.4×10^{2}
E05 Condenser of D01	6.4×10^{-2}	4.2×10^{2}	E03 Condensate cooler	1.6×10^{-1}	2.7×10^{3}	E06 Reboiler of C02	1.4×10^{-3}	1.4×10^{2}
G01 Phenol feed pump	4.9×10^{-2}	1.6×10^{2}	E04 Condenser of C03	4.5×10^{-2}	2.9×10^{2}	E07 Evaporator of D01	6.1×10^{-2}	2.1×10^{2}
G02 Cyclohexanone pump	2.9×10^{-2}	2.9×10^{2}	E05 Reboiler of C03	8.8×10^{-2}	8.0×10^{2}	G01 Cyclohexanone pump	3.1×10^{-2}	3.1×10^{2}
G03 Bottom pump	5.9×10^{-3}	5.9×10^{1}	E06 Condenser of D01	1.5×10^{-3}	7.6×10^{1}	G02 Cyclohexanol pump	5.9×10^{-3}	5.9×10^{1}
G04 Recycle pump	3.8×10^{-2}	8.5×10^{1}	E07 Recycle cooler	1.5×10^{-3}	7.6×10^{1}	G03 Recycle pump	5.9×10^{-3}	5.9×10^{1}
P01 Hydrogen compressor	3.9×10^{-1}	4.8×10^{2}	G01 Cyclohexanone pump	2.9×10^{-2}	2.9×10^{2}			
			G02 Recycle pump	8.8×10^{-3}	8.8×10^{1}			
	HI	**PI**		**HI**	**PI**		**HI**	**PI**
	2.3×10^{0}	2.3×10^{4}		2.0×10^{0}	9.7×10^{4}		7.4×10^{-1}	1.6×10^{4}

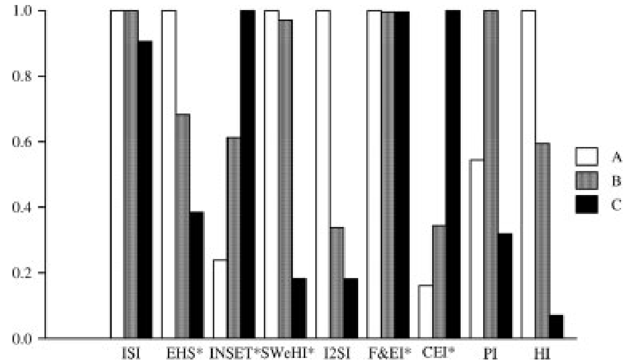

Figure 4. Inherent safety indexes calculated by different methods (see Table 1) for the hydrogenation reactor present in all the three alternatives considered in the case study.

have different scales, the index values reported in Figure 4 were normalized dividing them by the higher value obtained for each methodology. In the case of I2SI, that has a higher value for an inherently safer option, the inverse of the index was considered for normalization.

A first remark that comes from the analysis of the figure is that there is no agreement in the results obtained by the different methods, both from a qualitative and a quantitative point of view. The differences are likely to arise both from the different level of detail required by the application of the method (see Table 1), and by the different penalization factors considered. For instance, the reversed behavior of INSET method compared to EHS is mainly due to the penalization parameters used in the former, that do not consider the high operating pressure of the units. As a consequence, the inventory of phenol, which is linked to the conversion, becomes determinant in the ranking by the INSET method, since it has a prevailing role among the toxic material hazard.

Moreover, the results in Figure 4 show that the less information demanding indexes yield poor evaluation of single units. PIIS is not at all suitable for the analysis of a single reaction unit, being designed to address the process as a whole. On the other hand, the scoring of ISI, that can be applied to the sole reaction section, seems not sensitive to differences in unit operating conditions. Even the more detailed approaches are not able to consider all the hazards evaluated by the UPI: the SWeHI is strongly influenced in the results by the data on inventory value and, on the other hand, the F&EI is quite unable to consider the specific unit characteristics. Both these indexes base the assessment of the reactor only on the flammable proprieties of materials, respectively, identifying as secondary issues or neglecting the toxic dispersions. On the other hand, the CEI index is limited to considered toxic effects, thus, it only takes into account phenol releases, since this is the only substance that has available ERPG data. Finally, I2SI seems to have a behavior similar to UHI, but it shall be recalled that the results of this index partially reflect the expertise of the analyst, being thus "tailored" on the specific cases.

Figure 5 shows the comparison of the overall inherent safety indexes calculated by different methods. The results show that also the values of the overall indexes largely differ among the different methods. In quite all the overall indexes represented in Figure 5, the reactors play a dominating role in determining the index values, as evident from the comparison with Figure 4. Despite the large differences shown by the different methods, most of them indicate that option C is preferable, in accordance with the results of HI.

The results reported above allow some general conclusions to be drawn. No coherence exists among the available methods for the quantitative assessment of inherent safety. Several factors are responsible of the disagreement in the results, evidenced by Figures 4 and 5. In particular, the detail of information required for the application of each method influences the results. Thus, procedures based on general data do not allow a detailed hazard identification. Moreover, subjective assumptions on material quantities resulted a significant issue for the reliability of some literature methods. Furthermore, not all the tools attribute the same importance to different potential hazard factors. These elements, if added to built-in assumption, and to some degree of freedom left to the experience of the analyst, may well justify the differences in the results obtained.

As expected, the results obtained for the overall potential hazard index (PI) are frequently in line with those obtained using the more detailed methods proposed in the literature (e.g., EHS, SWeHI), since in the methodologies considered the potential severity of the scenarios is the prevailing factor in the analysis. On the other hand, the inherent safety hazard index (HI) introduced in this study adds further details to the results, accounting for the recorded safety scores of the different units, thus, assessing the hazards coming from auxiliary equipment, as compressors, filters, and heat exchangers, that are often overlooked in conventional severity-based inherent safety assessment methods.

The application to the case studies also allowed outlining some general considerations about the potential advantages of the proposed method:

• The method is based on the consequence assessment of reference accidental scenarios, taking advantage of the pro-

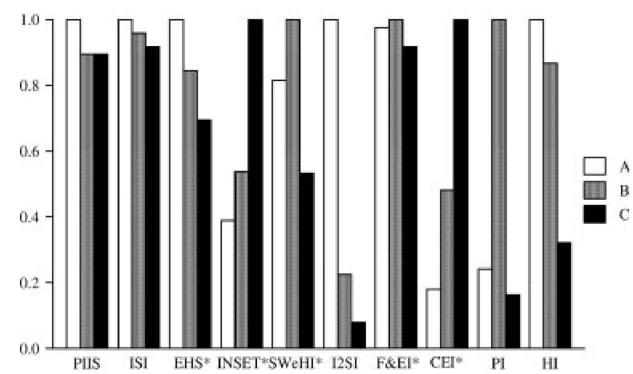

Figure 5. Comparison of the overall inherent safety indexes calculated by different methods (see Table 1) for the case study.

(A) liquid-phase pressurized hydrogenation, (B) liquid-phase hydrogenation and striping, and (C) gas-phase hydrogenation. (*) Aggregation was obtained by the assumptions discussed in the text.

gress in the availability of user-friendly commercial software, that significantly reduced the time requirements for consequence analysis. The use of consequence modeling of reference accidental scenarios, and of credit factors derived from statistical data limit the requirements for built-in expert judgment, and for the introduction of subjective elements within the analysis. The final result is expected to be a more realistic and sound representation of the inherent safety performance.

• Through the use of credit factors, the method considers the inherent safety performance of the single pieces of equipment (i.e., the credibility of the LOCs). This feature is not present in most of the other methods.

• The method is extremely flexible allowing the application of the more appropriate model for the analysis of each specific scenario. As a consequence, built-in assumptions and generalizations typical of other tools are avoided, yielding a more specific assessment of the expected accident severity. On the other hand, the method has no limitations in considering specific and nonstandard pieces of equipment, since LOCs and credit factors may be determined by the application of well-known specific methods (e.g., FMEA). This possibility is not present in most of literature tools, due to built-in assumptions that may not be easily modified by the user.

• The method yields quantitative indexes that allow an easy interpretation and communication of the results. Transparent rules are defined for the combination of the KPIs of the single units to give overall indexes for the process. Moreover, the results are obtained on a fixed scale. Therefore, it is possible to compare the inherent safety indexes obtained even for very different units or processes. This is an important feature in order to address the absolute ranking of the inherent hazard, and the requirements for add-on safety devices or other risk control and risk management measures.

Conclusions

A consequence-based method for the quantitative assessment of the inherent safety of processes was developed. The method is based on the evaluation of two KPIs, related to the severity of potential accidents, and to the recorded safety scores of process equipment. In the framework of a comparative assessment of the inherent safety of alternative processes, the methodology developed in this study overrides several problems present in previous methods proposed for quantitative inherent safety assessment. Introducing a direct relation among hazard factors and consequence analysis of potential scenarios, the proposed methodology avoids the use of arbitrary indexes. The comparison of the results with those obtained from other literature methods for inherent safety assessment showed that the KPIs introduced allowed considering the hazards coming from auxiliary equipment, that are often overlooked in conventional inherent safety assessment methods.

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