Journal of Loss Prevention in the Process Industries 91 (2024) 105382

Contents lists available at ScienceDirect

Journal of Loss Prevention in the Process Industries

journal homepage: www.elsevier.com/locate/jlp

An artificial neural network approach to enrich HAZOP analysis of complex processes

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ARTICLE INFO

Keywords:
HAZOP study
Dynamic simulation
Artificial neural network
Complex processes
Styrene polymerization process

ABSTRACT

This paper proposes an innovative approach to enrich Hazard and operability (HAZOP) analysis for complex processes using process simulators and artificial neural networks (ANNs). HAZOP study is a systematic qualitative procedure aimed at identifying potential hazards and operability issues. It heavily relies on the collective knowledge and experience of the team during brainstorming sessions. Traditionally, HAZOP considers only "one failure at a time," overlooking the effects of deviation causes amplitudes, their propagation, and subsequent domino effects. This simplification is necessary to manage time and costs during sessions. However, in complex systems, neglecting certain scenarios may result in overlooking critical situations. In our proposed method, we leverage process simulators to simulate upset scenarios comprehensively. By systematically varying all possible deviation causes and their combinations, we generate a substantial amount of simulation data. To facilitate evaluation, we introduce novel evaluation indexes. Additionally, we define a sensitivity index for ranking HAZOP scenarios based on severity of consequences. Furthermore, we classify scenarios into three severity levels according to their consequences. To enhance HAZOP analysis, we employ ANNs. These networks learn process behaviors and predict the evaluation indexes. They also classify scenarios based on pre-simulated data. With this approach, the HAZOP team can efficiently analyze the consequences of nearly any combination of deviation causes and failures, even with varying amplitudes. We validate our method by applying it to a real-world complex polymerization plant, demonstrating its value in practical scenarios.

1. Introduction

Artificial Intelligence (AI) is a wide-ranging area of computer science dealing with construction of machines to imitate the problem-solving and decision-making capabilities of the human mind. With the wide availability of process data and powerful computational tools, the hype around AI approaches has accelerated today, since they can solve complex problems in a wide range of applications such as process modeling and digital twins, quality control, optimization, process monitoring, fault detection and diagnostics, maintenance, etc. (Sanikhani et al., 2019; Rahmanifard and Plaksina, 2019; Arunthavanathan et al., 2020; Kaur et al., 2020). However, in some applications due to complexity of subject matter, lack of sufficient data and less knowledge on how to formulate the problem, AI approaches have less been used. Hazard and Operability (HAZOP) study or HAZOP analysis is the one which is the focus of this paper.

HAZOP study is a systematic procedure used to review chemical process design and operation to identify potential hazards and operability problems. This analysis is intrinsically a qualitative approach performed by a multidisciplinary team of experts during brainstorming sessions (CCPS, 2008). Therefore, the quality and success of HAZOP analysis mainly depend on the knowledge, experience, and training level of the HAZOP facilitator and the team members (Baybutt, 2015). In other words, HAZOP is a human-centered activity prone to human error.

Conventional qualitative HAZOP works well for safety analysis of simple systems. For HAZOP analysis of more complicated systems, some

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https://doi.org/10.1016/j.jlp.2024.105382
Received 9 January 2022; Received in revised form 7 April 2024; Accepted 28 June 2024
Available online 1 July 2024

simplification rules are assumed to keep the HAZOP brainstorming sessions time and cost affordable (Mokhtarname et al., 2022).

- Effects of "amplitude and duration" of deviation causes or failures are commonly ignored in the brainstorming sessions. However, for instance, how much exactly does the deviation "less flow" mean: 80%, 50% or 20% of the normal operation condition value? Does the deviation occur as a step change? Does the deviation last 5 min or more, or is it only an impulse? These may have different consequences.
- One deviation cause or failure at a time is only considered in the HAZOP brainstorming session while multiple deviation causes (e.g., multiple failures of equipment and devices) could have greater consequences.
- Effects of domino events are commonly ignored in the HAZOP brainstorming. Domino effect in context of HAZOP study is defined as "an event at one unit that causes a further event at another unit".

In general, such simplification rules could lead to missing the rare but important critical scenarios (i.e., in terms of safety or operation). In the best case, these scenarios are identified empirically during commissioning and operation. In the worst case, these scenarios remain unidentified and could contribute to some major problems.

Considering the afore-mentioned limitations and knowing the power of computer applications, methodologies to combine computer-aided approaches with the HAZOP study have become among the most studied topics in the field of hazard identification improvement. "Automated HAZOP" has been a widely focused research topic in academia for about 30 years. However, very few of these approaches have been used in the chemical process industry. There are several researchers and research groups that investigated the status of HAZOP studies automation and the general improvement in this area (e.g. Dunjó et al., 2010; Taylor, 2017; Cameron et al., 2017; Single et al., 2019). Automated HAZOP refers to a computer-based program that tends to automate HAZOP analysis fully or partially. For automatic analysis of potential hazards and operability issues within HAZOP studies, conclusions regarding cause-and-effect relationships or consequences need to be identified. This process of inferring conclusions is called reasoning. Reasoning is an important module for conducting HAZOP automation. Single et al. (2019) provided a classification of major reasoning techniques within the context of HAZOP automation as illustrated in Fig. 1.

Basically, there are qualitative and quantitative reasoning approaches. Single et al. (2019) reviewed the qualitative reasoning approaches and grouped them into three generations: rule-based expert systems (Karvonen et al., 1990), integrating models with rule-based systems (Cui et al., 2008), and integrating models with case-based reasoning (Zhao et al., 2009) based on the literature in the 80s until today. Quantitative model-based approaches (i.e., which are based on first principles models) are among the many ways for supporting conventional HAZOP towards automation and are usually implemented using process simulators. This area has gained more importance in the last years (Danko et al., 2018, Murillo et al., 2018; Raoni et al., 2018; Danko et al., 2019; Mokhtarname et al., 2020; Mokhtarname et al., 2021a). Thus, process simulators seem to be promising tools to provide more accurate causes and consequences analysis beside of reducing the required time and effort and minimizing human factors.

Fig. 2 illustrates the sequence of HAZOP study through an Engineering, Procurement, and Construction (EPC) of a project. Preliminary coarse HAZOP uses the full HAZOP procedure in early phase of project where there is still the "ability to change the design, operating and maintenance policy". During coarse HAZOP, qualitative consequences of HAZOP scenarios are commonly put in evidence to highlight the scenarios that require further simulation analysis. Such scenarios are simulated outside HAZOP brainstorming session and then reassessed in a "complementary main HAZOP". Main HAZOP is held at the front-end engineering phase and its objective is the assurance of the current safety design ("Will it Work?") rather than making recommendations for change.

The scope of further simulation analysis is first based on the team engineering judgement and therefore some credible scenarios may be overlooked. On the other hand, to perform a thorough quantitative HAZOP analysis, all possible deviation causes as well as their combinations and propagation effects are required to be scrutinized in order to prioritize the possible scenarios that can result in hazardous situation or undesired operability issues. But this would be very time and effort consuming and therefore would not happen during HAZOP sessions. For more complex HAZOP nodes, where many process variables interact, consequence analysis of deviation scenarios is a more difficult and time-consuming task. In research investigations focusing on combination of dynamic simulation and HAZOP study, the range of HAZOP deviations are commonly kept uniform, and a limited number of simulations are analyzed for their explanatory purpose (Labovský et al., 2007; Kang and Guo, 2016; Carlos et al., 2018; Danko et al., 2019). Besides, propagation of deviation causes on all critical process variables are not commonly investigated. Therefore, to continue in the HAZOP automation progress, other issues like simultaneous deviations and processing and evaluation of a large amount of data in form of simulations outputs must be considered.

With the wide availability of process data and process simulators, artificial intelligence can play new roles in enhancing safety analysis of industrial process design and operation. The novel idea of this research is the use of process simulators and artificial neural networks (ANN) to

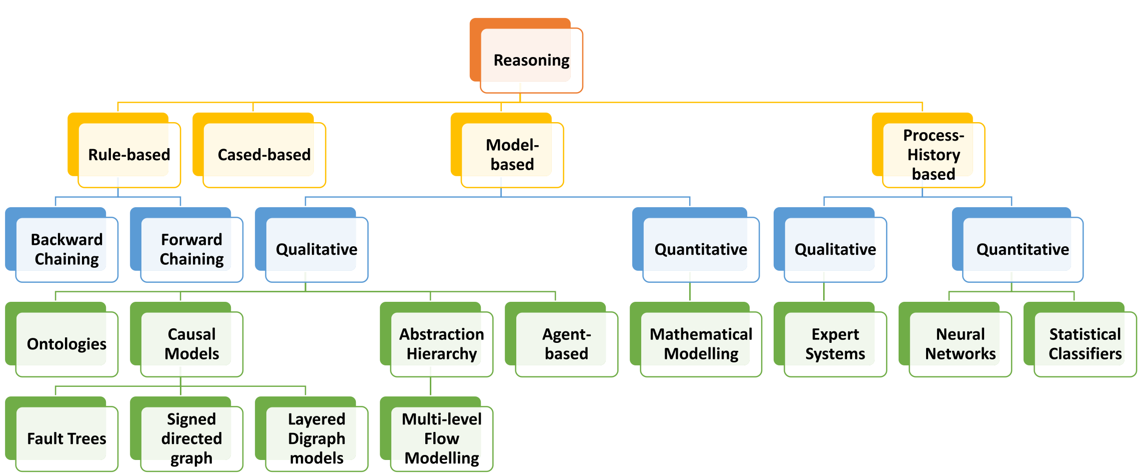


Fig. 1. Reasoning technique classes for HAZOP studies (Single et al., 2019).

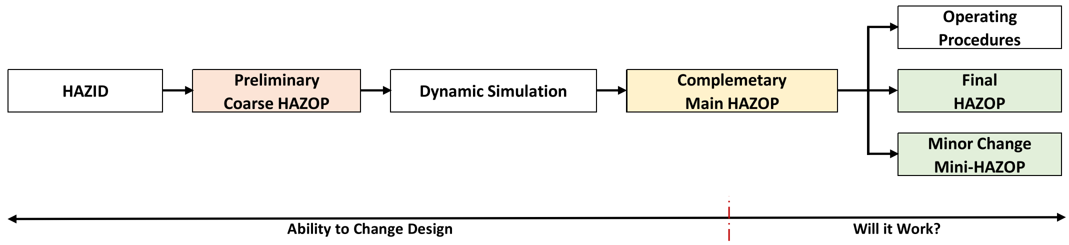


Fig. 2. Sequence of HAZOP studies during EPC of a project.

aid HAZOP decision-making. Process simulators are first used to simulate upset scenarios as much as possible. In this regard, systematic variations of all possible and important deviation causes and their combinations are suggested which result in a large amount of data in form of simulation outputs. For easy evaluations of simulation results some new evaluation indexes are proposed. A sensitivity index is also defined for ranking of HAZOP scenarios. Furthermore, three severity levels are defined to classify HAZOP scenarios regarding severity of consequences. ANNs are then used for learning process behaviors and prediction of the evaluation indexes and classification of scenarios based on the pre-simulated scenarios. Using the proposed method, the HAZOP team could easily analyze consequences of almost any combination of deviation causes or failures with different amplitudes in a very short time. The effectiveness of the proposed method is verified by investigations on an operating styrene polymerization plant.

As a final word, although process simulators are commonly used within HAZOP analysis, the resulting accuracy depend on the accuracy of the developed process model. Therefore, the results need to be checked and verified by HAZOP expert team. Today, process industries are turning to a new generation of simulators called digital twins which are virtual representations of the real-world. Digital twins can seek to identify breakages in process plants before they happen and then provide solutions. There are many reasons for developing such twins in the process industries such as product development, design customization, optimization, etc. Having this in mind, the assumption of having good simulators for process plants during the design and operation phases seems to be reasonable.

The remainder of this paper is organized as follows. The details of the proposed methodology of this paper is provided in Section 2. In Section 3, the proposed methodology is applied to an operating styrene polymerization process. Discussions are presented in Section 4. Finally, in Section 5, conclusions are discussed.

2. The proposed methodology

To understand the results of a deviation cause by simulation, one typically looks at the related output trends from simulators. These trends help interpret the behavior or outcomes resulting from such a deviation cause. The process involves applying various variations and waiting for the simulator-generated outputs, which may include plots, graphs, and other visual representations. The expert then delves into these trends to assess their effects. Now, consider a scenario where an operator must apply various deviation causes and their combinations, creating numerous trends to comprehend the outcomes. Depending on the dynamic nature of the process, this analysis can be time-consuming and is not feasible during HAZOP brainstorming sessions. To address this, initially, we define indexes derived automatically from the resulting trends. These indexes facilitate easier interpretation. More importantly, we suggest formulating the problem using an ANN. The ANN takes deviation causes as typical inputs and the resulting evaluation indexes for some limited variations as typical outputs. After offline training, the neural network creates a model capable of predicting evaluation indexes for any possible variation of the deviation causes. Notably, once trained, the neural network provides rapid predictions based on input data. Our study found this approach highly effective. Additionally, we classify each scenario into three severity levels based on the consequences. Another ANN is employed to predict severity levels. By adopting this method, the HAZOP team can efficiently analyze the consequences of nearly any combination of deviation causes or failures, even with varying amplitudes, in a short timeframe.

The proposed methodology can be divided into three steps: (1) deviation analysis, (2) data collection process, and (3) artificial neural networks for the prediction of simulation results and classification of HAZOP scenarios which are described in detail in the following subsections.

2.1. *Deviation analysis*

During a typical HAZOP analysis, process plants are initially divided into sections called nodes. Next, all possible guidewords are combined with process variables to generate HAZOP deviations. All possible causes or failures associated with these generated HAZOP deviations are then identified. To assess adverse consequences, different possible causes or failures are commonly investigated independently during the brainstorming session.

In the first step of the proposed procedure, critical process variables are determined. In the context of this research, critical process variables refer to those process variables in which deviations could lead to major hazardous situations and/or operability issues. Experienced plant operators are often considered the best experts for identifying these variables. Following this, all possible deviation causes or failures are identified. This paper emphasizes evaluating multiple deviation causes or failures and systematically varying the amplitudes of these causes or failures, rather than solely relying on qualitative assessment of single deviation causes or failures.

2.2. *Data collection process*

Once process critical variables are determined and all possible deviation causes or failures are identified, in the next step, the required data are collected. The data collection process includes performing simulation of deviation causes or failures and calculating evaluation and sensitivity indexes described in the following subsections.

2.2.1. *Performing simulation of deviation causes or failures*

To collect information of the process abnormal conditions, process simulators are required. For operating plants, the plant actual data of process faults can be very helpful; however, it may be insufficient. In fact, the operating condition of the actual operating plant may not be changed due to safety and economic issues. Therefore, acquiring sufficient abnormal condition data by directly imposing the process faults to the actual plant is impossible. Besides, the records of the previous abnormal conditions cannot guarantee that all types of deviations have been included. Therefore, process simulators not only help during the design stage, but also could help during operation as well.

In this research, to assure that all process upsets are seen, almost all combinations of various deviation causes with different amplitudes are considered. Thanks to powerful computer systems, all deviation scenarios can be simulated with a reasonable time and effort utilizing available process simulators. Therefore, as the next step, a large amount of data in form of simulations outputs must be processed and evaluated. It should be noted that in practice you do not need to make all possible combinations with quite a large range of amplitude variations as these may be unnecessary and very time consuming. Instead, the most important combinations and some amplitude variations (with experts view) could be sufficient.

2.2.2. Calculating the evaluation and sensitivity indexes

Having simulated a deviation cause, the process dynamic behavior is commonly characterized by different indexes. The behavior indexes can be used to understand the sensitivity of deviation causes. A typical sensitivity evaluation model of the deviation cause was first introduced to HAZOP analysis by Kang and Guo (2016). There, a sensitivity evaluation model was proposed to measure the effect of each deviation cause on the target process variable included in the deviation. In their research, three evaluation indexes were considered, and effects of deviation causes on only one target process variable were investigated. Besides, amplitudes of all deviation causes have been uniformly set only at 10% of the departure from the normal operation condition.

In this paper, a new sensitivity evaluation model considering some other complementary indexes (i.e., total of five evaluation indexes are considered) is introduced with emphasis on effects on all critical process variables within a node. Besides, multiple deviation causes or failures with variations of amplitudes are investigated in the evaluations rather than qualitative single deviation cause or failure. Using the proposed sensitivity evaluation model, the deviation causes are ranked based on the sensitivity value. This enables the operators to focus on more sensitive causes. Higher sensitivity value of a deviation cause means that this deviation cause could result in more significant changes in the process variables. Finally, the ranking results are documented in HAZOP analysis report. It is worth noting that the sensitive causes resulting in deviation can be further screened out in the process monitoring and fault diagnosis.

The comprehensive sensitivity index for a deviation cause can be expressed as the weighted sum of the variation degree of the critical process variables multiplied by fluctuation degree and time coefficients. The sensitivity index (S) of a deviation cause is thus formulated as:

$$S = \sum_{i=1}^{n} w_i \left(V_d \times C_f\right) \tag{1}$$

where V_d is considered as the main evaluation index representing variation degree of the target process variable compared to normal value condition, n is the number of critical process variables, and w_i is the weight factor representing the importance degree of each critical process variable. Weight factors may be determined by various methodologies. In this paper, we invoke "expert's view" in specifying these weights.

V_d is not the only effective index on the sensitivity value. Therefore, another indicator named as C_f is also considered which is representative of a combinatory effect of the fluctuation degree and time coefficients. C_f is defined as follows:

$$C_f = \frac{F_d \times \theta_{ss}}{\theta_p \times \theta_c} \tag{2}$$

The evaluation indexes of (1) are described in the following:

- V_d is a ratio defined as the difference between the maximum (or minimum) value of deviation in the target process variables and normal operating value when a failure occurs divided by the difference between its high and low alarm limits as follows:

$$V_d = \frac{\left|V_{\max(or\ \min)} - V_N\right|}{V_{alarm}^{H} - V_{alarm}^{L}} \tag{3}$$

where $V_{max\ (or\ \min)}$ indicates the maximum (or minimum) value of the deviation after the occurrence of the deviation cause and V_N is the value of the target process variable in normal operating condition. The V_{alarm}^{H} and V_{alarm}^{L} are the high and low alarm limits of the target process variable, respectively. In Equation (3), V_{max} (V_{min}) is used when the target process variable under consideration is ascending (descending) relative to the normal value V_N. In many process plants we are worried about increasing the critical process variables such as pressure, temperature, etc., since they could lead to hazardous situations. On the other hand, decreasing these parameters could lead to some major operability problems. Since both hazardous situations and operability issues are scopes of HAZOP analysis, in this research, both increasing and decreasing behavior of process variables are considered in this evaluation index.

- Parameter V_d is multiplied by C_f which includes fluctuation degree (F_d) of the target process variable under abnormal process condition. F_d is a ratio to show the difference between maximum and minimum values of the target process variable divided by the difference between its high and low alarm limits as follows:

$$F_d = \frac{V_{max} - V_{min}}{V_{alarm}^{H} - V_{alarm}^{L}} \tag{4}$$

F_d is an indicator of the stability degree of the target process variable under abnormal condition.

In both the variation degree and fluctuation degree, division by the difference of high and low alarm limits is performed to make these indexes dimensionless and their related values somehow normalized and comparable with other indexes.

- The duration time it takes for the target process variable to reach the maximum (or minimum) value is represented by T_p and is somehow normalized as follows:

$$\theta_p = \frac{T_p}{T} \tag{5}$$

where T represents the duration of the simulation process.

- The duration time required for the target process variable to reach and remain within a given tolerance band is represented by T_s and is somehow normalized as follows:

$$\theta_s = \frac{T_s}{T} \tag{6}$$

- The duration time it takes for the target process variable to reach the high high/low low alarm limit is another important index represented by T_c. This index shows the criticality of process condition and is somehow normalized as follows:

$$\theta_c = \frac{T_c}{T} \tag{7}$$

Fig. 3 depicts dynamic simulation result of a deviation cause for a typical process variable. In this figure, parameters $V_{\max}$, $V_{\min}$, V_N, T_p, T_s, and T_c are visually illustrated for better understanding. These parameters are used to define the useful indexes of (3) to (7). Having calculated the evaluation indexes, the sensitivity index is then calculated to rank the scenarios.

So far, for each deviation scenario, a sensitivity value and five evaluation indexes are calculated using process simulator tools. The following subsection focuses on how ANNs could improve HAZOP analysis using the collected data.

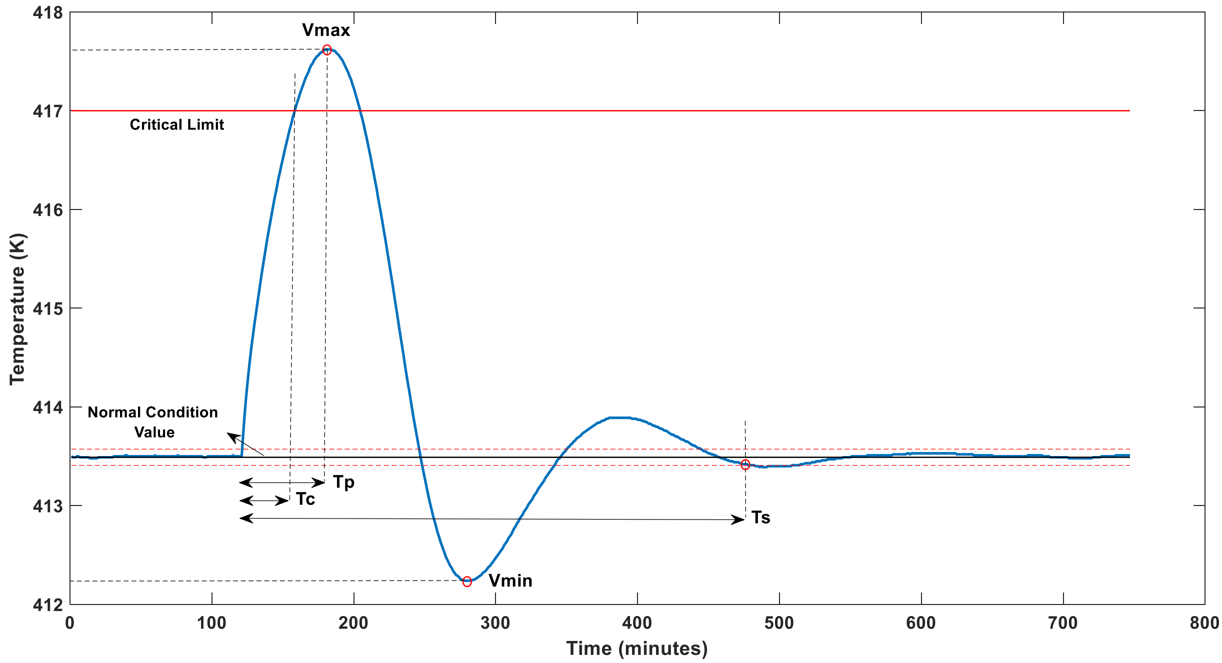


Fig. 3. Dynamic simulation result of a deviation cause for a typical process variable parameters (V_{max}, V_{min}, V_N, T_p, T_s, and T_c are visually illustrated in this figure which are used to define the useful indexes of (3) to (7)).

2.3. *Artificial neural networks for prediction of simulation results and classification of HAZOP scenarios*

Fig. 4 illustrates the flowchart of HAZOP analysis using the procedure suggested by this research. As previously mentioned, this paper suggests simulation of all combinations of deviation causes with systematic amplitudes variations to ensure that all possible and important HAZOP scenarios are considered. When we refer to systematic amplitude variations, one may think of variations in all ranges from very small to very large. However, implementing such a comprehensive range of variations is impractical and inefficient in terms of time and effort. Therefore, in this research, we propose 5 different amplitude variations in the range with 20% steps. Subsequently, ANNs are employed to predict other variations within the specified range for use in the HAZOP analysis. The details of the proposed procedure are discussed in the following.

Process upsets are typically classified into several classes based on the severity of their consequences. In this paper, three severity levels are defined.

- Severity level 1 represents process deviations where critical process variables falls within their high/low alarm limits. These scenarios result in process upsets or reduced productions. Properly functioning control systems and timely actions by plant operators can handle such situations.
- Severity level 2 refers to the cases where process variables are between their high/low and high high/low low limit alarms. These scenarios indicate more severe consequences compared to the first class.
- Severity level 3 represents critical scenarios that lead to hazardous situations and undesired plant shutdowns. Implementing safety instrumented systems is necessary for handling such scenarios.

As demonstrated in Fig. 4(a), once critical process variables have been selected, HAZOP deviations have been generated, and possible causes have been identified (i.e., using results of the preliminary coarse HAZOP), the next step is data collection. Data collection includes simulating deviation causes or failures, as well as calculating of the evaluation indexes for all critical process variables as explained in Subsection 2-2-2. Based on the evaluation results, the scenarios are also classified into the severity levels explained earlier. Consequently, numerous collected deviation scenarios exist, where the inputs are different deviation causes with different amplitudes and the outputs are the evaluation indexes and the severity level that the deviation cause belongs to it. Once the data has been collected, ANNs are employed to create a model for predicting the evaluation indexes and the severity level for any possible variation of the deviation causes. This approach allows the determination of evaluation indexes and severity levels without the need for complex analysis and with reasonable time and effort. Fig. 4(b) illustrates how the trained neural networks are utilized within HAZOP analysis. It's important to note that the training phase of the proposed ANN (depicted in Fig. 4(a)) occurs outside HAZOP brainstorming session after simulations with the process model. Subsequently, the trained ANN (shown in Fig. 4(b)) is used during the "main HAZOP" brainstorming as an aid decision tool (refer to Fig. 2).

3. Implementation of the proposed HAZOP procedure on a polymerization process

In this section, implementation of the proposed methodology is investigated in an operating styrene polymerization plant.

3.1. *The case study process description and establishment of the process dynamic model*

Fig. 5 illustrates the schematic of the real operating styrene polymerization plant under consideration. In this process, fresh styrene monomer from the storage tank is mixed with the feed from the recycle drum V101, which includes unreacted styrene monomer and ethylbenzene (as solvent) recycled from the output of the 2nd reactor. The combined feed then passes through the mixer MX-1 and is preheated by the heat exchanger E−1 to reach the design temperature before entering the 1st reactor. The polymerization reaction is thermally initiated and progresses through two cascade Continuous Stirred Tank Reactors (CSTRs). Styrene polymerization is highly exothermic and the heat of reaction in both reactors is removed by heat exchangers E−2 and E−3,

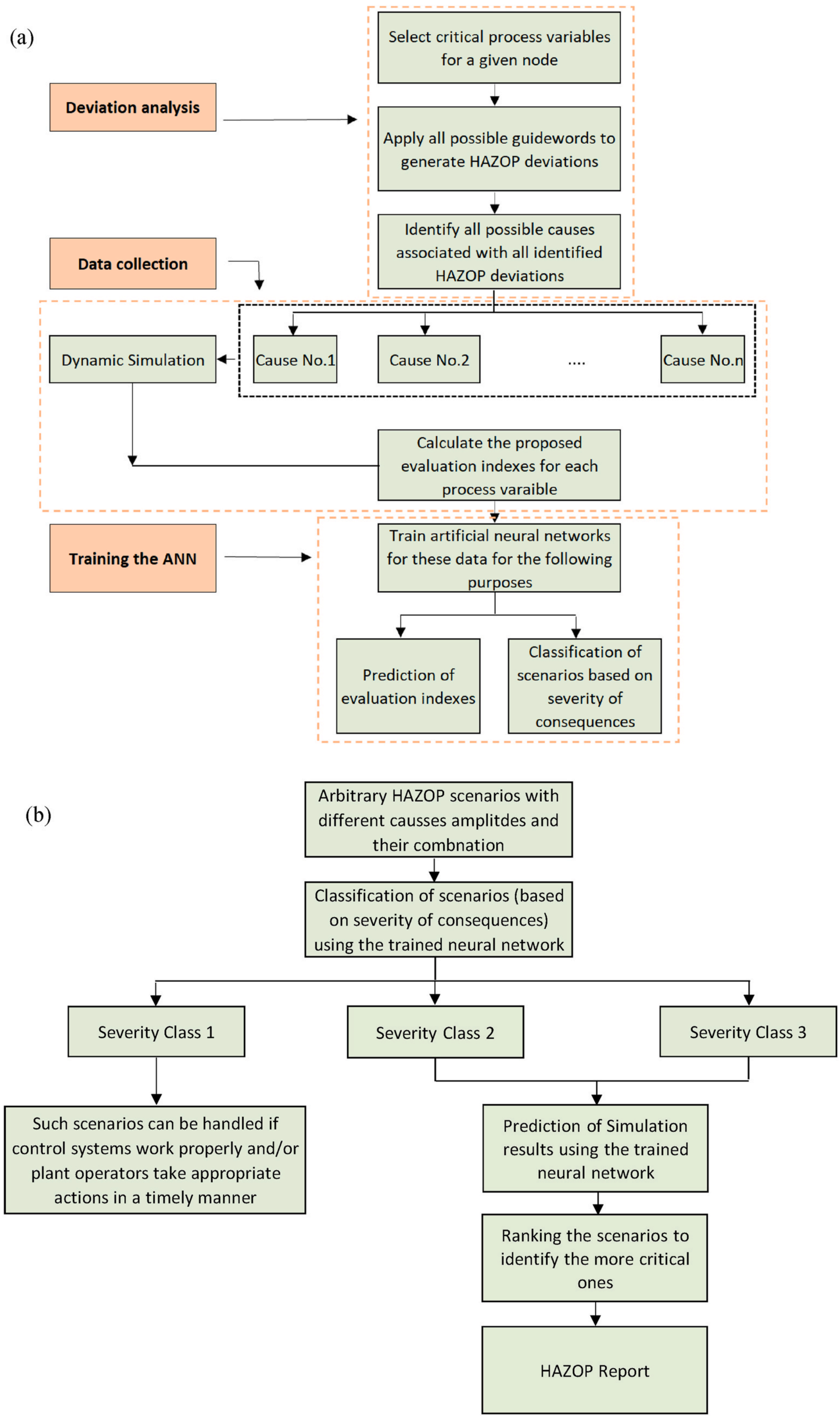


Fig. 4. The proposed HAZOP procedure using artificial neutral networks; (a) the training phase, (b) employing the trained neural network within the HAZOP analysis.

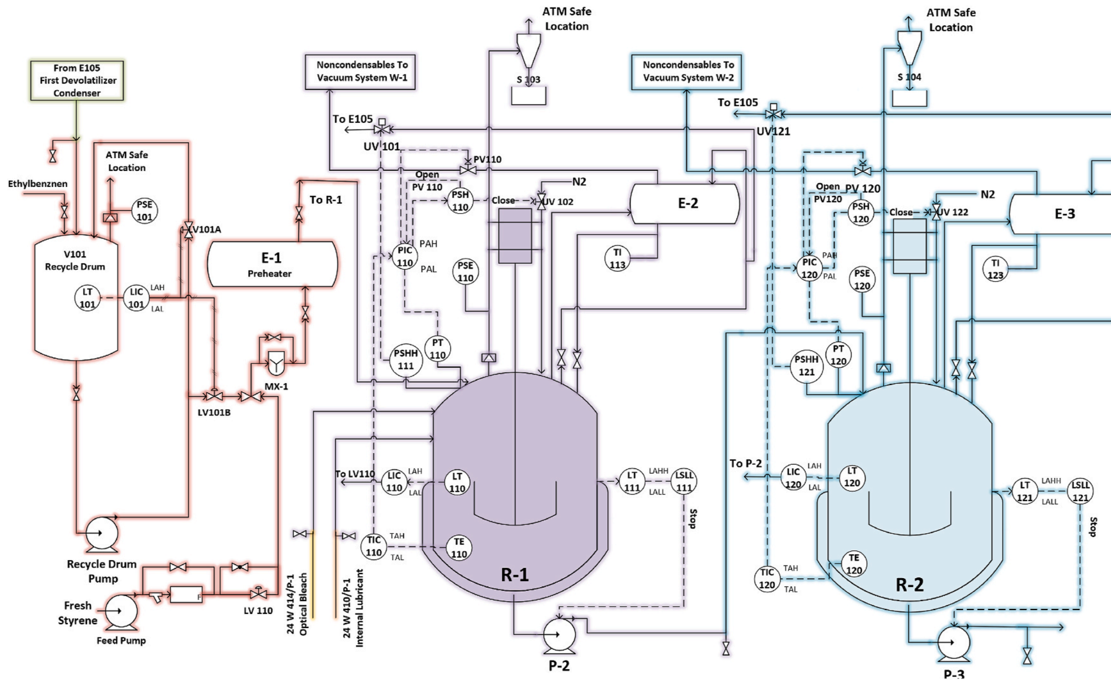


Fig. 5. Schematic of the polymerization process under consideration.

utilizing auto-refrigeration cooling mechanism. For more detailed information on the reaction kinetics and mechanisms, readers are referred to our previously published research (Mokhtarname et al., 2021b). There, the dynamic process models of the polymerization reactors nodes have been also developed and verified based on the actual plant data and historical records.

3.2. Deviation analysis

The polymerization plant in this study is divided into three nodes including "Feed and Recycle System", "1st Polymerization Reactor", and "2nd Polymerization Reactor". These nodes are highlighted in different colors as illustrated in Fig. 5. In this research, we consider HAZOP deviations and their corresponding causes associated with the 1st polymerization reactor node as the case (see Table 1). Based on the deviation causes reported in Table 1, a total of seven parameters associated with this node are considered for further simulation analysis as illustrated in Table 2.

Table 1
HAZOP deviations and their corresponding causes for the 2nd node.

No.	Deviation	Causes
1	No flow to the first polymerizer	- Feed pump failure, failure of LV110 or its control system to close more (i.e., less styrene feed to the first reactor), Any plugging or closed manual valve in upstream of 1st polymerizer
2	More flow to the first polymerizer	-Failure of LV110 or its control system to close more, Opened LV110 bypass valve due to operator mistake
3	High pressure in the reactor	-Failure of PV110 or its control system to close more -Less cooling in the condenser due to failure of cooling water or operator mistake -Excess injection of N_2 due to operator mistake.
4	Low pressure in the reactor	-Failure of PV110 or its control system to open more
5	High temperature in the reactor	-More heating of feed in preheater E−1. -Lower concentration of ethylbenzene
6	Low temperature in the reactor	-Less heating of feed in preheater E−1 -Higher concentration of ethylbenzene due to leakage or human mistake
7	High level in the reactor	-Failure of LV110 or its control system to close more -LIC120 failure to decrease speed of P-2
8	Low level in the reactor	-LIC110 failure to close LV110 more -LIC120 failure to increase speed of P-2

An experienced plant operator was interviewed to identify the critical process variables of the case study under consideration. Critical variables of Node 2 are reactor pressure (P_R), temperature (T_R), level (V_R), and condenser output temperature (T_C). The same variables are also considered for Node 3 to analyze the effect of deviation propagations.

3.3. Data collection

3.3.1. Performing the process dynamic simulation

In this paper, deviation causes are applied to the developed process simulation model individually and simultaneously. Here, for sake of simplicity (and saving pages on this paper) up to three simultaneous deviation causes are considered. Generalization to higher number of deviation causes can be similarly performed for a complete study in the industry. Each deviation cause is inputted to the simulation model in the form of a step disturbance. Deviation cause amplitudes significantly influences the operation condition of the plant. If the disturbance amplitude is too small, the deviation from process target variable may not be seen due to automatic adjustment of the control system; therefore, the plant is under normal operating conditions. Therefore, in this research, the amplitudes of all the step disturbances have been set

Table 2
A total of seven parameters associated with Node 2.

No.	Parameter
1	Flow of styrene feed flow rate
2	Pressure valve 110 opening percentage
3	Condenser coolant water flowrate
4	Flow of N_2 gas
5	Input feed temperature
6	Solvent concentration
7	Flow of 1st reactor output

between 0% and 100% of the possible deviation from the normal operation conditions with uniform steps of 20% changes. In simulation of all scenarios, disturbances are initiated 2 h after simulation begins. This time is used for better presentation of simulation results and can be chosen as desired without affecting the final results. Afterwards, the dynamic response of critical variables is recorded for an additional 13 h for this case study. This time would be different for different systems. In other words, this time is chosen such that the system reaches its steady state value after the disturbance is loaded. This way the effect of deviation propagation in process critical variables is better seen. The sampling interval of the data is 1 min, and 867 sample data are obtained for each simulation scenario.

3.3.2. Calculating the evaluation and sensitivity indexes

In this research 37170 deviation scenarios (i.e., for seven failures and five different amplitudes variations) were first simulated including single failure and simultaneous double and triple failures scenarios with different amplitudes. These simulations were performed by a computer system of core i5 and 8G RAM in 3.5 days. As the next step, the evaluation indexes, introduced in Subsection 2-2, were calculated for each simulation scenario. In other words, for each deviation cause, process variables are characterized and analyzed by the five indexes. Calculations of the evaluation indexes for all simulation trends were performed by a computer program in a few minutes.

Having available such pre-simulated scenarios, another evaluation is also performed to aid decision-making during HAZOP analysis. As mentioned in Subsection 2-3, the consequences of process faults are categorized into three severity levels based on the results of the evaluation model. Therefore, there are 37170 collected scenarios which are different deviation causes with different amplitudes and the corresponding severity levels that the deviation cause belongs to it (i.e., severity levels 1, 2, and 3).

Deviation scenarios of severity level 1 commonly result in reduced production and could be easily handled by the control systems and/or timely intervention of plant operators. The HAZOP team should pay more attention to the scenarios of severity level 2 and especially level 3 which may lead to hazardous process conditions and operability issues. Therefore, it is important to provide such classification for the HAZOP team to help prioritize the deviation scenarios.

3.4. Training the artificial neural networks for classification of HAZOP scenarios and prediction of simulation results

Havin collected simulation data, first, an artificial neural network is trained to classify each deviation scenario to the three severity levels. The input/output configuration is illustrated in Fig. 6. Next, an artificial neural network is trained for such classification purposes. Probabilistic neural network (PNN) introduced by Specht (1990) is used in this paper. Such neural network is essentially based on the well-known Bayesian classifier commonly used in many classical pattern-recognition problems. The network is trained with 80% of the scenarios and tested with the next 20%. The spread value of PNN was chosen 0.03 by trial and

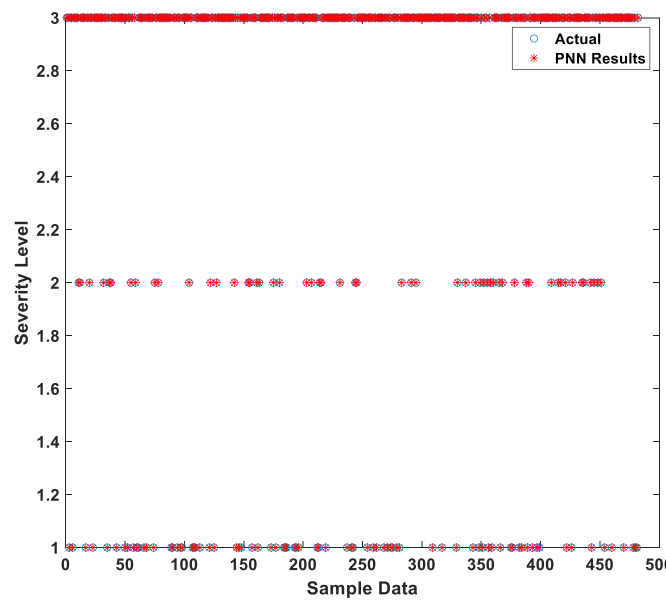


Fig. 7. Comparison of the actual severity levels of scenarios (blue circles) with the predictions of the PNN (red star) emphasizing on a very good approximation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

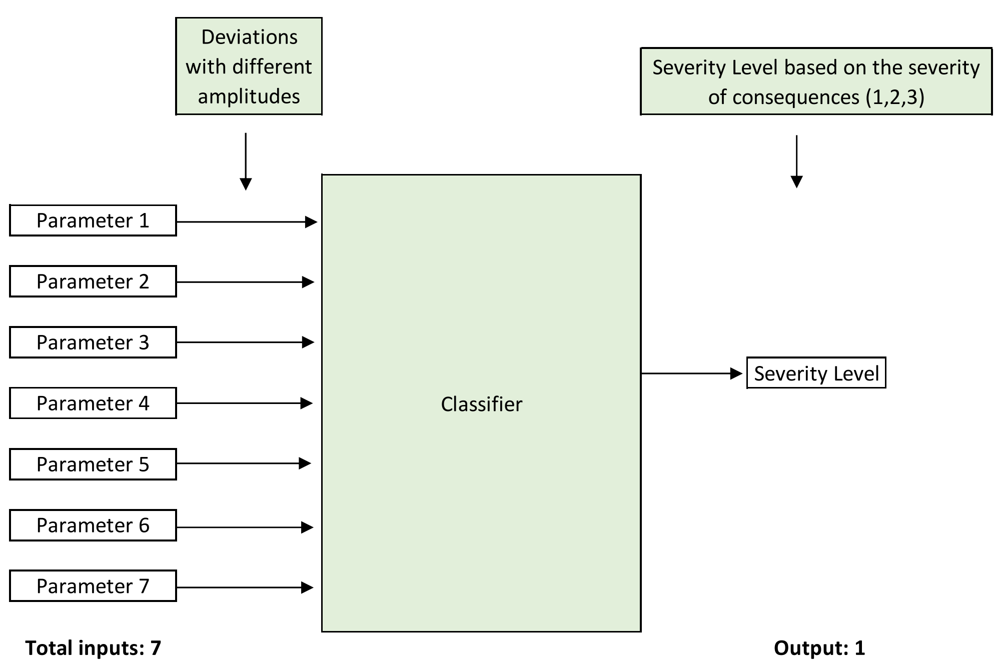


Fig. 6. Input/output configuration of network for the classification problem in this research.

error to obtain the minimum square error. Fig. 7 shows comparison of the PNN results and actual data for some of the test scenarios. In this figure, x axis shows the HAZOP scenarios and y axis is the severity level of each scenario (i.e., severity levels 1, 2 and 3 explained above). As can be seen the blue circles which are the results of PNN best fit to the actual severity levels (i.e., red cross) emphasizing on good approximation.

Having such a network, severity level of any arbitrary deviations cause can be determined with no need to any further simulation. Besides, the scenarios of the same severity levels can be ranked using the sensitivity formulation introduced in (1). This can help the HAZOP team to highlight the scenarios that are more critical in terms of consequences.

As the next evaluation step, another artificial neural network is trained to predict the evaluation indexes of any deviation cause with arbitrary amplitude within reasonable time and effort. The configuration of inputs and outputs of the neural network is illustrated in Fig. 8. There are 7 parameters with different amplitudes variations ranging from −100% to +100%, and 40 outputs (i.e., eight process variables with 5 indexes for each variable). To facilitate training of the ANNs, 40 independent networks are trained for each output separately. With such a network, one can request simulation results.

The famous and efficient multi-layer perceptron (MLP) is investigated for the collected simulation data. The performance of several MLP structures is evaluated for this purpose. The networks are trained using a random 80% of the total scenarios and tested with the remaining 20%. To achieve somehow an optimal network structure, an optimizing algorithm is developed to adjust the number of neurons in each layer of a three-layer MLP. An incremental approach is used to identify the best number of neurons for each layer. The study involved 180 iterations for each neural network. Additionally, four different learning algorithms were considered during the process of selecting the optimal structure.

Due to space limitations in this paper, only two evaluation indexes related to the reactor temperature are presented. First, MLP network is investigated for the output V_d of the reactor temperature. Four different algorithms, as listed in Table 3, were tested for training the MLP network. Each entry in Table 3 presents 180 different trials of a three-layer network with "tansig" neurons in all layers, aiming to find the optimal number of neurons that minimize the mean square error (MSE).

Table 3
The performance of the various algorithms for the MLP network (i.e. 4 different learning algorithms, each with 180 different choices of the neurons of the three layers).

Performance Algorithm	# of neurons for three layers	MSE (for train data)	MSE (for test data)
trainlm - Levenberg-Marquardt	[18 10 10]	4.8e-04	1.23e-03
trainrp - Resilient Backpropagation	[20 25 5]	2.8e-03	1.3e-02
traincgb - Conjugate Gradient with Powell/Beale Restarts	[25 25 5]	4.1e-03	3.2e-02
OSS trainoss - One-Step Secant	[30 20 10]	5.3e-03	4.3e-02

The results of training this network with the different algorithms are summarized in Table 3. Notably, using the "trainlm" algorithm with 18, 10, 10 neurons in the hidden layers achieved the minimum MSE. For all other indexes and other process variables, the same procedure was followed to train the appropriate network. Figs. 9 and 10 depict the regression plot of the train and test data for V_d and F_d indexes of the reactor temperature, respectively. These figures illustrate the approximated values of train and test data obtained using the MLP network compared to their actual value. Data points close to the x = y line indicate good performance of the MLP network, while dispersion of data points reflects approximation errors. Overall, the results demonstrate the good performance of the developed MLP network.

3.5. Results and analysis

Some interesting results based on the proposed methodology are explained in the following.

- First the proposed sensitivity evaluation model is investigated for the case study process. In this case study, increasing the reactor pressure, temperature, and level (i.e., which are considered as critical process variables) could lead to more severe consequences than their decreasing. Therefore, we pay more attention to these scenarios. Besides, the reactor pressure and temperature are more critical than the reactor level. As a result, in the sensitivity formula of (1), weight factors for pressure and temperature are considered ten times larger.

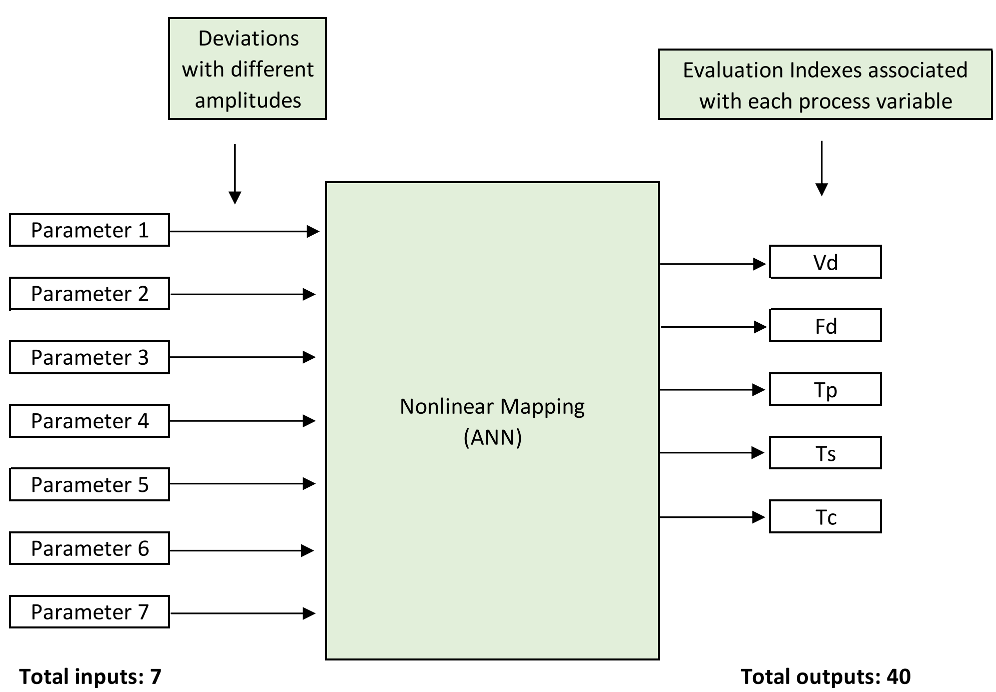


Fig. 8. Input/output configuration of networks for the nonlinear mapping problem in this research.

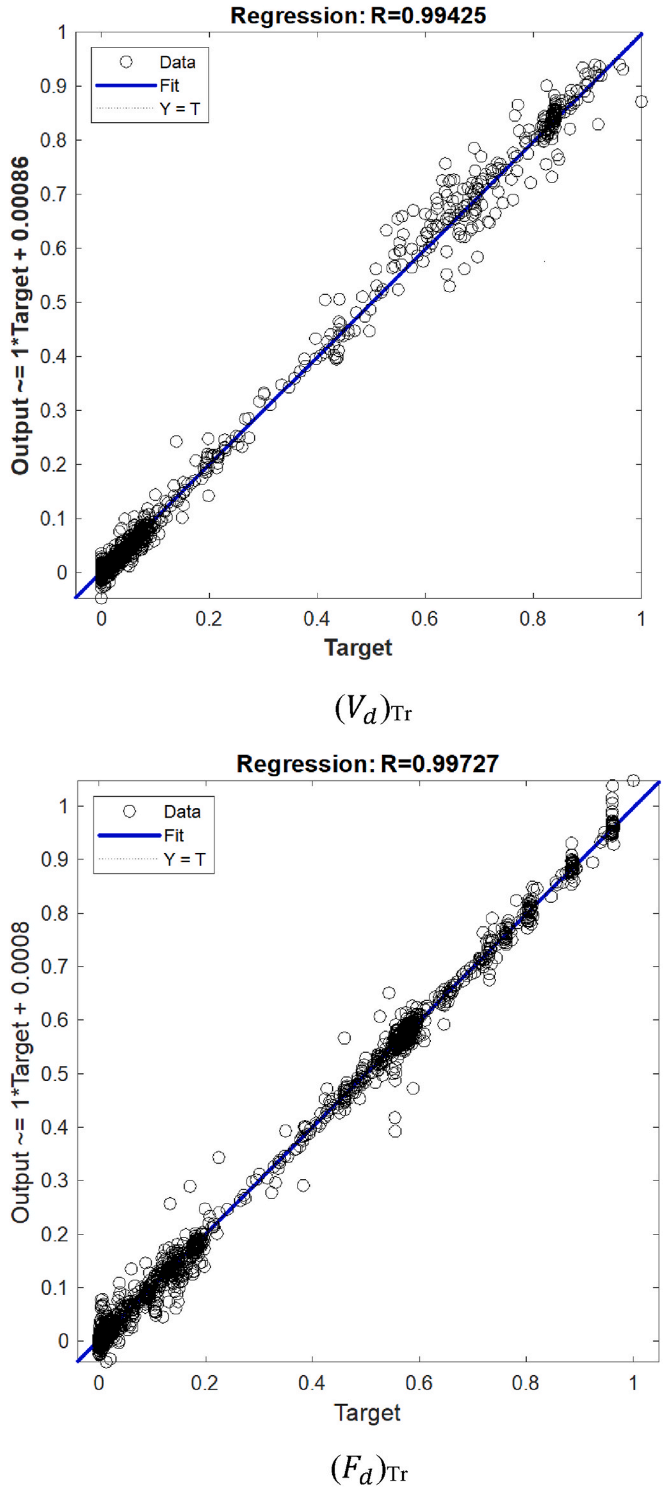


Fig. 9. Regression analysis of the train data.

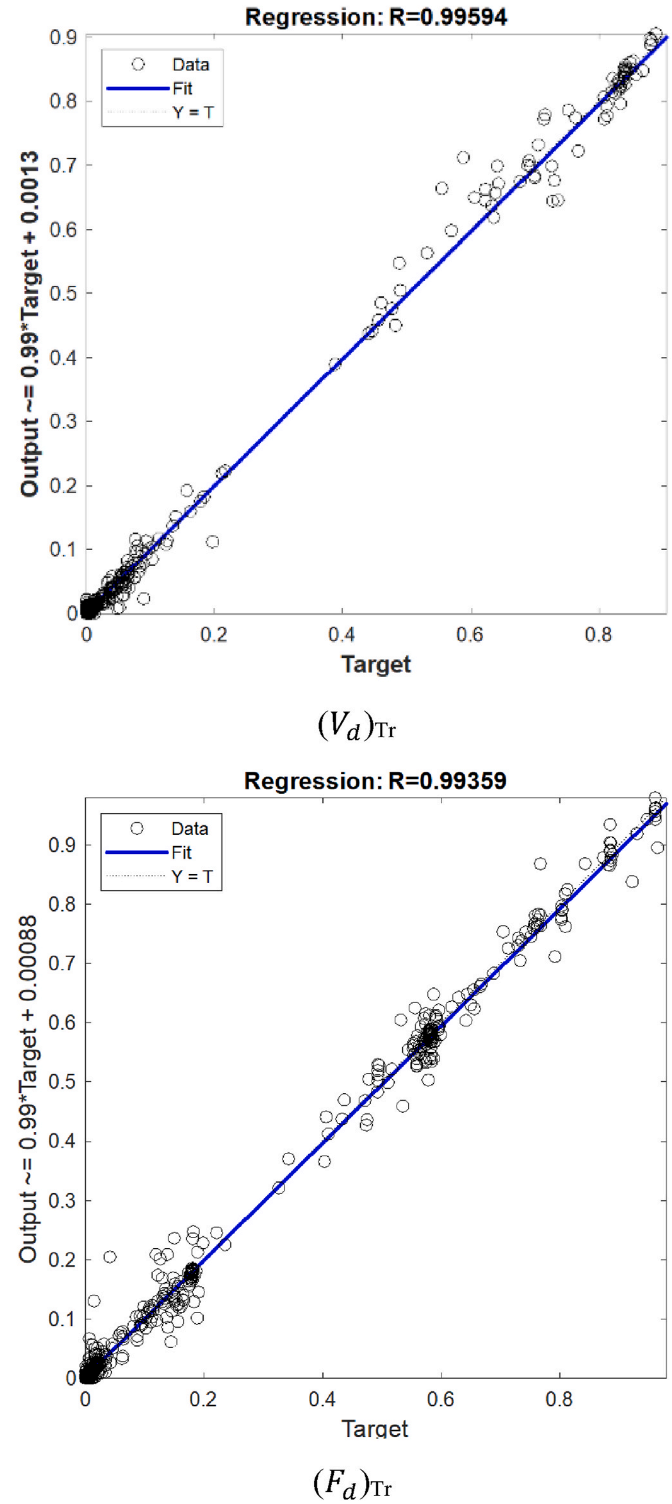


Fig. 10. Regression analysis of the test data.

Some of the deviation causes considering two simultaneous failures are given in Table 4. In this table, evaluation indexes are predicted for the 1st polymerization reactor. The first scenario (S_1) is to completely close valve PV110 and simultaneously cutting of styrene fresh feed flow rate. In this scenario, in addition to temperature/pressure control system failure, the total fresh feed styrene which is an important source of cooling the reactor content is also cut off. As can be seen in Table 4, the reactor temperature and pressure are increased reaching their critical limit (see V_d and T_c values). Reactor level is decreased (i.e., V_d is zero since the maximum value is equal to the normal value), however, the critical limit is not reached. Besides, these variables have ascending and descending behaviors and do not reach their steady state values (see T_s value that is close to 1 which means the steady state value is not reached during the total simulation time). The second scenario (S_2) is to completely close valve PV110 and simultaneously cutting of the output of the first reactor pump P-2. This scenario is almost the same as the scenario S_1. Styrene feed flow rate is cut off as the response of control system LIC110 to reactor level increase. Nevertheless, the reactor level

Table 4
Evaluation indexes for some of the deviation causes.

Target variables	Evaluation indexes	S_1	S_2	S_3	S_4	S_5	S_6
T_r	V_d	3.868	3.955	3.44	3.783	3.573	3.605
	F_d	3.868	3.955	3.44	15.138	3.573	3.605
	θ_p	0.031	0.032	0.029	0.079	0.048	0.049
	θ_s	0.996	0.995	0.994	0.994	0.993	0.987
	θ_c	0.027	0.028	0.028	0.049	0.043	0.043
P_r	V_d	1.987	2.041	1.732	2.278	1.8	1.824
	F_d	1.987	2.041	1.732	4.474	1.8	1.824
	θ_p	0.031	0.032	0.029	0.080	0.482	0.049
	θ_s	0.990	0.987	0.982	0.987	0.982	0.969
	θ_c	0.020	0.021	0.020	0.036	0.032	0.032
V_r	V_d	0	1.022	0	5.322	0	0
	F_d	1.142	1.022	0.005	5.322	0.004	0.004
	θ_p	0.001	0.032	0.007	0.751	0.007	0.007
	θ_s	0.944	0.991	0.009	0.999	0.009	0.010
	θ_c	Not reached	Not reached	Not reached	0.652	Not reached	Not reached
Normalized sensitivity value		1	0.95	0.79	0.75	0.34	0.33

Scenario Description:
S_1: Closure of PV110 and cutting of styrene fresh feed flow rate.
S_2: Closure of PV110 and cutting of the output of the 1st reactor pump P-2.
S_3: Closure of PV110 and increasing the input feed temperature.
S_4: Closure of PV110 and more concentration of ethylbenzene in the reactors.
S_5: Closure of PV110 and cutting of condenser coolant flowrate.
S_6: Closure of PV110 and excess injection of nitrogen gas.

cannot not be controlled and is increased due to existence of recycled flow. The behavior indexes and sensitivity value are given in Table 4. The third (S_3) is to completely close valve PV110 and simultaneously increasing the input feed temperature. This results in reactor temperature and pressure increase which cannot be controlled and runaway reaction may occur. In this scenario, reactor level remains almost constant (see V_d and F_d values which are almost zero and indicating very small fluctuation around the normal value). Scenario S_4 is to close PV110 valve and more concentration of ethylbenzene in the reactors. In this case, reactor pressure and temperature firstly increase due to PV110 closure (see V_d values). Over the time, with propagation of failures, reactor pressure and temperature decrease (see F_d values which indicates larger values compared to the V_d). Besides, reactor level increases which could lead to reactor overflow (see θ_c which show that the level critical limit has reached). Scenarios S_5 and S_6 are to completely close PV110 and simultaneously cutting of condenser coolant and excess injection of nitrogen gas, respectively. Evaluation indexes of these two other scenarios are also reported in Table 4. These two scenarios as well as the S_1 to S_3 scenarios could lead to runaway reaction since pressure and temperature values have exceeded their critical values.

Having obtained the evaluation indexes, the sensitivity index is then calculated for each scenario and reported in Table 4. Scenarios are sorted in descending order regarding the sensitivity value. Scenario 1 is identified as the most sensitive scenario in terms of consequences. This analysis can be easily done for all variations of deviation causes and their combinations. The most sensitive scenarios are finally marked in the HAZOP worksheets for further evaluations and required corrective actions.

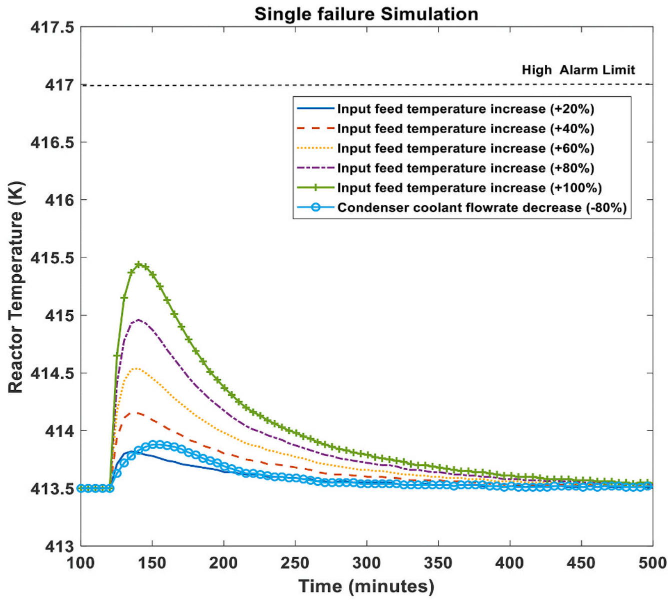
- As mentioned previously, HAZOP brainstorming discussion is commonly performed considering one deviation cause or failure at a time. This paper emphasizes evaluation of multiple deviation causes or failures with systematic variations of causes or failures amplitudes and watching for deviation propagations and domino effects. Simulation results of the case study in this paper clearly show the importance of such evaluation. For this purpose, simulation results of single deviation cause with different amplitudes, simulation results of all possible combinations of two simultaneous deviation causes with different amplitudes, and simulation results of all possible combinations of three simultaneous deviation causes with different amplitudes are individually analyzed. The severity levels of consequences of each case are illustrated in Table 5. As can be seen, from the total 70 simulations of single failure scenarios, 35 (45.45%) scenarios are classified as severity level 3. Similarly, for the double failure scenarios, 72.65% and for the triple failure scenarios 93.13% of the scenarios are classified as severity level 3. The greater the number of simultaneous events, the more severe results could be seen. This justifies the increasing percentage from single failure to double and triple failures scenarios. On the contrary, the decreasing percentage of the scenarios with severity level 1 and 2 for the double and triple failures scenarios reveal that the process variables remain less probable within their alarm ranges.

To better convey the concept, simulation results of two individual deviation causes, i.e., less flow of condenser coolant flowrate and more heating of feed in the preheater, are depicted in Fig. 11*(a)*. Simulation results show that for these individual deviation causes the outputs (i.e., reactor temperature) are at their safe operating limits which emphasizes that no preliminary caution or preventive action is needed. However, considering their simultaneous occurrences, reactor temperature exceeds the high alarm limit which could lead to runaway reaction as illustrated in Fig. 11*(b)*.

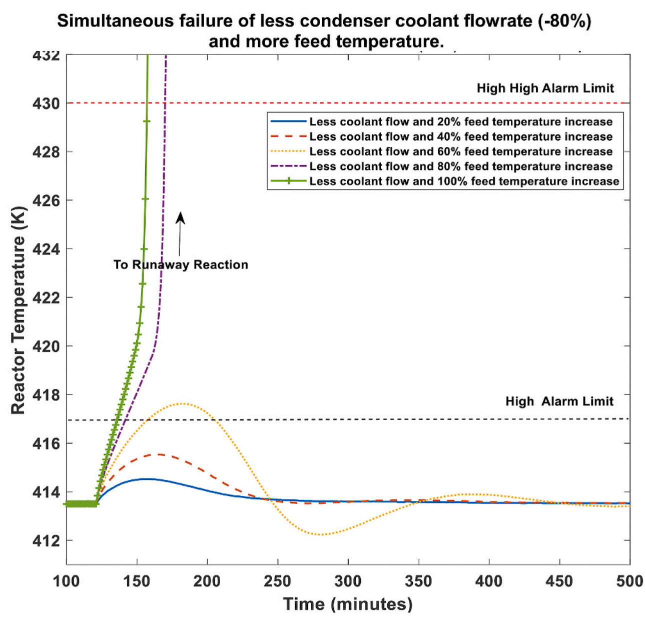
- Another important result is that the scenarios that exceed process high/low alarm limits (i.e., scenarios with severity levels 2 and 3) are more likely to exceed the high high/low low alarm limits (i.e., scenarios of severity level 3). Fig. 12 shows severity levels of scenarios that exceed the high/low alarm limits. The results show that 76% of

Table 5
Severity of consequences for single failure and multiple failures scenarios.

Scenario's type	Total # of simulation scenarios	# of scenarios with severity level 1	# of scenarios with severity level 2	# of scenarios with severity level 3
Single failure	70 (100%)	24 (31.17%)	11 (14.29%)	35 (45.45%)
Double failure	2100 (100%)	294 (14%)	280 (13.33%)	1526 (72.65%)
Triple failure	35000 (100%)	130 (0.37%)	2273 (6.5%)	32579 (93.13%)



(a)



(b)

Fig. 11. *(a)* Consequence analysis of individual deviation causes which shows safe operation of plant, *(b)* Consequences of their simultaneous occurrences which could lead to runaway reaction.

single failure scenarios that exceeds process high/low alarm limit, will also exceed the high high/low low alarm limits. This value is 84.5% and 93.5% for double and triple failure scenarios, respectively, which illustrates more severity of multiple failure scenarios rather than single failure scenarios in terms of consequences. Therefore, our hypothesis that multiple deviation causes or failures are quite important and need to be considered is verified.

4. Discussions

In this section, a summary of the strengths of the proposed methodology is provided.

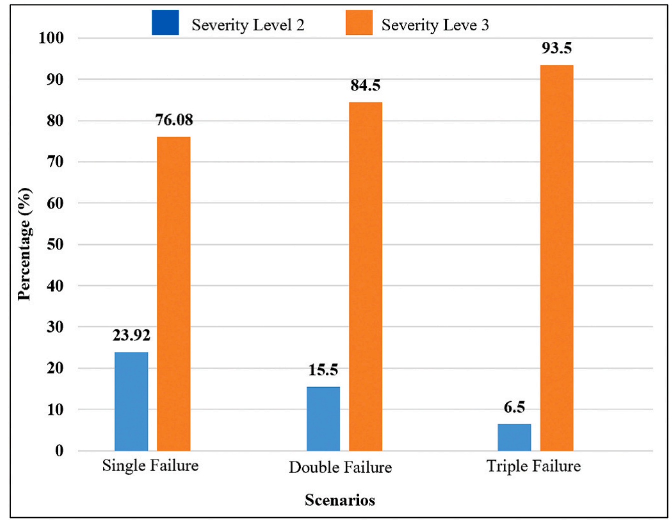


Fig. 12. Severity levels of scenarios that exceed the high/low alarm limits.

- Conventional Qualitative HAZOP is effective for safety analysis of simple systems. However, when analyzing more complex systems, several simplification rules are commonly applied. These rules include ignoring the effects of “amplitude and duration” of deviation causes or failures, considering only one deviation cause or failure at a time, and disregarding the effects of domino events. Unfortunately, relying solely on general impressions and limited human knowledge may result in overlooking critical consequences, potentially leading to major accidents in industrial settings. A historical review of both major and non-major accidents underscores the significance of addressing such oversights. Therefore, we advocate for a detailed and systematic analysis approach, which can significantly enhance the safety of industrial processes.
- In traditional HAZOP, dynamic simulation is either not used or only a few dynamic simulations are applied upon request. Consequently, most of the results heavily rely on expert knowledge and experience with some general understanding of the potential consequences. In our proposed research methodology, we adopt a highly precise and systematic approach that involves extensive dynamic simulations. As a result, the dependence on expert knowledge and experience has significantly diminished. Nevertheless, experienced experts can still intuitively evaluate our accurate analysis if they require further conviction.
- Traditional HAZOP does not consider simultaneous multiple deviation causes or failures, nor their propagations and domino effects due to the complexity of the problem and the limitations of human capabilities. However, by using the proposed systematic and AI-based approach, evaluations of such scenarios become straightforward, as we have demonstrated, and highly valuable.
- To generalize the proposed methodology to other plants, an accurate process dynamic model is required. Any modeling involves some assumptions. Therefore, the more accurate the process dynamic model, the more reliable the output of the proposed methodology. However, in general, the proposed methodology is not dependent on a particular simulation tool or approach.
- The ANN model, the algorithm, and the procedure suggested in this research are generally applicable to any similar problem and are not dependent on a particular class of neural network. This means that anyone following this approach may use any class of neural networks that they consider accurate enough for the collected data during such a study.
- There are no specific limitations to the proposed neural network approach, except for the general concept inherent in developing neural network models. In fact, many neural network structures

(such as MLP, RBF, etc.) are universal approximators capable of modeling any continuous nonlinear behavior. The primary considerations are the availability of a rich dataset and the appropriate model structure.
- As a final point, in terms of computational demand, a system with typical processing power is sufficient for the data collection process and training of ANNs.

5. Conclusions

AI can assume novel roles in enhancing safety analysis for industrial process design and operation. This is made possible by the widespread availability of process data and process simulators. In this paper, we proposed the utilization of process simulators in conjunction with ANN to assist HAZOP team members during brainstorming sessions. Process simulators are employed to simulate upset scenarios as comprehensively as possible. Subsequently, ANN learn process behaviors and predict simulation results. They also classify scenarios based on pre-simulated scenarios. By using this approach, the HAZOP team can easily analyze the consequences of nearly any combination of deviation causes or failures, even with varying amplitudes. To demonstrate the added value of our methodology, we applied it to an operating styrene polymerization plant. The results clearly underscore the importance and effectiveness of the proposed methods within HAZOP analysis.

Abbreviations

AI	Artificial intelligence	MSE	Mean Square Error
ANN	Artificial Neural Network	PNN	Probabilistic Neural Network
HAZOP	Hazard and Operability	RBF	Radial Basis Function
MLP	Multi-Layer Perceptron		

CRediT authorship contribution statement

Reyhane Mokhtarname: Investigation, Methodology, Writing – original draft, Writing – review & editing, Conceptualization, Formal analysis, Validation. **Leonhard Urbas:** Project administration, Supervision, Formal analysis, Writing – original draft. **Ali Akbar Safavi:** Conceptualization, Formal analysis, Methodology, Project administration, Supervision, Writing – original draft, Writing – review & editing, Validation. **Fabienne Salimi:** Project administration, Supervision. **Mohammad M. Zerafat:** Formal analysis. **Nasser Harasi:** Data curation.

Declaration of competing interest

I would like to submit the manuscript entitled "**An Artificial Neural Network Approach to Enrich HAZOP Analysis of Complex Processes**" by Reyhane Mokhtarname, Leonhard Urbas, Ali Akbar Safavi, Fabienne Salimi, Mohammad Mahdi Zerafat and Nasser Harasi to be considered for publication in the "***Journal of Loss Prevention in the Process Industries***".

We know of no conflicts of interest associated with this publication. As corresponding author, I confirm that the manuscript has been read and approved for submission by all the named authors.

Data availability

The authors do not have permission to share data.

Acknowledgement

The research work presented in this paper is partially supported by Iran's Ministry of Science, Research and Technology, Information and Communication Technology Park, and Fars Science and Technology Park under Javaneh grant number 129130003.

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