Making the chemical and process industries more sustainable

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Making the chemical and process industries more sustainable: Innovative decision-making framework to incorporate technological and non-technological inherently safer design (ISD) opportunities

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ABSTRACT

Inherent safety design principles have been used extensively to design safer plants. However, to date their application is merely limited to technical changes in the process. An unexplored area of ISD is related to all the non-technical aspects linked to the safety of industrial plants, such as the Human and Organizational Factors, often referred to as HOFs. This study presents an Inherent Safety Decision Making framework (ISDDM), with the objective to provide a structured tool that can be easily used by industrial practitioners. The novelty of the ISDDM is the provision of a structured framework where purely technical and non-technical ISD alternatives are categorized and analyzed, to check if possible interactions exist among the alternatives proposed. To prove the usefulness of the model, a case-study addressing a carbon capture plant is carried out. This technology will play an important role in the reduction of CO_2 emission in carbon-intense industrial processes, implying a rapid scale-up of these plants in the next years, therefore justifying the analysis of this green technology. Adopting the proposed ISDDM, the improvements in terms of safety from the base case ranged from 58% to around 70% for the best design solution, while from an economic perspective, cost variations were comprised between 16% and 22%. The results of the study demonstrate that the framework can be rigorously implemented and that it provides a considerable number of additional alternatives due to the inclusion of HOFs in the analysis. In conclusion, an improved and adequate ISD is a key to environmental sustainability.

1. Introduction

Process risk management consists of inherent, active, passive, and procedural strategies (Hendershot, 1997). According to Mannan (2012), inherent and passive approaches offer the highest reliability. Inherent Safety Design (ISD) is at the top of this hierarchy because it introduces intrinsic changes that are woven in the process and in the organizational structure of the company to eliminate the hazards or dramatically reduce their impact. As reported by CCPS (2009), the resulting chemical plants are more robust, more reliable, easier to operate, and economically more sound.

Although ISD concepts date back to the 70s of the previous century they are not widespread in real industrial practice (Khan and Amyotte, 2008a,b). This fact is not justified since there is no clear downtrend in the number of major accidents that happened in the last twenty years (European Commision, 2020). The trend demonstrates that if companies want to achieve a dramatic reduction of the major accidents, avoiding losses of life, money, and reputation, they should give priority to a more reliable, effective, and sustainable safety strategy as ISD.

Accident analysis of famous major accidents in the chemical and process industries with the ISD view usually is focused on implementing technological solutions. However, human and organizational factors (HOFs) are an unexplored field where multiple ISD initiatives could be adopted through the entire life cycle of industrial facilities.

Therefore, this study aims to develop a framework that can encourage the application of ISD procedures in chemical and process industries, at all life cycle stages and that it is accessible to ISD experts as well as industrial practitioners' novel to the subject. To achieve these goals, Section 2 presents the main barriers that prevent the diffusion of ISD, the unexplored sources of ISD

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innovations, and the impact of human errors in the rate of accidents. By using this information, in Section 3 an Inherent Safety Design Decision Making (ISDDM) framework is proposed. The novelty compared to previous works, is related to the clear distinction between purely technological and non-technological ISD opportunities so that the spectrum of possible safety improvements is enlarged. In the framework developed, Human and Organizational Factors are explicitely accounted, introducing a clear progress with respect to the structure proposed by Hurme and Rahman (2005), Therefore, the analysis extends beyond the typical manner in which ISD studies are performed. An additional new element of the procedure consists in the analysis of the array of ISD alternatives to identify possible interaction among the various ideas which combined may exploit a bigger advantage in terms of safety, economics, and sustainability.

The framework is tested in Section 4 with a case study regarding an industrial plant for capturing CO_2. The reason is twofold: first, there is a lack of complete ISD practical studies that demonstrate the full potentialities of this approach, especially regarding technologies that are gaining relevance in the sustainable industry. Secondly, Carbon Capture Utilization and Storage (CCUS) will play an important technology in the reduction of CO_2 emissions in carbon-intensive industrial processes such as in steel, cement, and chemical production, and in fuel transformation sectors. In the International Energy Agency- Sustainable Development Scenario (SDS), CCUS accounts for 7% of the cumulative emissions reductions needed globally to 2040. This implies a rapid scale-up of CCUS deployment, from around 30 million tonnes (Mt) of CO_2 currently captured each year to 2300 Mt per year by 2040 (IEA). It is clear that in the imminent future the facilities related to CCS will process a considerable amount of CO_2 and all the chemicals involved in the process. For this reason, it is important to analyze the possible hazards and consequences involved in these plants. The results and the discussion of the case study are discussed in Section 5, while conclusions are provided in Section 6.

2. The pivotal role of ISD in the chemical and process industry

Major accidents in chemical and process industries are events with relatively low frequency but with extremely severe consequences. Therefore, the chemical industry has developed different approaches to decrease the number of accidents. As was mentioned in the introduction, the inherent approach offers the highest reliability. Five main principles can be identified as the basis of the ISD philosophy, named Substitute, Minimize, Moderate, and Simplify (CCPS, 2009; Kletz et al., 2010). The investigation of well-known accidents such as the Bhopal toxic gas cloud disaster (India, 1984) and the Flixborough accident (Edwards, 2005) give different points of reflection from an ISD perspective. The use of the ISD principles could have prevented or dramatically reduced the consequences of these catastrophes. Table 1 reports some examples of ISD options that could have been implemented in the cases of the Bhopal and Flixborough accidents.

ISD can play a crucial role in the prevention of major accidents, however, it has not been widely adopted among the industries for a series of hurdles that are identified and classified in Section 2.1. To overcome some of the barriers described previously, in Section 2.2 a generic structure is proposed that connects ISD with the process of technological and non-technological sustainable innovation in companies. ISD approach is a design methodology that can lead to a more responsible industry based on sustainable values. Afterward, in Section 2.3, studies that conduct accident investigations are used to identify the most critical areas where ISD can act to prevent the creation of hazardous conditions. The last section of this section reports a holistic approach to incorporate ISD review procedures through the entire life cycle of an industrial plant.

2.1. Barriers in the implementation of IS

The development of an appropriate methodology requires, at first, the identification of the barriers that have hindered the development of ISD strategies among the industries during the last decades. Table 2 reports the literature studies which describe the barriers. Broadly, two types of barriers are identified, named *Technical barriers* and *Managerial barriers*. The former is related to the difficulties in applying ISD during the design of industrial processes, while the latter is linked to the management perspective and encloses the socio-technical issues that obstacle the introduction of ISD into companies' practices.

The hurdles for the implementation of ISD can be summarized in *Lack of awareness* both at the technical and managerial levels, *Lack of methodologies* that encourage the ISD application, and *Lack of evidence* of the economic benefits. Edwards (2005) marked the relevance of the last point. In particular, he stated that all these barriers have a common problem, which is the base of all of them, that is "*the inherent conservatism or (business) risk-aversion to new approaches of the industry*". This *inherent conservatism* indicates the industry's aversion to the business risk of using safety as a key driver in early project development. Therefore, it is usually not possible to show the full potential of this approach, in terms of risk and costs reduction. It results in low or no corporate commitment with a consequent lack of resources for the integration of ISD during early design stages. To obtain the approval at the managerial level, and consequently obtaining the resources required for its application, it is necessary to stress not only the advantages in terms of process safety but also the opportunities to bring innovations. Indeed, this usually results in more sustainable plants, both from the economic and environmental point of view. The following section describes how the ISD approach can be used as the connection between the safety domain and the process of sustainable innovation.

Table 1
Examples of ISD principles applied to the Bhopal and Flixborough accidents.

Accident	ISD Principle	Description
Flixborough 1974, England	Attenuate by limitation of effects	Of the 28 deaths at Flixborough, 18 occurred in the control room. It demonstrates as an opportune siting of the facilities could have limited the impact of the accident.
	Simplify	The process was neither user-friendly nor easy to operate, in fact as stated in the *Flixborough Report*, "*greater attention to the ergonomics of plant design could provide rewarding results*"
Bhopal 1984, India	Substitute	The reaction product, carbaryl, could have been made using the same raw materials, phosgene, and methylamine, but reacting them in a different order to avoid the production of MIC
	Minimize	Although the on-site storage of MIC was convenient, it was not essential. In fact, the MIC was reduced by 75% within the year of the accident.

Table 2
Type of barriers related to the integration of ISD in companies.

Type of barrier	Barrier
Technical barriers	*No definitive methodologies are available to evaluate ISD. Also, the tools being developed appear to complicate* (Gupta and Edwards, 2002; Khan and Amyotte, 2008a,b).
	The application of ISD methodologies is time and expertise intensive (Gupta and Edwards, 2002).
	Lack of information about successful uses of ISD with regards to safety and costs (initial/lifetime) (Edwards, 2005; Gupta and Edwards, 2002)
Managerial barriers	*No corporation commitment* (CCPS, 2009; Gupta and Edwards, 2002)
	Low or nil focus on ISD during feasibility studies (Edwards, 2005; Khan and Amyotte, 2002)
	Lock of Training and organizational culture toward ISD (CCPS, 2009)

2.2. *ISD as a source of innovation*

According to the second and third editions of the Oslo Manual (Oslo Manual, 2005), there are mainly three sources of innovation: technological innovation in the products, processes, and non-technological innovation in organizations. *Technological product innovation* can take two broad forms, named *technologically new product* and *technologically improved product.* The former is a product whose technological characteristics or intended uses differ significantly from those of previously produced products. The latter is defined as the adoption of technologically new or significantly improved production methods. These methods may involve changes in equipment, or production organization, or a combination of these changes.

On the other hand, *non-technological innovations* represent all the innovation activities of firms that do not relate to the introduction of technologically new or substantially changed goods, services, or processes. The major types of organizational innovation are related to the introduction of significantly changed organizational structures, the implementation of advanced management techniques, and the implementation of new or substantially changed corporate strategic orientations.

But how does ISD fit the process of innovation in the chemical and process industries? The main objective of ISD is to seek alternative materials, processes, and procedures for addressing safety issues in facilities that deal with hazardous chemicals. To achieve these results, it is often necessary to adopt novel technologies, for instance, chemical routes, manufacturing routes, process units, but also to review the organizational structure of a company with consequent changes in human aspects as working and training procedures, the relation with contractors and suppliers, communication and so on. Usually, this creative process, if applied systematically and through the entire life cycle, leads not only to a *safer plant* but also to a *more sustainable plant*. Therefore, the general concepts of technological and non-technological innovation can be adapted to the safety domain using the Inherent safety design philosophy as the connection between innovation and safety in the process industries. Consequently, the proposed general framework that could be used to induce the incorporation of ISD in company practices requires both technological and non-technological innovations.

The *non-technological innovation* is induced at first by a cultural emphasis on ISD as an important organizational value and tool for the risk control of industrial facilities. At the same time, the support at the corporate level is necessary being essential to provide the resources and establish policies and procedures to integrate the use of inherent safety into the *"way in which companies do business"*. *Technological innovation* requires simultaneously a methodology to apply ISD systematically through the entire life cycle and technicians who have the knowledge to put it into practice.

Edwards (2005) pointed out that while most safety advisers know about ISD and most engineers have heard about it, most managing directors know nothing about it. Therefore, until there is no visible body of knowledge and experience that ISD can make a significant positive contribution to competitive advantage and profitability, as well as offering significant hazard reductions and greener processes, little will happen. In conclusion, one important goal of the methodology developed in this work is to demonstrate how relevant is the impact of ISD concepts both in terms of safety and sustainability. It will prompt the managers to introduce ISD in their standards, by showing evidence of its benefits using case studies.

2.3. *The impact of poor safety management on major accident hazards*

Gaining a deep understanding of the mechanisms that caused major accidents as well as the errors that induced the hazardous condition is crucial to avoid that the same situation will occur in the future (Kletz, 2002). To achieve this result, it is necessary to ensure that as much information as possible is extracted from the available description of an accident. Accident databases are an important source of this information.

Around the world, some agencies collect and classify accident reports from the chemical and process industry. For instance, in Europe, the Major Accident Reporting System (MARS) has the purpose to facilitate the exchange of lessons learned from accidents and near misses involving dangerous substances, to improve chemical accident prevention and mitigation of potential consequences. Several studies have conducted an analysis of the causes that induced major accidents in the chemical and process industry based on information retrieved from accident databases. The results of the literature review are reported in Table 3.

From the studies reported in Table 3, the human error condition plays an important role in the accident process. A deeper analysis of the accidents identifies a series of underlying errors that are purely related to Human and Organisational Factors (HOF), as managerial omissions, ineffective training, unclear procedures, etc. Fig. 1 provides a graphical representation of the conclusions obtained by Nivolianitou et al. (2006).

From these studies, it is possible to state that HOFs have a great impact on the overall safety of a plant. In terms of numbers, the statistical contribution of HOFs in the studies ranges from a minimum of 40% up to 80%. An important point regarding the magnitude of the accident is that ones that are induced by latent safety management system failures have significantly higher 'severities' than accidents caused by more immediate failures. In conclusion, despite most of the frameworks and research conducted about ISD focus on purely technical aspects, it is worthwhile to develop a framework that can explicitly consider HOFs.

2.4. *A holistic and sustainable approach to incorporate ISD concepts into the entire life cycle of a plant*

Generally, there are opportunities to apply ISD concepts through the entire life cycle of a plant, although the number and the type of

Table 3
A literature review of the accident investigation report.

Author	Title	Findings
Drogaris (1993)	Learning from major accidents involving dangerous substances	The study analyzed 121 accident reports retrieved from the MARS database. For most of the accident reports, both the immediate causes and the underlying causes have been identified.
Kawka and Kirchsteiger (1999)	Technical note on the contribution of sociotechnical factors to accidents notified to MARS	It analytically demonstrates that around 66% of the accidents reported in the MARS database are caused by latent safety management system failures.
McCafferty (1995)	Successful system design through integrating engineering and human factors	Human errors in the chemical process industry account for up to 80%.
Nivolianitou et al. (2006)	Statistical analysis of major accidents in the petrochemical industry notified to the major accident reporting system (MARS)	The study, that analyzes with the same approach adopted by Drogaris (1993) 85 accident reports in the MARS database shows that human factors related to the organizational structure that deals with safety account for more than 40% of the cases.
Kidam and Hurme (2012)	Statistical Analysis of Contributors to Chemical Process Accidents	It analyses accidents from the FDK database and provides an extensive analysis of which contributors to accidents are the most common, how they act as a contributor and how they are connected. HOFs are present in almost 40% of the cases.

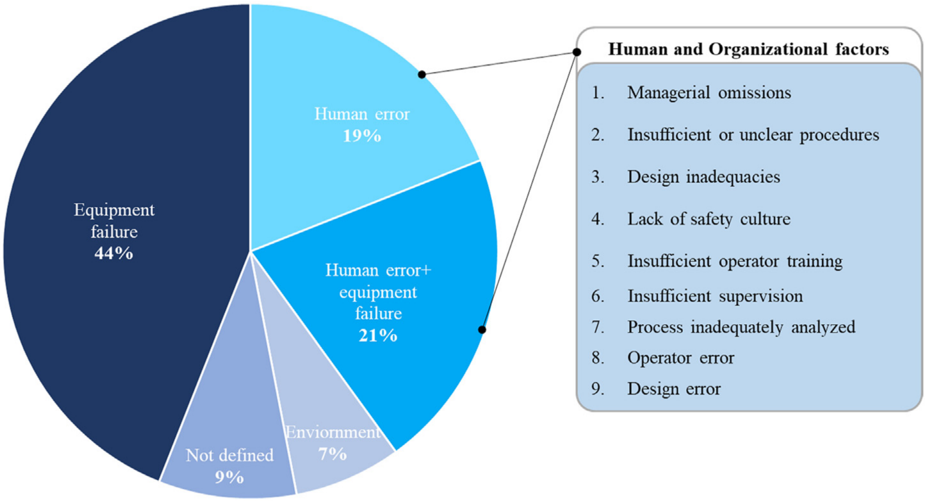

Fig. 1. Immediate and underlying causes of accidents in petrochemical industries. Adapted from Nivolianitou et al. (2006).

opportunities dramatically change moving from early design stages to detailed design or operations. During design stages, it is possible to make major technical changes in the process structure, from the substitution of a chemical route to the physical arrangement of the units to avoid domino effects. Nevertheless, HOFs should be considered in these preliminary stages as well, even with a qualitative analysis. Having a preliminary understanding of the non-technical issues associated with a process can help during the advanced design stages. When the plant is already operating, it is more difficult to introduce technical changes for two reasons: first, changes during operations can create hazardous conditions, so a detailed program for the management of change is required; secondly, modifications may be unfeasible from the economic point of view. However, there are plenty of opportunities to make the organizational structure inherently safer. Fig. 2 summarizes the general road map for the incorporation of ISD concepts through the life cycle.

One possible solution to implement ISD during operations and maintenance is to develop policies that require the integration of ISD concepts into the process safety management plan. The European Industrial Gases Association (EIGA) provides a structured guideline to implement the process safety management program (PSM) in the industry (EIGA, 2014). Eight (8) elements are particularly suitable for the introduction of ISD concepts, for instance, the periodic training sessions for employers, review of the periodic hazards' analysis, the definition of maintenance and inspection procedures. The following section describes the structure of the decision-making framework that could be used to evaluate systematically the ISD options, during the life cycle of an industrial plant.

3. ISD framework for technical and non-technical initiatives

As discussed in the previous sections, the opportunities to implement ISD concepts are numerous, especially when non-technological aspects are considered. Theoretically, this is an important point in favour of ISD as it demonstrates that the application of the principles is not limited to purely technical aspects. However, in practical terms, it could be complex to deal with numerous initiatives, and arriving at the final decision could not be straightforward. One possible solution is to use a structured approach that guides step-by-step the entire challenging process of generating, evaluating, and selecting the optimal ISD alternatives. The methodology should be *flexible* so that it can be used for all the life cycle stages of a plant, *compatible* with the well-established methods and standards used by the companies, and as *simple* as possible, to avoid complexities that may discourage its application. In Fig. 3 the general structure of the ISD approach adopted is proposed. This is an inherent safety design decision-making framework (ISDDM) that can be used to implement ISD systematically, starting from the definition of the base case, until the final design selection.

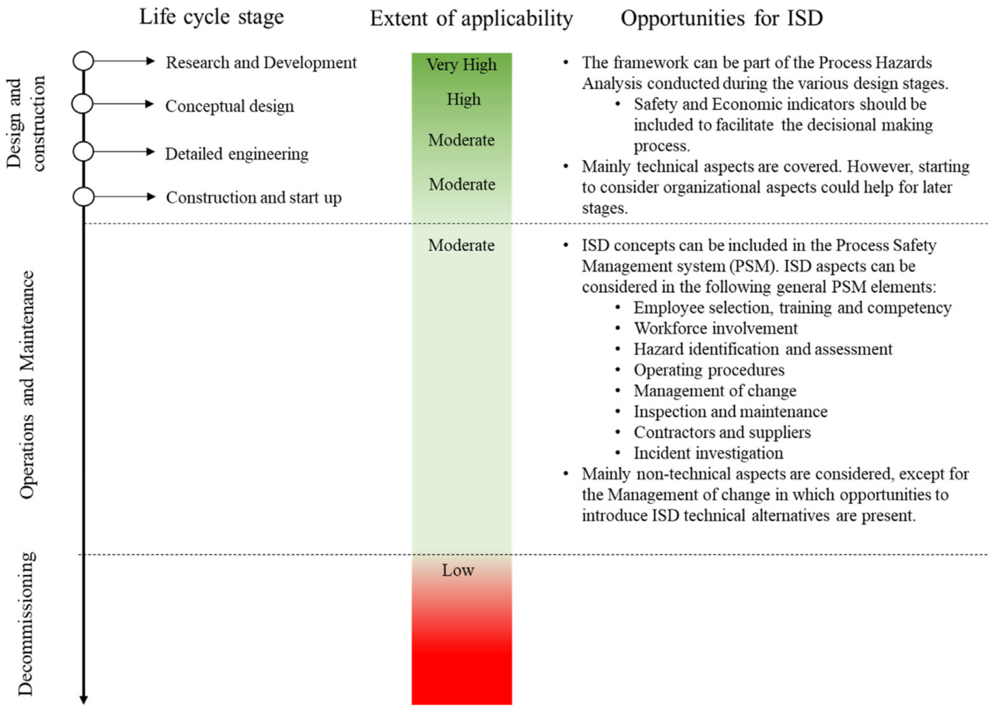

Fig. 2. Generic road map for the incorporation of ISD concepts through the whole life Cycle.

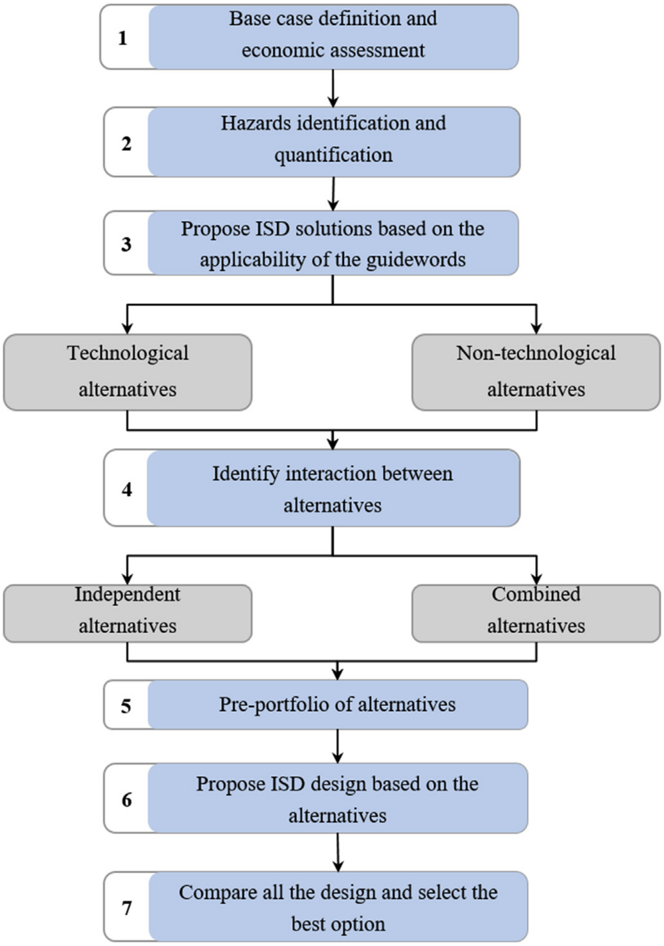

Fig. 3. Inherent safety design decision-making framework (ISDDM).

The first step of the procedure, called *Base case definition*, requires a detailed description of a base design, procedure, or strategy that will be used as a metric for comparison with ISD alternatives. The next step is *Hazards identification and quantification*. This is a fundamental step as, without a deep understanding of the hazards involved, the results obtained by the overall procedure may be compromised. Depending on the stage analyzed, different tools can be used for hazard identification. With these data, it is possible to evaluate the performance in terms of safety and economics of the base design, which are usually evaluated through indicators. When the base case is fully defined, it is possible to enter the core of the procedure, which consists of *Proposing ISD options based on the applicability of the guidewords*. This is the section in which the team is challenged to identify alternatives based on the critical issues identified in the previous analysis. The resulting ISD alternatives are classified into two categories, named *technological* and *non-technological*. All the ISD alternatives that introduce purely technical changes in the process structure belong to the technological category, while the proposed opportunities that may induce changes in the organizational structure that deals with safety, belong to the non-technological category. Some examples of non-technological alternatives are novel training, inspection, or maintenance procedures, the integration of ISD review during the periodic safety audits, and hazard identification procedures. At this point, the database of ISD alternatives is deeply analyzed to identify possible interactions between alternatives that may exploit greater improvements in terms of sustainable safety and cost-benefits. The output of this process is a list of two types of ISD options: *Independent alternatives* and *Combined alternatives*. Independent alternatives cannot be implemented in the same design (or operations) because they may introduce new hazardous conditions, or they may not be feasible from an economic point of view. Some alternatives, if combined, may exploit bigger advantages and, in this case, they are classified as combined alternatives. It is likely to arrive at this point in the procedure with a long list of opportunities to implement ISD. However, because of time constraints, it will not be possible, in most cases, to consider all the alternatives in detail. For this reason, a *Pre-portfolio of alternatives* is required, where a first pre-feasibility check is performed based on available information, as feedback from operation and maintenance technicians, pilot projects, laboratory data, patents, etc. Based on the pre-ranking, the safety and economic indexes of the ISD designs are evaluated and, finally, the best design option is selected by finding the optimal solution.

One of the biggest challenges of ISD implementation is determining the inherent safety level of a plant. Generally, the approaches for assessing inherent safety are classified into three categories: models, qualitative reviews, and metrics. Metrics, more commonly called index-based approaches, have been widely used since they are user-friendly and time effective than other approaches (Jafari et al., 2018). Some studies provide a list of the indexes developed and with their potentialities and weaknesses such as the work of Athar et al. (2019) and Jafari et al. (2018). A general rule for the selection among the index is that it should be a compromise between complexity and applicability, concerning the level of details available and the life cycle analyzed. Based on the research, the Safety Weighted Hazard Index (SW&HI) index satisfied the previous requirements, allowing a preliminary estimation of the impact of technical and non-technical changes including HOFs. Indeed, the SW&HI is a hybrid index, where the relative ranking approach is used to evaluate the impact of HOFs while the graphical, equational, and risk-based approaches can be used to estimate the area impacted by the incidental event (Khan et al., 2001). The SW&HI is structured as follow:

$$SW\&HI_{Tot,n} = \sum_{i}^{j} SW\&HI_{i,n} = \sum_{i}^{j} \frac{Hazard\ impact_{i,n}}{A_{i,n}}$$
$$= \sum_{i}^{j} \frac{max(B_{1,i,n}; B_{2,1,n})}{A_{i,n}}$$

Where B_1 addresses the damage due to fire and explosions, B_2 considers the damage due to toxic release and dispersion while factor A incorporates the quantification of the various safety measures adopted by the industry as well as the safe operation practices related to the HOFs.

To investigate the trade-off between the safety level and the costs induced by the changes from the base case, it is necessary to perform an economic analysis of each case proposed. Indeed, the final objective of the procedure is to find the optimal solution that maximizes safety and costs. To achieve this goal, an additional indicator is required to evaluate the economic performance. The Net Present Value (NPV) is a widely applicable indicator used to evaluate the profitability of a project and to compare the performance of different design solutions. However, if a specific economic indicator to examine the performance of a technology exists, it is strongly recommended to employ it. The reason is that it will make the results of the analysis easier to compare with the market' benchmarks or with previous studies. This specific situation is clarified in the following case study.

4. Case study

To demonstrate the applicability of the ISDDM framework, a case study, that covers all the seven steps discussed previously, is presented. The input data used come from a technical feasibility study conducted by Berghout et al. (2017) where is reported the technical information from a heterogeneous cluster of 16 companies. In this study only 4 of the companies from chemical production are considered, with an overall CO_2 production of 375 kt per year, corresponding approximately to 35400 kmol/h of inlet flue gas in the carbon capture plant.

According to the procedure, the first step requires the complete definition of the base case. The post-combustion structure consists of two columns, an absorber and stripper, two heat exchangers, and a kettle reboiler. The solvent used in the base case is Ethanolamine (MEA), which is often adopted as a benchmark for other solvents (Wang et al., 2017), while the base arrangement consists of a carbon capture unit installed in each chemical plant. The overall amount of CO_2 produced by the 4 companies is 375 kt per year. The percentage of carbon captured usually achieved using MEA technology is around 85−90%. In all the simulations, 90% of CO_2 is captured from the flue gas. The rigorous calculations for the overall material and energy balances, liquid and gas side mass transfer coefficient, and interfacial equilibrium for the absorber and the stripper have been solved by using Aspen Hysys. The absorption process is governed by reactions between the solvent and the CO_2 so it cannot be modeled by conventional thermodynamic packages. For this reason, the *Acid gas* model is used, as it considers the chemical reactions that take place. The process flow diagram used in Hysys is reported in Fig. 4.

The specifications used for the simulation are based on previous studies that focused on finding the optimal operative conditions for this configuration. In the absorber, temperature, pressure, composition, and flow rate are required for the inlet flue gas and the lean solvent. The inlet flue gas and the lean solvent flow rates change from case to case, while the other inlet parameters and specifications remain constant. Table 4 summarizes the constant input data employed for all the cases.

For the calculation of the lean solvent required, the following equation has been used (Agbonghae et al., 2014):

$$F_{Lean} = \frac{F_{FG} x_{CO_2} \phi_{CO_2}}{100z(\alpha_{Rich} - \alpha_{Lean})} \bullet \left[\frac{M_{Amine}}{44,009}\left(1 + \frac{1 - \omega_{Amine}}{\omega_{Amine}}\right) + z\alpha_{Lean}\right] \tag{1}$$

Where:

- F_{Lean}: mass flow rate of the lean amine solution.
- F_{FG}: mass flow rate of the flue gas.
- x_{CO2}: mass fraction of CO_2 in the inlet flue gas.
- M_{Amine}: molecular weight of ethanolamine.
- ϕ_{CO_2}: percentage of CO_2 in the flue gas that is recovered.
- α_{Rich}: Rich amine CO_2 loading.
- α_{Lean}: Lean amine CO_2 loading.
- ω_{Amine}: mass fraction of amine in the unloaded solution.
- z : number of equivalents per mole of amine (1 for MEA).

The adaptive solver is used to reach the convergence of the stripping column. In most of the simulations, the head key component fraction (CO_2) and the reboiler temperature are controlled/tuned since they are systems constraints. The purity of the CO_2 outlet stream needs to be high, at least 98%, to avoid the problem in the compression stage. The recommended reboiler temperature is around 120 °C, a higher value will induce solvent degradation. Despite this measure, some amine is lost during the operation. Then, a Make-up block is added, as can be seen from Fig. 4. When the heat and material balances for the absorber and stripper are solved, their diameters have been calculated using design specifics available in the literature for similar plants. The following criteria have been used (Dutta et al., 2017):

- Max flooding 80%.
- Superficial gas velocity <2.5 m/s.
- Maximum allowable pressure drops 4.1 mbar/m of packing.

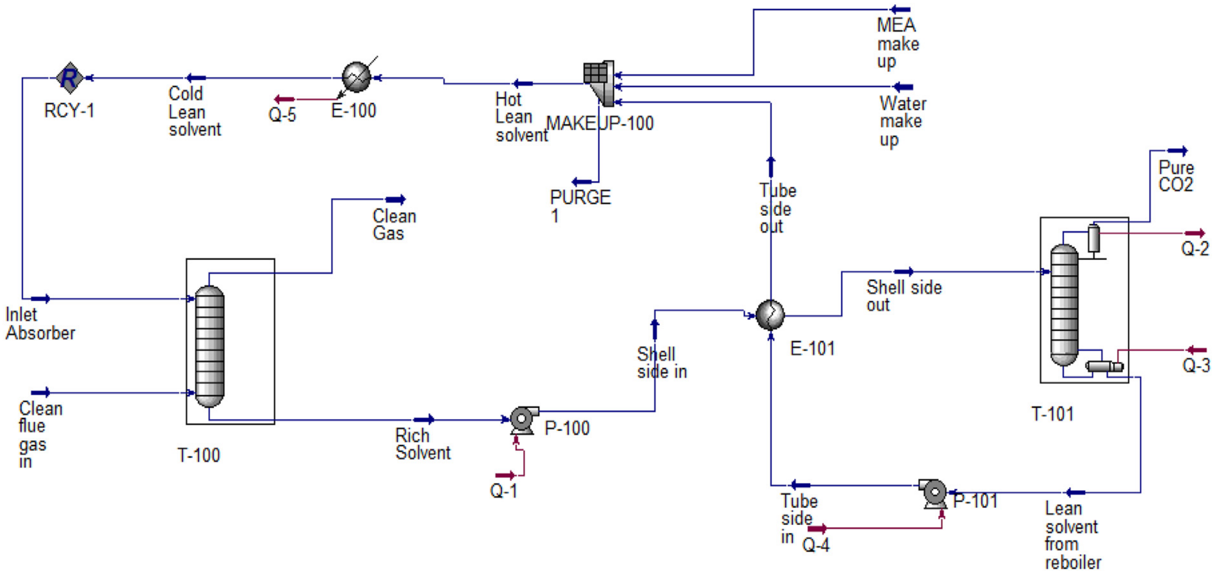

Fig. 4. Hysys flowsheet for Carbon Capture using chemical absorption.

Table 4
Compositions and specifications of the absorber' inlet streams.

	Inlet flue gas	Inlet Lean Solvent	
Parameter	Value	Value	Units
Temperature	40	40	°C
Pressure	1,2	1,2	bar
Molar fractions			
Carbon dioxide	4,04	2,54	%
Nitrogen	74,32	0	%
Water	8,67	85,88	%
Oxygen	12,09	0	%
Argon	0,89	0	%
MEA	0	11,58	%

According to the literature, the Flexipac 2.5X structured packing is recommended for the absorber, while Mellapak 250Y for the stripper.

A preliminary geometrical design of the cross-heat exchanger, reboiler, and condenser has been performed to obtain the specifics necessary for calculating the cost and for estimating the capacity of the units. The units' capicities have been used for the safety index estimation. The design procedures, the equations for the heat transfer coefficients, and the relations for the pressure drops have been retrieved from technical books (Robert Hood Perry, 2008; Sinnott (1993)). The total capital investment of a facility (CAPEX) has been estimated considering the *fixed capital costs* and the *working capital costs*. The former, which represents the total costs of the plant ready for start-up, can be divided into four investments:

1. The inside battery limit (ISBL) investment.
2. The Outside battery limit (OSBL) investment.
3. Engineering and construction costs.
4. Contingency charges.

The ISBL investment is estimated by using the equipment's installation costs obtained from the Aspen Hysys proprietary software. For what concerns the remaining indirect costs, percentages retrieved from the literature have been used to provide a preliminary estimation. Their values are reported in Table 5.

During preliminary cost analysis, the *working capital* is usually estimated as a percentage of the fixed capital cost (Robert Hood Perry, 2008). In this work, 20% of the fixed capital is assumed. The *operative costs* are estimated considering the *variable costs of production* and the *fixed costs of production*. For the variable costs of production, the raw materials considered in this analysis are the amine and the water needed for the solvent make-up, while the utilities considered are the electricity used for pumping and steam required for the reboiler in the regeneration section. The fixed costs of production are incurred regardless of the plant operation rate or output and include costs for maintenance, operating labor, salaries, taxes, and insurance, etc. The operating labor costs are estimated assuming an average salary of 2000 €/month, and that one operator per shift requires 4.2 operators if it is assumed that 21 shifts cover the operation and each operator works five, 8-h shifts per week (Robert Hood Perry, 2008). According to guidelines found in the literature, this kind of process requires at least three operators per shift, resulting in a cost of 302400 €/year. For preliminary analysis, the remaining fixed costs can be estimated using percentages of other costs. The values are reported in Table 6.

The next step of the procedure requires the identification and quantification of the hazards involved in the base design solution. For this work, the Preliminary Hazard Analysis (PHA) has been selected and two categories of trigger events are identified, named technological and non-technological. The first category considers events as mechanical failures, process deviations, abnormal conditions, etc., which are related to purely technical features of the process units and can be considered as the immediate causes that triggered the accident process. They lead to the hazardous condition *Loss of containment* and, being MEA a moderately flammable and highly toxic chemical, possible accident scenarios would be the pool fire or the toxic dispersion. All the underlying causes or latent errors related to the HOFs belong to the non-technical category, for instance, insufficient operator training, insufficient supervision, insufficient or unclear procedures, process not adequately analyzed, etc. Table 7 lists the results of the hazards identification procedure, where purely technological and non-technological causes were identified.

At this point in the procedure, it is necessary to evaluate the performance in terms of safety and economics of the base alternative. As described previously, the SW&HI index is selected to

Table 5
Factors considered for the estimation of the Fixed capital costs.

Factor	Value	Reference
ISBL	Variable according to the case analyzed	Aspen economic analyzer (8.8)
OSBL	15% (Restructuring of already existing site)	Robert Hood Perry (2008)
Engineering and construction	20% ISBL + OSBL	Sinnott and Towler (2020)
Contingency	10% ISBL + OSBL	Sinnott and Towler (2020)

Table 6
Factors considered for the estimation of fixed cost of production. Adapted from (Sinnott and Towler, 2020)\.

Factor	Value
Supervision	25% of operating labor
Direct salary overhead	40% of operating labor + supervision
Maintenance	3% of the ISBL
Taxes and insurance	1% of ISBL
General plant overhead	65% of total labor + maintenance

measure safety performance. For what concerns the economic indicator for the CCS project, the *CO_2 avoidance cost* is used. The results will be compared with studies of CCS available in the literature. The *CO_2 avoidance costs* represent the CO_2 tax at which the product cost is the same for either a fossil fuel plant without CO_2 mitigation (but paying the CO_2 tax) or the same fossil fuel plant that includes the added capital and efficiency losses of adding CCS (but avoiding most of the CO_2 tax). The CO_2 tax must be higher than this CO_2 avoidance cost to justify the higher risks, capital, and lower efficiency of utilizing CCS (Simbeck and Beecy, 2011). Different methods can be used to calculate the CO_2 avoidance costs. The approach used in this work consists in the evaluation of the total annual cost associate with each CCS structure and the net amount of CO_2 emissions avoided per year (Roussanaly, 2019):

$$CO_2 avoidancecosts = \frac{Annualizedcapitalcosts + AnnualOperativecosts}{AnnualCO_2 emissionsavoided}$$

The relation between the CO_2 avoidance costs and the SW&HI is mainly exploited in the increase (or decrease) of the capital and operative costs induced by the employment of the ISD solutions. After these two preliminary steps, the base case is fully defined, and the team should have a good understanding of the hazards involved as well as the technological and non-technological causes that may induce the hazardous events. The next step corresponds to the proposal of ISD alternatives. The output of this brainstorming exercise is reported in Table 8, where each critical issue is assigned to a specific category and the corresponding ISD alternative is classified according to the ISD principle used.

As reported in Table 8, a total of 23 ISD alternatives are proposed, among them 7 are purely technical while the remaining address human and organizational factors as working and training procedures, ergonomics aspects, communication, or a combination of technological and non-technological aspects. An additional analysis of the proposed alternatives is necessary for two reasons: at first, some alternatives can be combined as they may exploit bigger advantages, secondly, some alternative proposed may be unfeasible or novel approaches without any real industrial application. For these reasons, a pre-ranking of the alternatives is

Table 7
PHA covering technological and non-technological aspects for CCS.

ID[a]	Cause	Hazardous condition	Consequence
T	Corrosion, mechanical failure, or human error in Column vessel (T-100)	Loss of containment	Pool fire or Toxic cloud
T	Leakage from the Heat exchanger (E-101) (caused by corrosion, mechanical failure, or human error)		
T	Leakage from the column vessel (T-101) (caused by corrosion or mechanical failure)		
T	Leakage from the reboiler (R-100) (caused by corrosion, mechanical failure, or human error)		
T	Leakage from the condenser (C-100) (caused by mechanical failure or human error)		
T/NT	Not reliable material supplier. Storage conditions are inadequate.	Contaminants in the solvent	Sub reactions which induce economical loss (higher solvent make up because of degradation; higher replacement of items because of corrosion)
NT	Inadequate maintenance program.	Dangerous maintenance or inspection conditions	Serious injury or fatality. E.g. Operator falls from the absorption or stripping column during an inspection
NT	Inadequate inspection program.		
NT	Lack of accessibility for maintenance and inspection procedures.		
NT	Inadequate maintenance program.	Unclear maintenance or inspection procedure	Maintenance error can lead to an economic loss (plant shut down) or LOC.
NT	Inadequate inspection program.		Inspection error. E.g. Inspection failure can lead to wrong analysis or missed information in the final report.
NT	Not adequate training program	Lack of awareness of the worker	Human error (LOC); Serious injury or fatality; Economic loss.
NT	Workload conditions are not properly analyzed resulting in inadequate management.	Excessive or very low workload conditions	Human error (LOC); Serious injury or fatality; Economic loss.
NT	Inadequate analysis of the environmental factors	Air quality is not monitored appropriately	Workers may be exposed to toxic chemicals during activities with possible health problems in the medium or long term.

[a] T: technological; NT: non-technological; T/NT: the combination of technological and non-technological aspects.

Table 8
Inherently safer design alternative identified in step 3 for the Carbon capture process.

Category	Critical issue	Alternative	Principle
Process (technological)	Toxicity of the solvent (MEA)	1. Membrane separation process (Wang et al., 2017). 2. Replace MEA with a less hazardous amine (MDEA, DEA, etc.)	Substitute and Attenuation by moderation
Process (technological)	Corrosivity of the solvent (MEA)	3. Ionic liquids (Luis, 2016) 4. Replace MEA with a less hazardous amine (MDEA, DEA, etc.)	Substitute
Process (technological)	Amount of hazardous material processed and column dimensions	5. Ionic liquids P 6. Rotating packed bed (Wang et al., 2015) 7. Replace the recovery shell and tube with a more compact solution (plate and frame, spiral heat exchanger, etc.) (Wang et al., 2015).	Minimize
Process (Layout) + Organizational (Communication and job design)	Lack of accessibility for maintenance and inspection procedures. Complexity of the plant. Area exposed to dangerous conditions.	8. Agreement for clustering the process to reduce the plant complexity and decreasing the unit's congestions (Berghout et al., 2017). 8.1. Partially centralized process (One shared stripper) 8.2. Fully centralized process	Simplify
Organizational (Human system interface design)	Make incorrect assembly impossible during construction and maintenance activities	9. Design components with unique shapes or with male-female fitting pairs (CCPS, 2009)	Simplify (error-proof)
Organizational (Human system interface design)	Erroneous maintenance	10. Dashboard with main features and comprehensible visualization for Operation and Maintenance, without overload with alarms. (CCPS, 2009) 11. Use clear signage and labeling	Simplify
Organizational (Human system interface design)	Inspection procedures in hazardous working areas	12. Remote monitoring during the inspection using drones (mainly for the absorption and stripping columns).	Substitute and Simplify
Organizational (Job design)	Lack of an adequate maintenance program	13. Assign clear roles and responsibilities for each maintenance task. 14. Establish appropriate maintenance procedures. 15. Provide enough access for maintenance. 16. Use permit to work system if hazardous units are involved. 17. Avoid fatigue through *smart shift* working (Amyotte et al., 2007)	Simplify
Organizational (Job design and Digitalization)	Chronic or long-time exposure to toxic compounds	18. Use Internet of Things (IoT) wearable technologies to monitor continuously the worker safety.	Simplify
Organizational (Digitalization)	Time of inspection (worker exposition to toxic compounds)	19. Agile data processing (Digital solutions with Natural language processing (NLP) Textual and voice recognition).	Simplify
Organizational (Training and Digitalization)	Lack of awareness and training	20. Training with augmented reality 21. Establish periodical training sessions	Simplify
Organizational	Solvent with composition out of specific (impurities, low)	22. Leasing of solvent	Simplify
Organizational (Digitalization)	Inappropriate predictive maintenance	23. Use big data collected from sensors to make a predictive analysis of the unit conditions.	Simplify (error prevention)

Table 9
Pre portfolio of ISD alternatives for increasing sustainable safety.

ID[a]	Alternative	Comments	Pre-ranking[b]
IA1	Base case	Each company implements its own CCS process.	-
IA2	Absorption with Ionic liquids	Nowadays, large scale-up is not realistic.	NF
IA3	Rotating packed bed (RPB)	RPB is a promising technology as studies show that its dimensions are around 10 times lower than common packing bed systems (Borhani et al., 2019). However, the technology has only pilot plant scale applications.	NF
IA4	Less hazardous amine (DEA or MDEA)	A deeper analysis is required to check the impact on the safety and economic domain.	L
IA5	Partially Centralized solution with common stripper and reboiler	May lead to an improvement in terms of safety and economic, therefore, a deeper analysis is required	M
IA6	Fully centralized solution, with one single CCS plant for all the companies	May lead to an improvement in terms of safety and economic, therefore, a deeper analysis is required	M
IA7	Drones and IoT technologies for worker safety and training sessions with augmented reality	Drones are quickly entering the chemical processing space as more companies begin to embrace their use for inspection and monitoring tasks. Both IoT technologies and augmented reality are promising technologies for improving safety.	H
CA1	Fully centralized solution using DEA as a solvent; improved working conditions and workers monitoring; novel training sessions; clear and structured maintenance and inspection procedures.	Probably the most feasible solution from the safety perspective. A deeper analysis is required to confirm the positive effect on safety and to check the impact on the economic domain.	H
CA2	Same structure of CA1 but the use of a compact cross heat exchanger (plate and frame)	Same consideration of CA1	H

[a] IA: independent alternative; CA: combined alternatives.
[b] H= High; M = Moderate; L = Low; NF= Not feasible.

required before starting feasibility studies. An example of the pre portfolio of alternatives is provided in Table 9.

The alternatives with the higher score are analyzed to check their technical feasibility and to investigate the performance in terms of safety and economics. In the next section, the results of alternatives IA5, IA6, CA1, and CA2 are reported and the decision-making process is discussed.

5. Results and discussion

The performance of the base design in terms of SW&HI and CO_2 avoidance cost is reported in Fig. 5, where the bubble radius represents the amount of CO_2 emitted per year by each plant in kilo tonnes.

The two indicators show opposite trends: the SW&HI decreases for smaller CCS structures while the CO_2 avoidance cost increases as the size of the plant increases or, in other terms, for stronger CO_2 emitters. The first behaviour can be easily justified by the fact that as the amount of CO_2 processed increases, the unit's dimensions, the solvent flow rate, the utilities required, etc., increase, resulting in structures with a higher damage potential, if the same safety measures are adopted in all the plants. The trend of the economic index demonstrates that as the amount of CO_2 processed increases, the economic feasibility of the CCS structure increases. This behavior can be justified by the fact that usually, CCS facilities process large amounts of CO_2 so the effect of the economy of scale becomes relevant. Nevertheless, it is possible to improve the design by using ISD approaches. Different studies have been focused on the purely technical improvements of the post-combustion technology, to make the process more feasible from the economic and environmental point of view. Therefore, this study uses the previous technical options and combines them with ISD strategies that focus on human and organizational factors. For instance, as reported in the Pre-portfolio of alternatives, the agreement to cluster the entire process seems the most promising alternative, at first, because the overall area exposed to hazardous conditions is dramatically reduced and secondly, the entire process structure is simplified. These improvements in the HOFs are reflected in the SW&HI on the term $A_{i,n}$. The improvement from the base case of the design alternatives IA5, IA6, CA1, and CA2 are reported in Fig. 6.

From Fig. 6, it is clear that the solutions resulted in an improvement from the base design both in terms of safety and economic perspective. The decrease of the safety index is the most remarkable effect between the two indicators that, in other words, indicates that the overall area exposed to the hazardous condition is reduced. This dramatic reduction is mainly due to the new arrangement of the structure, that is changed from a fragmented to a centralized plant and by the substitution of the original amine with a less toxic and flammable solvent. The final task of the ISDDM is the selection of the final alternative which matches the objectives. Fig. 7 shows the trade-off between costs and safety, expressed as an area with a 50% probability of fatality/damage.

It is clear from Fig. 7 that the alternative IA2 is dominated by the other design solutions, therefore it is rejected. The choice among the remaining alternatives, forming a Pareto front, cannot be decided a priori. Thus, a subjective criterion needs to be introduced in the decision-making process. In this case, the safety domain was selected as prevalent, since the future carbon tax will be much higher than the calculated CO_2 avoidance costs. Actually, according to the Government of the Nivolianitou et al. (2006), the tax will increase gradually until 150€ per ton in 2030. Therefore, the difference between each design alternative is not enough to justify the selection of one case to the other. In conclusion, the final design solution adopted is the CA2, with a CO_2 avoidance costs of 92 €/ton CO_2 and an SW&HI of 6.3 m. It combines the use of the ISD principles of simplification, substitution, and minimization, both for technological and non-technological aspects, resulting in the optimal design solution.

5.1. Practical implications of this study

Despite the results are in line with the objectives, different challenges can be used as starting points for future works. First, the SW&HI provides a specific sub-index to consider HOFs aspects. However, further research could include specific items that allow a clear distinction of innovative non-technical alternatives like administration and management aspects, distribution and logistics, and information and communication systems. Second, to test the flexibility claimed by the approach proposed, future work could be the further analysis of the CCS technology in a more advanced stage of design, where detailed safety analysis will be performed to obtain an estimation of the risk involved in the plant.

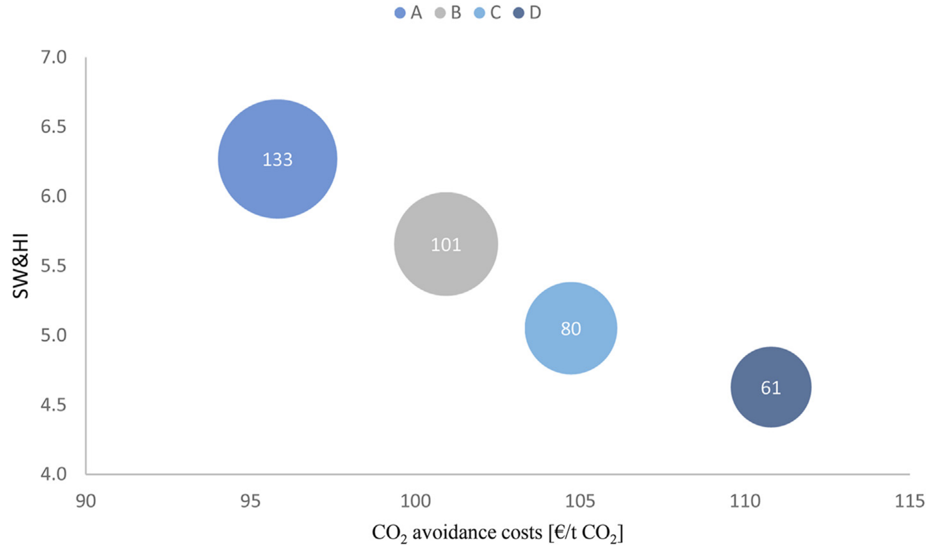

Fig. 5. SW&HI and CO_2 avoidance cost function of the CO_2 emitted for a year in kt. The bubble radius represents this value.

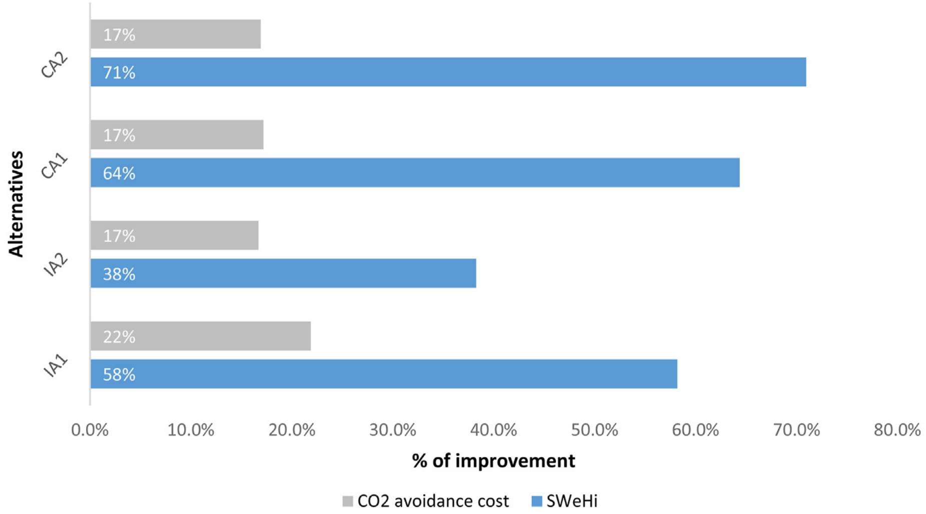

Fig. 6. % of improvement of ISD alternatives from the base case.

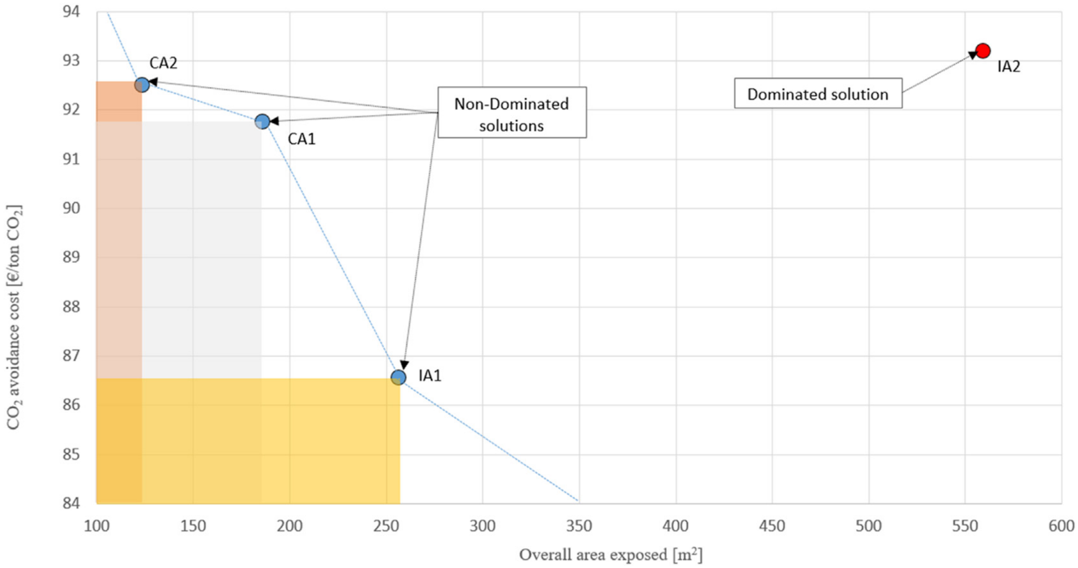

Fig. 7. Decision making graph showing the trade-off between safety and cost.

Third, the results obtained demonstrated that the CCS structure is not feasible with the actual carbon tax in The Netherlands. Nowadays, the carbon tax in The Netherlands is 30 € per ton of CO_2 emitted, while the average CO_2 avoidance cost is around 3 times this value. The results are in line with results obtained by Berghout et al. (2015), where the average cost is around 90 € per ton. However, according to the government of The Netherlands, the tax will increase gradually until 150€ per ton in 2030 (Government of the Netherlands, 2019).

6. Conclusions

An Inherent Safety Design Decision Making (ISDDM) framework is developed and proposed for systematic identification, classification, and evaluation of both technological and non-technological ISD alternatives, explicitely addressing HOFs. The applicability of the ISDDM is tested using a carbon capture plant as a case study. The final design selected has an improvement from the base case of 17% in terms of CO_2 avoidance costs and around 70% in terms of the radius of the area exposed to moderate hazard. The analysis provides an increase of ISD alternatives exploring HOF aspects compared with just technical studies. The resulting plant would be safer and more sustainable, both from the environmental and economic point of view. The results of the case-study demonstrate the applicability and flexibility of the ISDDM developed, which allows the qualitative analysis of organizational and human factors also during early design stages when the low level of details available usually discourage their analysis.

CRediT authorship contribution statement

Yuri Di Martino: Conceptualization, Methodology, Software, Writing – original draft, Validation, Investigation. **Santiago Echeverri Duque:** Project administration, Visualization, Validation, Investigation. **Genserik Reniers:** Supervision, Writing – review & editing, Resources. **Valerio Cozzani:** Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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